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DOE HANDBOOK

HAZARD AND ACCIDENT ANALYSIS HANDBOOK

Interim Use

U.S. Department of Energy
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FOREWORD

This U.S. Department of Energy (DOE) Handbook is approved for use by all DOE elements and their contractors. It may be applied to upgrading existing Documented Safety Analyses (DSAs) to the requirements of DOE-STD-3009-2014, *Preparation of Nonreactor Nuclear Facility Documented Safety Analysis*, or to revising DSAs for existing facilities based on their current safe harbor methodology. The Handbook may also be used to prepare and document hazard and accident analyses during facility design.

This Handbook is intended to assist DOE and its contractors in preparing and reviewing DSAs that are cost-effective and consistent in quality and content. To this end, the Handbook provides information on applicable scientific theories, analysis techniques, practical examples, and lessons learned from DOE applications and experience.

The Handbook addresses these subjects:

- Process for preparing a safety analysis, specifically the Chapter 3 portion of the DSA,
- Major accident types, such as fires, explosions, loss of confinement, chemical reactions, and natural phenomena events,
- Criticality accident analysis,
- Source term analysis,
- Radiological dispersion and consequence analysis, and
- Chemical dispersion and consequence analysis.

DOE Order 252.1A, Admin. Chg. 1, *Technical Standards Program*, states that DOE handbooks provide “a compilation of good practices, lessons-learned, or reference information that serve as resources on specific topics.” The guidance provided in this Handbook is not mandatory and may be used at the discretion of DOE contractors and field offices.

This Handbook is being issued for “Interim Use” because it is the first publication of a very large and technically complex document. While great efforts have been made to achieve completeness and accuracy, comments and feedback are welcome from users during the initial two-year period of availability. Beneficial comments (recommendations, additions, and deletions), as well as any pertinent data that may be of use in improving this document, should be emailed to nuclearsafety@hq.doe.gov or addressed to:

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ACRONYMS

AC	Administrative Control or Alternating Current
ACGIH	American Conference of Government Industrial Hygienists
AED	Aerodynamic Equivalent Diameter
AEGL	Acute Exposure Guideline Level
AICC	Adiabatic, Constant-Volume Combustion
AIHA	American Industrial Hygienist Association
AMAD	Activity Median Aerodynamic Diameter
ANS	American Nuclear Society
ANSI	American National Standards Institute
APAC	Accident Phenomenology and Consequence
ARF	Airborne Release Fraction
ASCE	American Society of Civil Engineers
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
BC	Building Construction
BDBA	Beyond Design Basis Accident
BEBA	Beyond Evaluation Basis Accident
BEU	Beyond Extremely Unlikely
BLEVE	Boiling Liquid Expanding Vapor Explosion
BNL	Brookhaven National Laboratory
BR	Breathing Rate
BST	Building Source Term
CCPS	Center for Chemical Process Safety
CDC	Centers for Disease Control
CFAST	Consolidated Model of Fire and Smoke Transport
CFD	Computational Fluid Dynamics
CFR	Code of Federal Regulations
CMM	Chemical Mixture Methodology
CR	Central Registry
CSE	Criticality Safety Evaluation
CTH	Cloud Top Height
CW	Co-located Worker
DBA	Design Basis Accident
DCF	Dose Conversion Factor
DDT	Deflagration to Detonation Transition
DF	Decontamination Factor
DG	Dense Gas
DNFSB	Defense Nuclear Facilities Safety Board
DOE	Department of Energy
DOS	Disk Operating System
DOT	Department of Transportation
DR	Damage Ratio
DSA	Documented Safety Analysis
DTA	Differential Thermal Analysis

EBA	Evaluation Basis Accident
EDE	Effective Dose Equivalent
EEGL	Emergency Exposure Guidance Level
EFCOG	Energy Facility Contractor Group
EG	Evaluation Guideline
EPA	Environmental Protection Agency
ERPG	Emergency Response Planning Guideline
EU	Extremely Unlikely
FDC	Flood Design Category
FDT	Fire Dynamics Tool
FGR	Federal Guidance Report
FHA	Fire Hazards Analysis
FMEA	Failure Modes and Effects Analysis
FTF	Filter Test Facility
FW	Facility Worker
GEP	Good Engineering Practice
GNB	Gaussian Neutrally Buoyant
GRF	German Research Foundation
HA	Hazard Analysis
HAZOP	Hazard and Operational Analysis
HC	Hazard Category
HCN	Health Code Number
HDBK	Handbook
HE	High Explosive
HEPA	High Efficiency Particulate Air
HPR	Highly Protected Risk
HRR	Heat Release Rate
HSDB	Hazardous Substances Data Bank
IACR	International Association of Cancer Registries
ICRP	International Council on Radiation Protection
IDLH	Immediately Dangerous to Life and Health
IEEE	Institute of Electrical and Electronics Engineers
ILA	Immediate Landscaped Area
INL	Idaho National Laboratory
IST	Initial Source Term
JFD	Joint Frequency Distribution
LANL	Los Alamos National Laboratory
LCF	Latent Cancer Fatality
LEL	Lower Explosive Limit
LET	Linear Energy Transfer
LFL	Lower Flammability Limit
LOC	Level of Concern
LPF	Leak Path Factor
LPG	Liquified Petroleum Gas

MAR	Material at Risk
MAK-Wert	Maximale Arbeitsplatz-Konzentration
MOI	Maximally Exposed Offsite Individual
MW	Molecular Weight
NAC/AEGL	National Advisory Committee for Acute Exposure Guideline Levels
NARAC	National Atmospheric Release Advisory Center
NASA	National Aeronautics and Space Administration
NCRP	National Council on Radiation Protection
NDC	Natural Phenomena Hazard Design Category
NEPA	National Environmental Policy Act
NFDRS	National Fire Rating Danger System
NIOSH	National Institute for Occupational Safety and Health
NIST	National Institute of Standards and Technology
NNSA	National Nuclear Security Administration
NNSS	Nevada Nuclear Security Site
NOAA	National Oceanic and Atmospheric Administration
NPH	Natural Phenomena Hazard
NQA	Nuclear Quality Assurance
NRC	Nuclear Regulatory Commission
NTSB	National Transportation Safety Board
OSHA	Occupational Safety and Health Administration
PAC	Protective Action Criteria
PBL	Planetary Boundary Layer
PC	Performance Category
PDC	Precipitation Design Category
PEL	Permissible Exposure Level
PHA	Preliminary Hazard Assessment
PISA	Potential Inadequacy of the Safety Analysis
PNNL	Pacific Northwest National Laboratory
PRA	Probabilistic Risk Assessment
PrHA	Process Hazard Analysis
PSO	Program Secretarial Office
PUREX	Plutonium Uranium Redox Extraction
PWHA	Probabilistic Wind Hazard Assessment
RCRA	Resource Conservation and Recovery Act
REL	Recommended Exposure Level
RF	Respirable Fraction
RG	Regulatory Guide
RTECS	Registry of Toxic Effects of Chemical Substances
SAC	Specific Administrative Control
SAWG	Safety Analysis Working Group
SBAA	Safety Basis Approval Authority
SC	Safety Class
SCAPA	Subcommittee for Consequence Assessment and Protective Actions
SDC	Seismic Design Category

SDS	Safety Data Sheet
SFPE	Society of Fire Protection Engineers
SIH	Standard Industrial Hazard
SIZ	Structure Ignition Zone
SME	Subject Matter Expert
SMP	Safety Management Program
SNL	Sandia National Laboratories
SNM	Special Nuclear Material
SQA	Software Quality Assurance
SRDT	Solar Radiation Delta Temperature
SRNL	Savannah River National Laboratory
SRS	Savannah River Site
SS	Safety Significant
SSC	Structures, Systems, and Components
ST	Source Term
STD	Standard
STEL	Short-Term Exposure Level
STP	Standard Temperature and Pressure
TBP	Tri-Butyl Phosphate
TED	Total Effective Dose
TEDE	Total Effective Dose Equivalent
TEEL	Temporary Emergency Exposure Limit
TF	Topographical Feature
TLV	Threshold Limit Value
TNO	The Netherlands Organization
TNT	Trinitrotoluene
TRU	Transuranic
TSL	Technical Support Level
TSR	Technical Safety Requirement
TWA	Time-Weighted Average
UEL	Upper Explosive Limit
UFL	Upper Flammability Limit
UL	Underwriters Laboratories
USQ	Unreviewed Safety Question
V & V	Verification & Validation
VDC	Volcanic Design Category
VP	Vapor Pressure
WDC	Wind Design Category
WEEL	Workplace Environmental Exposure Limit
WIPP	Waste Isolation Pilot Plant

Note: Definitions related to the DOE hazard and accident analysis process can be found in 10 CFR §830.3, DOE-STD-3009-2014 (or other Part 830 safe harbor), or DOE-HDBK-3010-94, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities*. Other definitions related to accident phenomenology for evaluation of potential consequences, such as physical and chemical effects, are provided in references cited in the text.

1 INTRODUCTION

This Handbook contains methodology, data sources, and subject matter references for performing and reviewing hazard and accident analysis for Department of Energy (DOE) nonreactor nuclear facilities. The guidance offered supports development of a Documented Safety Analysis (DSA) required by 10 CFR[1] Part 830, *Nuclear Safety Management*, Subpart B, "Safety Basis Requirements."

The Handbook uses as a starting point drafts of a report prepared by the Safety Analysis Working Group of the Energy Facility Contractors Group. This early effort was sponsored by DOE's Office of Defense Programs (predecessor of NNSA) in the early 2000s. Although that report was not completed, some of its technical content has been incorporated into this Handbook.

The Handbook describes best practices gleaned from development of DSAs throughout the DOE complex and from insights acquired in the development of DOE-STD-3009-2014, *Preparation of Nonreactor Nuclear Facility Documented Safety Analysis.* The Handbook provides many application examples that will be helpful to the analyst.

1.1 PURPOSE

The principal purpose of this Handbook is to guide development of the DSA safety analysis for nuclear facilities in order to satisfy the requirements of a safe harbor method set out in 10 CFR Part 830, Subpart B. The safety analysis process consists of three main steps:

- Hazard analysis (including hazard identification and evaluation);
- Accident analysis (including accident scenario definition and consequence analysis); and
- Preventive and mitigative control selection.

DOE-STD-3009-2014 provides criteria and guidance organized in the above manner. Further, it includes lessons learned from use of DOE-STD-3009-94, Change Notice 3 (CN3), *Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Documented Safety Analysis,* and other safe harbor methods. Therefore, this Handbook uses excerpts from DOE-STD-3009-2014[2] as the starting point for the amplifying guidance and good practices, but the scope of the Handbook is not limited to that standard.

The information in this Handbook is also relevant to other safe harbor methods for developing a safety basis document, such as DOE-STD-3011-2016, *Preparation of Documented Safety Analysis for Interim Operations at DOE Nuclear Facilities,* and DOE-STD-1120-2016, *Preparation of Documented Safety Analysis for Decommissioning and Environmental Restoration Activities*. The Handbook may also be use for upgrading existing DSAs to the new requirements of DOE-STD-3009-2014, or for updating DSAs for existing facilities based on their current safe harbor methodology.

1.2 OUTLINE

This Handbook is organized as follows:

- Chapter 2, *Hazard Analysis*, addresses hazard identification and evaluation, including hazard evaluation methods and safety control identification.

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[1] Code of Federal Regulations.

[2] When used without a 2-digit or 4-digit year number after "DOE-STD-3009," the term refers to both the 1994 and 2014 versions. If a specific version is meant to the exclusion of the other, the year will be stated.

- Chapter 3, *Accident Analysis*, provides a high level overview of the events that were identified in the hazard evaluation table to be evaluated for further accident analysis, provides an overview of the accident analysis process, and discusses two key topics: (1) assumptions and initial conditions; and (2) conservatism in analysis.
- Chapter 4, *Evaluation of Effects of Major Accident Types*, addresses the analysis of accident scenarios. The various topics covered provide information for evaluating the magnitude of the accidents and the resulting accident environments, so that the amount of radioactive or other hazardous material affected is defined. Toxic chemicals are a subset of hazardous materials that require additional dispersion and consequence assessment. In addition to evaluation of potential consequences to facility workers, this information is necessary to determine the source term available for release from the facility, and to evaluate the capability of safety structures, systems, and components (SSCs) to survive the accident environments and provide required safety functions when called upon.
- Chapter 5, *Source Term Analysis*, addresses development of the amount of radioactive material or toxic chemical released from a given confinement volume under the stress posed by insults from a hypothetical accident. Source term estimations include quantifying radioactive or toxic chemical material at risk, damage ratio, airborne release fractions or release rates, respirable fractions (for radioactive materials only), and leakpath factor.
- Chapter 6, *Atmospheric Dispersion*, addresses atmospheric transport and diffusion, meteorological data, and the models available for consequence assessment of radioactive releases to the atmosphere.
- Chapter 7, *Aquatic Dispersion and Groundwater Transport*, addresses surface water and ground water pathways, and the models available for consequence assessment of radioactive releases to aquatic water bodies and ground water.
- Chapter 8, *Radiological Consequence Assessment*, addresses the different types of radiation and the health effects they can have on the human body, its organs, and its tissues, and how radiological doses to receptors of interest may be estimated.
- Chapter 9, *Chemical Dispersion and Consequence Analysis*, addresses toxic chemical releases, their potential health effects and methods for estimating concentration at various distances.
- Chapter 10, *Hazard Control Selection and Classification*, addresses selection of safety significant and safety class controls that are credited in the hazard evaluation or accident analysis.
- Chapter 11 provides a complete list of references cited in the text.
- Appendix A, *Hazard Analysis Table Development*, provides guidance on constructing this table which is discussed in Chapter 2.
- Appendix B, *Criticality Accidents*, addresses this type of accident in greater detail.

2 HAZARD ANALYSIS

This chapter addresses hazard analysis (HA) techniques for the identification and evaluation of hazards, and the *identification* of controls to prevent or mitigate accidents. Hazard control *selection* is addressed in Chapter 10.

2.1 ELEMENTS OF HAZARD ANALYSIS

DOE-STD-3009[3] states that an HA consists of (a) hazard identification, (b) hazard categorization,[4] and (c) hazard evaluation. Hazard evaluation includes identification and safety classification of controls to prevent or mitigate potential hazard or accident scenarios.[5]

2.2 HAZARD IDENTIFICATION AND CHARACTERIZATION

The objective of hazard identification and characterization is to systematically and comprehensively identify radioactive and other hazardous materials within the facility, as well as natural phenomena hazards (NPHs) and external man-made events that may impact the facility and result in the release of these materials within the facility and to the environment. The hazard identification process includes characterizing hazardous materials (radiological and non-radiological) and energy sources, in terms of quantity, form and location. Examples of energy sources are falling objects, NPH-driven missiles, and other kinetic energy sources. Nuclear Criticality Hazard Evaluations are addressed in Section 2.3.2.

For DSAs prepared in accordance with 10 CFR Part 830, Subpart B, the key to successful hazard identification is ensuring comprehensive identification of the hazards associated with the full scope of facility processes, associated operations such as handling of fissionable materials, radioactive or hazardous wastes, and work activities covered by the DSA. Hazard identification does not yield specific hazard scenarios to analyze. Rather, it yields initial data from which hazard scenarios are subsequently developed. The overall quality of hazard scenario definition will be in direct proportion to the accuracy and completeness of the initial hazard information gathered.

The hazard identification process involves:

- Hazard data gathering;
- Summarizing hazard data in tables or data sheets; and
- Identifying standard industrial hazards (SIHs) needing further evaluation.[6]

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[3] As discussed in Section 1.1, when used without a 2-digit or 4-digit year number after "DOE-STD-3009," it refers to both the 1994 CN3 and 2014 versions of the DOE Standard. Otherwise, specific versions of DOE-STD-3009 are referenced throughout this Handbook.

[4] This Handbook does not address hazard *categorization*. Requirements and guidance for performing hazard categorization are provided in DOE-STD-1027-92, CN1.

[5] DOE-STD-3009-2014 defines a "hazard scenario" as "An event or sequence of events associated with a specific hazard, having the potential to result in undesired consequences identified in the hazard evaluation" and defines an "accident" as "A specific event or progression of a sequence of events resulting from an initiating event that is followed by any number of subsequent events that may lead to a release of radioactive or other hazardous material and/or exposure to a predefined receptor." The term "hazardous condition" has often been used in previous safety basis hazard evaluations instead of "hazard scenario." For the purposes of this Handbook, both terms are used interchangeably in Chapters 2, 3, 4, and 10 and in Appendix A when referring to the hazard evaluation.

[6] Such hazards might include electrical faults that could lead to a fire, or explosions harmful to nearby workers.

Comprehensive identification of hazards is best accomplished by a team comprised of safety analysts, system/process engineers, operational and support staff, industrial hygienists, and various subject matter experts (SMEs), as needed.

2.2.1 HAZARD DATA GATHERING

Gathering of hazard data commences with review of existing documentation, which includes the following:

- Facility and process descriptions (including available drawings and flow sheets);
- Historical radioactive and hazardous material inventory records;
- Existing safety documentation;[7]
- Operating and support procedures;
- Previous occurrence reports for the facility and relevant reports from general industry; and
- Facility design reports setting out the scope of new operations.

Once documented sources of hazards have been reviewed, a physical walkdown of the facility is undertaken to verify them and their locations. Such walkdowns are conducted with a floor plan noting the most significant details. Useful details may include information such as gloveboxes or containers, inventories and energy sources, system interconnections, and piping routes. Other details can be recorded during the walkdown in checklists and notebooks for completeness. If the facility is being designed, the floor plan can still be conceptually walked down using process and instrumentation drawings and process engineering drawings at whatever stage of development they are available. Hazard analysis is performed early in the project justification phase and during development of the Safety Design Strategy, continues during development of safety design basis documents as the design progresses, and is updated during development of the final DSA to authorize operations. If process and instrumentation drawings are based on evolving design of a new facility, the hazard identification will need to be reverified against the final design and as-built construction to support authorizing operations. The overall hazard identification and analysis is an iterative process during the design and construction phase of the project.

2.2.2 HAZARD DATA RECORDING

Checklists are used to ensure the hazard identification process is comprehensive and thorough. Checklists provide a generic list of hazards to look for in terms of radioactive and hazardous material types, energy sources, moving components, and the potential for falling objects. Hazard identification preparers use such checklists to systematically identify the presence or absence of hazards for a given area, from individual components/operations (e.g., gloveboxes) to entire rooms.

The raw data of a hazard identification can be recorded in a variety of ways. The critical information to be specifically noted in any recording mechanism is the hazard itself, its type, its magnitude and location, and sufficient descriptive notes to allow the HA team to place individual hazards in an appropriate context.

Materials of concern for release (or potential hazards in direct contact with materials of concern) are identified separately. Bounding inventory values of radioactive or hazardous materials are needed for the development of scenario-specific material at risk (MAR) for the hazard evaluation and accident analysis, consistent with the maximum quantities of material that are stored and used in facility processes.

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[7] Safety data sheets (SDSs); waste data sheets; health and safety plans; procurement and inventory records; and annual reports, such as the Emergency Planning and Community Right-to-Know Act, Tier II Chemical, and EPA Toxic Release Inventory.

Inventory data may be obtained from flowsheets, vessel sizes, contamination analyses, maximum historical inventories, and similar sources.

An example of a checklist for a DOE nuclear facility is shown in Table 2-1. The “Disposition” column is optional and is discussed in Sections 2.2.3 and 2.2.4. Other types of checklists that have been developed in the DOE Complex, and which may reflect site-specific and facility-specific hazards. These can be used to identify hazards and energy sources. Commercial industry practices for hazard identification, such as those described in the Center for Chemical Process Safety’s *Guidelines for Hazard Evaluation Procedures (*CCPS, 2008), provide guidance for the development of a comprehensive identification of hazards.

Table 2-1. Hazard Identification Checklist Example.
(Identify facility, location, or process)

No.	Item	Hazard present (Y/N)	Description (quantity, form, location)	Disposition (SIH, accident initiator/contributor)
1.0	**Electrical**			
1.1	Battery banks			
1.2	Cable runs			
1.3	Diesel generators			
1.4	Electrical equipment			
1.5	Heaters			
1.6	High voltage (> 600V)			
1.7	Locomotive, electrical			
1.8	Motors			
1.9	Power tools			
1.10	Pumps			
1.11	Service outlets, fittings			
1.12	Switchgear			
1.13	Transformers			
1.14	Transmission lines			
1.15	Wiring/underground wiring			
1.16	Other			
2.0	**Thermal**			
2.1	Boilers			
2.2	Bunsen burners/hot plates			
2.3	Electrical equipment			
2.4	Electrical wiring			
2.5	Engine exhaust			
2.6	Furnaces			
2.7	Heaters			
2.8	Lasers			
2.9	Steam lines			
2.10	Welding surfaces			
2.11	Welding torches			
2.12	Other			
3.0	**Pyrophoric Material**			
3.1	Pu and U metal			
3.2	Other (e.g., Zr)			
4.0	**Spontaneous Combustion**			
4.1	Cleaning/decontamination solvents			
4.2	Fuels (gasoline, diesel)			

No.	Item	Hazard present (Y/N)	Description (quantity, form, location)	Disposition (SIH, accident initiator/contributor)
4.3	Grease			
4.4	Nitric acid and organics			
4.5	Paint solvents			
4.6	Other			
5.0	**Open Flame**			
5.1	Bunsen burners			
5.2	Welding/cutting torches			
5.3	Other			
6.0	**Flammables**			
6.1	Cleaning/decontamination solvents			
6.2	Flammable gases			
6.3	Flammable liquids			
6.4	Gasoline			
6.5	Natural gas			
6.6	Paint/paint solvent			
6.7	Propane			
6.8	Spray paint			
6.9	Other			
7.0	**Combustibles**			
7.1	Paper/wood products			
7.2	Petroleum-based products			
7.3	Plastics			
7.4	Other			
8.0	**Chemical Reactions**			
8.1	Concentration			
8.2	Disassociation			
8.3	Exothermic			
8.4	Incompatible chemical mixing			
8.5	Uncontrolled chemical reactions			
8.6	Other			
9.0	**Explosive Material**			
9.1	Caps			
9.2	Dusts			
9.3	Dynamite			
9.4	Electric squibs			
9.5	Explosive chemicals			
9.6	Explosive gases			
9.7	Hydrogen			
9.8	Hydrogen (batteries)			
9.9	Nitrates			
9.10	Peroxides			
9.11	Primer cord			
9.12	Propane			
9.13	Other (e.g., NiCd batteries)			
10.0	**Kinetic (Linear and Rotational)**			
10.1	Acceleration/deceleration			
10.2	Bearings			
10.3	Belts			
10.4	Carts/dollies			
10.5	Centrifuges			
10.6	Crane loads (in motion)			

No.	**Item**	**Hazard present (Y/N)**	**Description (quantity, form, location)**	**Disposition (SIH, accident initiator/contributor)**
10.7	Drills			
10.8	Fans			
10.9	Firearm discharge			
10.10	Fork lifts			
10.11	Gears			
10.12	Grinders			
10.13	Motors			
10.14	Power tools			
10.15	Presses/shears			
10.16	Rail cars			
10.17	Saws			
10.18	Vehicles			
10.19	Vibration			
10.20	Other			
11.0	**Potential (Pressure)**			
11.1	Autoclaves			
11.2	Boilers			
11.3	Coiled springs			
11.4	Furnaces			
11.5	Gas bottles			
11.6	Gas receivers			
11.7	Pressure vessels			
11.8	Pressurized system (e.g., air)			
11.9	Steam headers and lines			
11.10	Stressed members			
11.11	Other			
12.0	**Potential (Height/Mass)**			
12.1	Cranes/hoists			
12.2	Elevated doors			
12.3	Elevated work surfaces			
12.4	Elevators			
12.5	Lifts			
12.6	Loading docks			
12.7	Mezzanines			
12.8	Floor pits			
12.9	Scaffolds and ladders			
12.10	Stacked material			
12.11	Stairs			
12.12	Other			
13.0	**Internal Flooding Sources**			
13.1	Domestic water piping			
13.2	Fire suppression piping			
13.3	Process water piping			
13.4	Other			
14.0	**Physical**			
14.1	Sharp edges or points			
14.2	Pinch points			
14.3	Confined spaces			
14.4	Tripping			
14.5	Other			
15.0	**Radioactive Material**			

No.	**Item**	**Hazard present (Y/N)**	**Description (quantity, form, location)**	**Disposition (SIH, accident initiator/contributor)**
15.1	Radioactive material			
16.0	**Hazardous Material (Toxicological, Chemical, Biological)**			
16.1	Asphyxiants			
16.2	Bacteria/viruses			
16.3	Beryllium and compounds			
16.4	Biologicals/Biotoxins			
16.5	Carcinogens			
16.6	Chlorine and compounds			
16.7	Corrosives			
16.8	Decontamination solutions			
16.9	Dusts and particles			
16.10	Fluorides			
16.11	Hydrides			
16.12	Lead			
16.13	Oxidizers			
16.14	Poisons (herbicides, insecticides, fungicides)			
16.15	Other			
17.0	**Direct Radiation Exposures**			
17.1	Contamination			
17.2	Electron beams			
17.3	Radioactive material			
17.4	Radioactive sources			
17.5	Radiography equipment			
17.6	X-ray machines			
17.7	Other			
18.0	**Non-ionizing Radiation**			
18.1	Lasers			
18.2	Other			
19.0	**Criticality**			
19.1	Fissile material			
20.0	**External Man-made Events**			
20.1	Aircraft crash			
20.2	Explosion			
20.3	Fire			
20.4	Power outage			
20.5	Transportation accident			
20.6	Other			
21.0	**Vehicles in Motion**			
21.1	Airplane			
21.2	Crane/hoist			
21.3	Forklifts			
21.4	Heavy construction equipment			
21.5	Helicopter			
21.6	Train			
21.7	Truck/car			
21.8	Waterborne Vehicle			
21.9	Other			
22.0	**Natural Phenomena**			

No.	Item	Hazard present (Y/N)	Description (quantity, form, location)	Disposition (SIH, accident initiator/contributor)
22.1	Earthquake			
22.2	Flood			
22.3	Lightning			
22.4	Rain/hail			
22.5	Snow/freezing weather			
22.6	Extreme straight-line wind			
22.7	Tornado			
22.8	Tsunami, seiche			
22.9	Volcanic ashfall			
22.10	Other			

An HA team safety analyst should work one-on-one with an individual SME and operations representatives to fill out those parts related to the SME's area of expertise and portions of the facility that have been segmented into process or area nodes for analysis as discussed later in this chapter. The multiple checklists from all the process or area nodes can be integrated into a complete draft of a hazard identification table and presented to the HA team for review, or the checklist for each node can be presented separately. Past experience has shown that this is a much more efficient way to complete the exercise than to have the entire HA team meet to discuss every item for every process or area node.

2.2.3 HAZARD SUMMARY DEVELOPMENT

DOE-STD-3009-2014, Section 4.0, DSA Section [3.3.2.1], states that the hazard identification data sheets (checklists) may be included in the DSA, or referenced as needed, and that a summary table that identifies hazards by form, type, location, and total quantity be presented, as well as a summary of major accidents or hazardous situations (e.g., fires, explosions, loss of confinement) that have occurred in the facility's operating history. The integrated checklist for the facility can be included in the DSA hazard identification results section. The process or area node checklists can also be used to develop a summary table to be included in the DSA. The range of information captured in the DSA hazard identification table is designed to ensure that the minimum hazard identification results are established, appropriate screening of hazards is performed, and information needed to perform an effective and efficient hazards evaluation is established. Table 2-2 is an example Hazard Summary Table form for a facility.

Table 2-2. Building XXX Hazard Identification Summary Table.

Hazard Type	Location	Form	Quantity	Remarks / Screening	References
Radioactive materials					
Direct radiation exposure					
Criticality accidents					
Hazardous chemicals (corrosives, toxics, reactions)					
Flammable/ combustible materials					
Explosive materials					
Electrical energy					
Kinetic and potential energy					
Pressure-volume					
Thermal energy					
NPHs					
Other					

These compilations of information reviews and facility walkdowns constitute initial information. Iterations between the hazard identification and hazard evaluation phases are likely necessary in order to ensure completeness.

2.2.4 EXCLUSION OF STANDARD INDUSTRIAL HAZARDS AND OTHER HAZARDOUS MATERIALS

The comprehensive hazard identification process in Sections 2.2.1 through 2.2.3 addresses all radiological and non-radiological hazards and energy sources. However, SIHs are not normally analyzed in a DSA hazard evaluation, unless chemical and industrial hazards result in a release of nuclear material, or an operator is incapacitated or prevented from taking credited action to prevent or mitigate a hazard scenario. DOE-STD-3009-2014, Section 3.1.1 states:

> Although the hazard identification process is comprehensive of all radiological and non-radiological hazards, DSAs are not intended to analyze and provide controls for standard industrial hazards such as burns from hot surfaces, electrocution, and falling objects. These hazards are adequately analyzed and controlled in accordance with 10 C.F.R. Part 851, *Worker Safety and Health Program*, and are analyzed in a DSA only if they can be an accident initiator, a contributor to a significant uncontrolled release of radioactive or other hazardous material (for example, 115-volt wiring as initiator of a fire), or considered a unique worker hazard such as explosive energy. The basis for any identified hazards excluded from further evaluation shall be provided. See Appendix A, Section A.1 of this Standard for further discussion on screening of standard industrial hazards and Section A.2 for a discussion on screening out certain chemicals based on low quantities or low hazard.

DOE-STD-3009-2014, Section A.1, provides the following SIH guidance:

> The Department of Energy (DOE) recognizes, via Title 10 of the Code of Federal Regulations (CFR) Part 830, the importance of including worker safety in safety analyses by specifically noting the worker as a population of concern. Developing a conceptual basis for the methodology used in this Standard requires answering the fundamental question of how worker safety is most appropriately addressed in the DSA. DSAs include hazard analyses and hazard controls for worker safety, unless the hazards and their potential consequences are due to standard industrial hazards.
>
> Standard industrial hazards are hazards that are routinely encountered in general industry and construction. These workplace hazards are addressed by provisions of 10 CFR Part 851, *Worker Safety and Health Program*, which requires identification and assessment of worker hazards and compliance with safety and health standards that provide specific safe practices and controls. Based on these provisions, evaluation of standard industrial hazards within DSAs is needed to the extent that these hazards act as initiators or contributors to accidents, or result from chemical or radiological hazards (for example, when an explosion is caused by radiolysis inside a tank). When standard industrial hazards are excluded from further evaluation, Section 3.1.1 of this Standard requires such conclusions to be included in the hazard identification, along with the basis used for exclusion.
>
> Standard industrial hazards that may be considered for exclusion from the DSA hazard evaluation include those in which a national consensus code and/or standard … defines and regulates appropriate worker safety practices. Specifically, the codes and standards required by 10 CFR 851.23, *Safety and Health Standards*, may be considered. Examples of hazards addressed by these requirements include confined spaces, electrocution, falling objects, non-ionizing radiation, hot work, and lasers. Toxicity of hazardous chemicals is addressed in Section A.2 rather than this subsection.
>
> [Unique hazards …]

> Standard industrial hazards that have the potential to be an accident initiator involving chemical or radioactive material releases are retained as part of the DSA hazard evaluation. For example, the existence of 440-volt alternating current cabling in a glovebox could be identified as a potential accident initiator of a fire involving radioactive or other hazardous materials.

The evaluation of hazards associated with “other hazardous materials,” and especially a subset involving hazardous chemicals, warrants further discussion regarding which hazards can be screened out or screened in. Some of these non-radiological hazards may be determined to be SIHs, while others may require further evaluation in the DSA per 10 CFR § 830.204(b)(3) “that might contribute to the generation or uncontrolled release of radioactive and other hazardous material.” One aspect of the “generation or uncontrolled release of … other hazardous material” consideration is recognized in DOE-STD-3009-2014, Section A.1, which states: “Toxicity of hazardous chemicals is addressed in Section A.2 rather than this subsection” and is therefore not treated as a SIH. In addition to toxicity, other chemical hazards may require further evaluation.

The introduction of DOE-STD-3009-2014, Section A.2 clarifies that not all chemical hazards (even those that can cause serious injury or death) need to be evaluated in the DSA hazard evaluation:

> The DSA is not intended to deal extensively with chemicals that can be safely handled by implementation of a hazardous material protection program. Therefore, a screening process is established to select for DSA evaluation only those chemicals of concern (i.e., type and quantity that have the potential for significant health effect on the facility worker, co-located worker, or public) that are present in the facility or activity and present hazard potentials outside the routine scope of the hazardous material protection program.

The DSA hazard evaluation scope covers analysis of (a) hazardous chemicals affecting nuclear safety and (b) in some cases, chemical hazards that are outside the scope of the facility’s hazardous material protection program. The intent of DOE-STD-3009-2014 is to cover:

- radiation-related hazardous chemical events (examples: chemicals comingled with radiological waste, chemicals generated through radiological processes, and chemicals generated or released through processing of radioactive materials);
- nuclear safety-related hazardous chemical events (examples: events that affect a worker relied upon for a credited action, events that affect safety-related SSCs through corrosion, fire, or explosion); or
- unique hazardous chemical events, not addressed by 10 CFR Part 851, that could cause harm to workers, the public or the environment.

As an example of an excluded chemical hazard, consider a chemical supply tank in a nuclear facility that has no interaction with radioactive material until the chemical is discharged into the nuclear process. The chemical hazards presented by this tank, if they are routine and common in industry, should be screened out of the DSA hazard evaluation as an SIH because 10 CFR Part 851 requirements will apply.

However, when a chemical is used in or generated by a nuclear process (i.e., interacting with nuclear material), then such physical consequences from process accidents (e.g., over-pressurization) should be evaluated in the DSA hazard evaluation. DOE-STD-3009-2014, Section 3.1.3.1 states:

> Facility worker consequences, due solely to a standard industrial hazard, do not need to be categorized in the hazard evaluation if screened out per Section 3.1.1. However, the evaluation of radiological or chemical hazards that result in a prompt death or serious injury should be assigned a high consequence

> per Table 1. Examples of such hazards might include the generation of flammable/explosive hydrogen gas by electrolysis of uranium in water or a spill of sodium hydroxide used in radioactive waste processing.

Another chemical hazard not screened out is described in the DOE-STD-3009-2014, Section A.1 that states: “Significant quantities of cryogenic material or compressed gases/liquids may also warrant consideration because of asphyxiation hazards that might affect the ability of facility operators to safely manage the facility. Such unique hazards are not treated as SIHs and are evaluated in the DSA.” Note that the consideration is related to impacts on safely managing the facility. This situation would include incapacitation of operators required to perform specific administrative controls affecting critical safety functions.

In general, a chemical hazard should not be screened out if it affects a facility worker expected to perform safety-related actions. Control room workers are in this category, as are operators expected to carry out credited actions for a specific administrative control. DOE-STD-3009-2014, Section A.2 includes the following example: “chemicals that may be excluded from the DSA’s hazard evaluation include … chemical is not listed in OSHA or EPA toxic chemical regulations or is not assigned a PAC 2 or 3 value.”[8] Regarding toxicity, impact on a facility worker is defined as being exposed to a chemical concentration reaching Protective Action Criteria (PAC)-2 or PAC/TEEL-3 levels based on a qualitative evaluation. Typically, PAC concentrations are evaluated over a 15-minute period. However for a screening evaluation, a shorter time may be warranted if the worker becomes incapacitated due to the chemical exposure in a shorter than 15-minute time frame.

Section A.1 of DOE-STD-3009-2014 describes situations that should not be screened out when considering other unique hazards:

> Unique hazards may be present in facilities that are not specifically addressed by the above exclusion criteria, either because of quantities larger than typically used in general industry or because of unique DOE applications or operations. Such hazards may represent a potential hazard to an entire work area affecting multiple workers.

The intended distinction is to ensure analysis of “other hazardous materials” outside the scope of 10 CFR Part 851 that could affect nuclear safety. If these unique hazards could impair or disable control room operators or make uninhabitable entire rooms where nuclear operations are conducted, such hazards should be evaluated in the DSA.

DOE-STD-3009-2014 requires that “the basis for any identified hazards excluded from further evaluation shall be provided.” Excluding a specific hazard or class of hazards should be accompanied by recording the applicable code or standard and the relevant site safety management program for implementing the code or standard. This basis may be included on the hazard identification table (see the “References” column in Table 2-2), or for more complicated justifications, in the DSA hazard identification results section. Either approach is suitable, as long as there is clear documentation of hazards screened out from the hazard evaluation.[9]

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[8] See Section 9.3 for additional discussion of screening chemicals.

[9] Many SIHs are evaluated in the hazard evaluation as an initiator or contributor to a radioactive or other hazardous material release, which should be acknowledged somewhere in the hazard identification results section.

2.3 INITIAL HAZARD EVALUATION DEVELOPMENT

2.3.1 OVERVIEW

Hazard evaluation is the starting point for control set selection to prevent or mitigate potential hazardous conditions (or hazard scenarios as defined in DOE-STD-3009-2014) that could result in undesirable consequences, and for the subsequent quantitative accident analysis. The definitions section of DOE-STD-3009 states that the hazard evaluation portion of a hazard analysis includes an examination of "the complete spectrum of potential accidents that could expose members of the public, onsite workers, facility workers, and the environment to" radioactive and other hazardous materials. The DSA hazard evaluation provides: (a) an assessment of the facility hazards associated with the full scope of planned operations covered by the DSA, and (b) the identification of engineered and administrative controls that can prevent or mitigate these hazards or hazardous conditions. It analyzes normal operations (startup, facility activities, shutdown, and testing and maintenance configurations) as well as abnormal and accident conditions. In addition to the process-related hazards identified during the hazard identification process, the hazard evaluation also addresses NPHs and man-made external events that can affect the integrity of an SSC. DOE-STD-3009-2014, Section 3.1.3 provides requirements and guidance on how hazard evaluations are to be performed for DOE nuclear facilities.

The initial hazard evaluation is accomplished by the following steps:

1. Define the scope of the HA. This scope can vary from a single process in a single room to an entire facility with multiple processes. Evaluation of the entire facility may be more efficiently performed by dividing it into smaller process or area nodes. The scope of activities to be evaluated by the analysis includes any activities that can occur when significant quantities of hazardous materials are present. These activities include (a) DSA-authorized processes and experiments in the facility, (b) off-shift activities, and (c) any hazard associated with maintenance and support activities that can occur when significant quantities of hazardous materials are present. (Quantities are significant if they can cause injury, for example, as related to asphyxiation in DOE-STD-3009-2014.) Physical boundaries, process/support system interfaces, and interfaces with other facilities need to be defined.

2. From the hazard identification results, evaluate hazards associated with authorized activities, man-made external events, or NPHs. Develop a comprehensive list of postulated hazard scenarios.

3. From the hazard identification results, evaluate radioactive and other hazardous materials and energy sources to determine possible interactions that could lead to accident conditions.

4. Evaluate circumstances such as equipment failures, process material hazards and failure of barriers, and mission activities that could affect the initiation and progression of the accident conditions.

5. Review applicable safety documentation, process history, occurrence reports, and other information sources to identify postulated or historical hazardous conditions and accidents associated with the facility.

All activities within the facility boundaries are considered in the analysis. The HA team defines where these boundaries, or process or area nodes, start and stop. Considerations include:

- Do activities start at the door of the facility, at the loading dock, or at an outside staging or storage area?
- If two facilities share common space, at what point does one facility analysis start and the other stop?
- Do immediately adjacent facilities pose hazards such as toxic materials?
- Are any hazards associated with the process or area nodes or facility boundaries that may warrant consideration of controls?

Following this initial evaluation, the process continues with the documentation of hazardous conditions and selection of unmitigated hazard scenarios based on potential interactions between hazardous materials and energy sources.

Typical hazards commonly associated with DOE nonreactor nuclear facilities are identified in Table 2-3. The table provides a suggested causal correlation between hazardous energy and material sources and potential accident types or categories.[10] Hazards identified in Table 2-3 do not always result in an accidental release of radioactive or other hazardous material required to be evaluated by DOE-STD-3009.

Table 2 3. Correlation of Hazardous Energy and Material Sources to Accident Types/Categories.

Accident Category*	Hazard Energy and Material Source Groups
FR-1: Fire	Electrical Thermal Friction Pyrophoric Material Spontaneous Combustion Open Flame Flammables Combustibles Chemical Reaction
EX-2: Explosion	Potential (Pressure) Explosive Materials Chemical Reactions
LC-3: Loss of Confinement/Spills	Radioactive Material Other Hazardous Material Toxic Chemical Chemical Reaction
DE-4: Direct Radiological Exposure	Ionizing Radiation Sources
CR-5: Nuclear Criticality	Fissile Materials
EE-6: Man-made External Events	Non-Facility Events (e.g., aircraft crashes) Vehicles in Motion Cranes
NPH-7: Natural Phenomena Hazards	NPH Events - Seismic, Extreme Wind, Flood, Lightning, Extreme Precipitation, Volcanic Ashfall

*The number assigned to the accident categories is for ease of data management, and any numbering scheme could be used if deemed necessary.

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[10] A similar correlation is provided in DOE-STD-5506-2007, *Preparation of Safety Basis Documents for Transuranic (TRU) Waste Facilities*, Table 3.2-1, Hazard Sources and Potential Events.

A graded approach as defined in 10 CFR §830.3 and DOE-STD-3009 should be applied to the selection of hazard evaluation techniques and developing the hazard evaluations. The selection of techniques is based on several factors, including the complexity and size of the operation being analyzed, the type of operation, and the inherent nature of hazards being evaluated. A discussion of hazard evaluation techniques and recommendations can be found in Part I of CCPS, 2008, especially Chapters 4 and 5.

2.3.2 NUCLEAR CRITICALITY HAZARD EVALUATION

A criticality accident represents a special case for hazard evaluation. The criticality safety program requirements[11] are derived from the HA process established in the American National Standards Institute/American Nuclear Society (ANSI/ANS)-8 series of national standards (e.g., ANSI/ANS-8.1, *Nuclear Criticality Safety in Operations with Fissionable Material Outside Reactors*). These standards require a documented nuclear criticality safety evaluation demonstrating that operations with fissionable material remain subcritical under both normal and credible abnormal conditions. Criticality safety evaluations provide the technical basis for controls to prevent or mitigate criticality accidents. The ANSI/ANS-8 series requirements do not apply to critical assemblies or similar operations.

Section 3.1.3.2 of DOE-STD-3009-2014 provides requirements on what to include in the DSA hazard evaluation of criticality accidents, while Section 3.3.4 provides requirements on safety classification of criticality safety controls. Experience shows that only a few evaluations of criticality accident scenarios for a facility may need to be included in the qualitative hazard evaluation. Appendix B provides guidance on the magnitude and consequence analysis of criticality accidents and the estimation of fission product yield and particulate source terms.

2.3.3 CHEMICAL HAZARD EVALUATION

As discussed in Section 2.2.4, chemical hazards are screened to determine the need for further hazard evaluation. However, per DOE-STD-3009-2014, Section A.2, chemicals “that could otherwise be screened out, but have the potential to be an accident initiator involving radioactive or hazardous material releases, or could compromise the ability of the facility operators to safely manage the facility, are retained as part of the DSA hazard evaluation.” Chemical properties such as reactivity, toxicity, and incompatibility with other chemicals are thus included in the hazard evaluation.

Qualitative evaluation of toxic chemical consequences using any of the hazard evaluation techniques discussed later in this chapter is generally sufficient to provide a basis for comparison to consequence thresholds of interest for the selection of safety significant (SS) controls (i.e., serious injuries, fatalities, or significant chemical exposure).

However, for some situations, further quantitative analysis of consequences is necessary for control selection. [12] Later chapters of this Handbook will provide guidance on quantifying chemical source terms (Sections 5.3 and 9.5) and dispersion analyses to estimate concentrations to receptors (Chapters 6, 7

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[11] Criticality safety program requirements are established in DOE O 420.1C. This Order states that DOE-STD-3007-2007, *Guidelines for Preparing Criticality Safety Evaluations at Department of Energy Nonreactor Nuclear Facilities*, is the required method for performing criticality safety evaluations, unless DOE approves an alternate method. An update to that Standard has been issued in DOE-STD-3007-2017, *Preparing Criticality Safety Evaluations at Department of Energy Nonreactor Nuclear Facilities*, which will be invoked in a revision to DOE O 420.1C.

[12] For example, see DOE-STD-3009-2014, Section 3.2.3.3 and Section A.2 for further information for evaluation of the toxicity hazard and determination of concentrations for the co-located worker (CW) at 100 m and maximally-exposed offsite individual (MOI).

and 9). However, selection and application of appropriate source term and dispersion methods for evaluation of chemical hazards will need to consider special situations such as chemical reactions, chemical transformations in the plume, or heavier-than-air plume modeling.

2.4 HAZARD EVALUATION METHODS

2.4.1 COMMERCIAL INDUSTRY METHODS AND DSA HAZARD EVALUATIONS

Chapter 4 of CCPS, 2008 describes twelve methods that can be used in a hazard evaluation. The discussion is oriented toward the chemical industry, but the basic strengths and weaknesses of each method are generally applicable for the DSA hazard evaluation. The following sections discuss four of these methods as applied to several facilities described in DOE-HDBK-3010-94, *Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities,* Appendix B.

None of these industry hazard evaluation methods were designed to generate a DSA hazard evaluation and do not yield hazard scenarios, nor were they designed to identify SS and safety class (SC) SSCs or specific administrative controls (SACs). Those results are uniquely defined for DOE usage to develop a DSA. Thus, one does not normally see the raw information generated from the industry hazard evaluation in a DSA; however, it is a necessary step to developing hazard scenarios. The hazard evaluation is performed to understand facility vulnerabilities and potential hazard scenarios. Those insights are then distilled into a DSA hazard evaluation table and are used for safety classification of controls and derivation of TSRs.

The common methods utilized vary in both complexity and focus. Each method has strengths and weaknesses, and depending on the scope of the HA, multiple HA methods may be used. For example, the Hazard and Operational Analysis (HAZOP) methodology is effective for analyzing a chemical process within a facility, but the "What-If" methodology is better suited for evaluating NPH and man-made external events with the potential to affect the entire facility.

2.4.2 METHOD #1: WHAT-IF?

The "What-If" method is a loosely-structured, brainstorming technique commonly used in the DOE complex by itself or in combination with other hazard analysis techniques such as Process Hazard Analysis (PrHA). As with any other hazard analysis method, the analysis typically is organized by facility operations, process, or activity location (e.g., a production support laboratory). Analysts utilizing this method formulate a series of questions, each beginning with the phrase "What if…?" for each process or activity. An example might be "What if the liquid tank in the support laboratory overflows?"

The hazard evaluation would discuss ways in which the tank might overflow (e.g., initiators and overall event progression sequences), the potential consequences of overflow, what preventive and mitigative control responses are available, and what additional measures may be recommended for consideration. The extent of the discussion is based on increasing potential consequences. If the liquid in question is simply water with trace contamination or less harmful chemicals, the discussion will reach resolution much more rapidly than if the liquid is radioactive or a highly volatile, toxic substance.

To provide proper structure for comprehensive results, the examination progresses in an organized manner, from the beginning of the activity/operation to the end. Well-designed checklists can provide additional structure that limits the potential for important events to be missed. This approach combines the "What-If" method with the simplest method for hazard evaluation that is a checklist that identifies already-known or understood hazards such as fires and explosions and can be augmented with specific design information. Furthermore, while a variety of potential outcomes can be identified, it is important to identify the ultimate consequence that is physically plausible. Analysts should not stop with the assumption that a given control will function. To do so can result in failure to identify vulnerabilities, and is also inconsistent with DOE's stated intent for unmitigated analyses.

The strengths of the "What-If" method include broad applicability, ease of use, and its adherence to natural thought processes. Weaknesses include a greater potential for neglecting interaction issues and for missing some events altogether. Another weakness of the What-If analysis is that many scenarios identified may result in no or insignificant consequences; thus, creating a large number of scenarios of no interest to the DSA process. A modified What-If analysis has also been used to identify scenarios with significant consequence potential for further analysis. Further analysis may include the DSA-required evaluation of the frequency, consequence, and risk for such scenarios of interest, or combining the results of the What-If analysis with other hazard analysis techniques, such as Process Hazard Analysis (PrHA). The quality of "What-If" results can vary significantly based on the experience of the individual leading the team effort. Generally, "What-If" analysis is most suited to simple operations and activities where the potential end states of each step are discrete and easy to identify. Manual operations/activities are often ideal for "What-If" analysis.

The H-21 TRU Waste Facility and the H-7 Production Support Lab discussed in DOE-HDBK-3010-94, Appendix B illustrate examples of facilities amenable to a "What-If" analysis. The common feature of these facilities is that they do not have complex processes. They consist of discrete, manual operations with well-defined interaction boundaries.

Consider the liquid sampling glovebox in the Production Support Lab. It is a non-complex operation where a laboratory operator analyzes 20 ml sample vials. A simple walkdown of the process generates obvious "What-If" questions as shown on Table 2-4.

Table 2-4. "What-If" Hazard Analysis Example H-7 Production Support Lab.

"What if…?"	Possible Consequences
1. …a collection of vials is dropped while being entered into the glovebox?	1. Broken vials, small Pu airborne release, minor worker exposure.
2. …the sample recycle bottle is dropped while coming out of the glovebox?	2. Spill, small Pu airborne release, minor worker exposure.
3. …liquid is spilled within the glovebox?	3. See #1 and #2 above, without direct worker exposure potential.
4. …the sample recycle bottle is overfilled (i.e., double batch of high concentration of fissile solution)?	4.a. Criticality Safety Evaluation shows large margin = no issue or 4.b. Criticality Safety Evaluation shows limited margin = potential criticality event
5. …the glovebox inventory of hexone solvent ignites?	5.a. Potential glovebox confinement breach and/or 5.b. airborne Pu release (larger release potential than spill)
6. …more samples are brought into the glovebox than its allowable storage spaces?	6. No specific consequence (potential deviation in operational practice that should be evaluated).
7. …planchettes are dropped outside of glovebox	7. No significant consequence (quantities of material are too small)

The above list is not exhaustive, but demonstrates the basic concept. This questioning process would be repeated for each of the specific operations and general activities authorized in the facility. The resulting complete set of questions and answers would then be combined and amplified as necessary to generate specific hazard scenarios in the DSA hazard evaluation table. For example, if the potential exposure consequences are sufficiently limited, all liquid spills might be combined into one representative hazard scenario. Or, if only one or two of the liquid spill scenarios could pose significant exposure potential, those would be documented as individual events.

Care should be exercised when combining scenarios. There should be no attempt to combine scenarios until potential controls are identified. The considerations to determine if scenarios should be combined include identifying that proposed controls are either bounded or are the same for all bundled scenarios. In the hypothetical case presented in the previous paragraph, suppose one distinct spill with significant consequences is combined with all other spills. The hazard evaluation would then identify any credited controls for one scenario as applying to all glovebox liquid handling operations.

Dissimilar scenarios cannot be combined. For example, fires and spills should not be artificially combined into one event because they have differing consequences, separate initiators, and unlike controls. The required clarity of the analysis of the most important preventive and mitigative controls will be lost if these dissimilar scenarios are combined. Bounding scenarios is primarily a function of their controls. The example above only illustrates the identification of “what if” questions (which may help define initiating events or scenarios) for a single operation, and the associated possible consequences. It may not define a complete set of initiated events or define completely an accident scenario, nor include the controls to prevent or mitigate such scenarios.

2.4.3 METHOD #2: HAZARD AND OPERATIONAL ANALYSIS

This method, abbreviated “HAZOP,” is designed to investigate chemical process and complex system performance requiring a more methodical approach to ensure completeness, which cannot be effectively accomplished with the “What-If” technique. It requires a significantly greater investment of time and resources than a “What-If?” analysis because team members are required to identify and assess the significance of system malfunctions or improper operations at each step of a process using a highly formal, systematic approach.

The HAZOP method first divides a process or system into discrete sections (defined as process or system nodes), with the intent or function of each section being well-defined. Figure 2-1 illustrates the complete HAZOP method, after defining the process or system nodes.

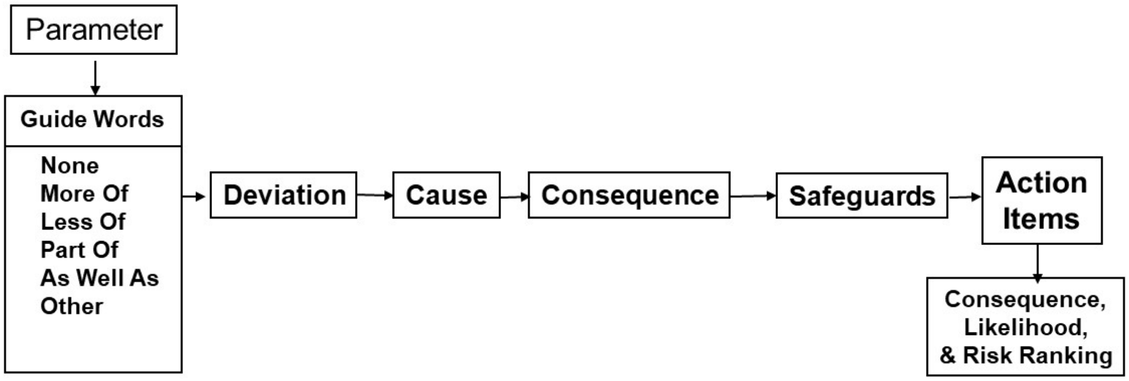
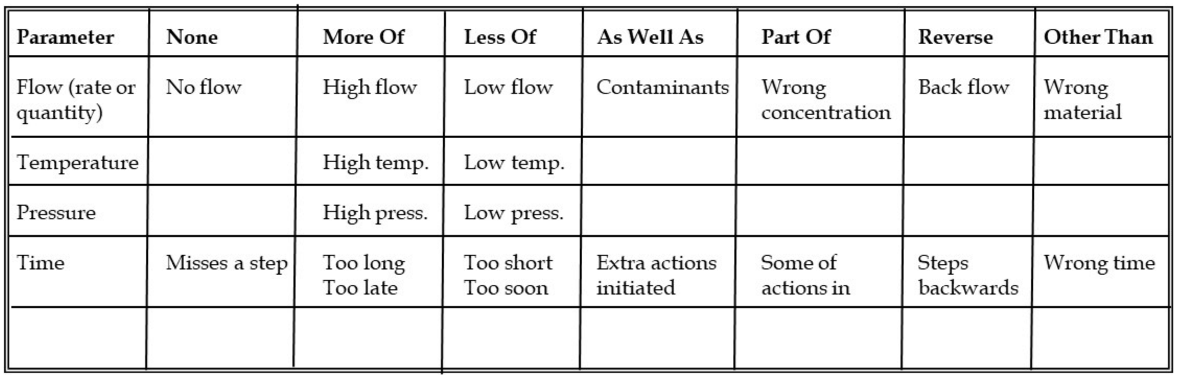


Figure 2-1. HAZOP Method Overview

The method then examines deviations in hardware and those caused by human interactions (such as those that occur during maintenance and operations) from design conditions by systematically combining each parameter of interest for the process or system with guide words. Examples of parameters include flow, pressure, temperature, composition, and even more conceptual items such as containment. Examples of guide words include “no, more, less, high, low, as well as, partial, reverse, wrong type, sooner than, later than, breach.” A HAZOP deviation matrix can be built to describe the evaluation criteria corresponding to a guide word for a given process or system parameter as illustrated in Figure 2-2.



Parameter	**None**	**More Of**	**Less Of**	**As Well As**	**Part Of**	**Reverse**	**Other Than**
Flow (rate or quantity)	No flow	High flow	Low flow	Contaminants	Wrong concentration	Back flow	Wrong material
Temperature		High temp.	Low temp.				
Pressure		High press.	Low press.				
Time	Misses a step	Too long Too late	Too short Too soon	Extra actions initiated	Some of actions in	Steps backwards	Wrong time

Figure 2-2. HAZOP Deviation Matrix

For example, the HAZOP team might start examining a process or system section by first identifying a parameter such as flow and the guide word “None”, and postulating a deviation of “no flow.” They would then identify the causes of no flow, qualitatively define the consequences of no flow, and what safeguards or controls are available or may be recommended for consideration, or other action items that may require further investigation. When significant consequence potential is identified, it is important to trace causality back to previous sections examined if the deviation of interest originates there. For additional perspective, consequence, likelihood, and risk rankings may be assigned to each of these significant deviations/cause conditions, or that may be accomplished in a subsequent DSA hazard evaluation. The team subsequently proceeds to other guide words for the selected parameter, such as “low flow,” followed by “high flow” and so on. This procedure yields an understanding of the integrated process or system behavior, as opposed to simply focusing on the discrete behavior of isolated components.

The HAZOP method brings to bear considerable structural rigor. It breaks down the entire process or system into a large number of discrete sections (pipe runs from Point A to Point B and individual vessels) and goes through a repetitive exercise to examine deviations in significant detail. Most deviations will not, in fact, involve any significant vulnerabilities, one reason that HAZOPs for large processes or systems are conducted over multiple days. The exercise simply takes time. Attempting to move swiftly through it tends to create an overload effect that defeats the purpose of this method.

The strengths of the HAZOP method are thoroughness enforced by structural rigor, focus on small details, adaptability to almost any process or activity, and generation of an organized evaluation record as an intrinsic part of the method. HAZOP also forces participants to properly define the process or activity at a detail level prior to beginning. Weaknesses include the fact that HAZOP is much more time and resource intensive than other methods. It is also vulnerable to poor initial organization. HAZOPs generally represent overkill for simple processes and predominantly manual activities, but are ideal for more complex processes, where the sheer magnitude of the potential deviations can overwhelm a “What-If” examination. Another weakness of the HAZOP method is that since it is focused on processes or systems, and their deviations, it often can miss more generic hazard scenarios such as external and natural phenomena events, or those not associated with process or facility systems.

Table 2-5 presents a HAZOP example for the Metal Dissolution Process described in DOE-HDBK-3010-94, Appendix B for the Plutonium Recovery Facility. This portion of the HAZOP evaluates a node defined by piping from the heat exchanger to the spray chamber as shown in Figure B.8 of DOE-HDBK-3010-94. The parameter examined is “Flow.” Compared to the previous “What-If” examples, the rigorous and repetitive nature of the method is clear. “What-If” relies on the ability and experience of the analysts to ensure completeness; HAZOP relies more on the method’s formal structure.

Table 2-5. HAZOP Example.

Note: Piping from Heat Exchanger to Spray Chamber (as shown in DOE-HDBK-3010-94, Figure B.6).

Parameter	Deviation (guide word)	Cause	Consequence	Safeguards or Controls	Likelihood	Consequence	Risk	Comments/Actions
Flow	No	1. Pump not working 2. Heat exchanger outlet valve incorrectly positioned 3. In-line filter clogged	Operational	Return line flow meter, Temperature sensors				Safe Condition: Dissolution reaction ceases without fresh acid flow Unsafe Condition: Potential to pressurize heat exchanger
Flow	No	1. Piping rupture	Plutonium solution spill	Glovebox, Glovebox ventilation, Critically safe drainage basin, Room air monitor, Room ventilation				
Flow	Low	1. Piping leak	Plutonium solution spill	Glovebox, Glovebox ventilation, Critically safe drainage basin, Room air monitor, Room ventilation				
Flow	High	1. Pump output excessive 2. Heat exchanger outlet valve incorrectly positioned	Temperature transient (more flow is heated less)	Temperature sensor on slab tank, Steam inlet control, Return line flow meter, Hydrogen detector, Shutdown interlocks, Air sparge				Unsafe Condition: More flow maximizes reaction. Unsafe Condition: Low acid temperature can yield undesired hydride sludge.
Flow	Wrong	1. Steam inlet off with heat exchanger leak	Plutonium solution enters heat exchanger condensate	Condensate collected in Raschig ring tank, Condensate samples				Action: Verify sampling frequency

As noted previously, the traditional HAZOP table is not an example of the hazard evaluation table expected in an actual DSA, but with modifications as suggested in Table 2-5, it may be suitable. The HAZOP identifies process vulnerabilities and interactions from which a set of hazard scenarios are usually derived for the DSA hazard evaluation table. For example, a runaway exothermic reaction generating hydrogen is an event that would be expected in the DSA hazard evaluation table.

Depending on the HAZOP results, there could be multiple entries for the same event to identify different progression paths, some of which would be of concern, while others may not. Alternatively, one entry could cover all potential progression paths; however, all paths should still be assessed to determine which, if any, warrant specific control. Example outcomes include:

1. The hydrogen detector and shutdown interlock is adequate to credit for all scenarios; or,
2. An individual control in a specific progression path may require crediting as well, either due to the high likelihood of that progression path or its ability to minimize the effect of the hydrogen detector and associated interlocks.

These methods were not developed to credit SSCs. They are intended to address problems that may arise when deviations from design conditions occur. The method (or any HA method) may uncover safety issues to be further evaluated.

2.4.4 METHOD #3: FAILURE MODES AND EFFECTS ANALYSIS

The failure modes and effects analysis (FMEA) is a flexible tool for examining equipment, a process, or system failures (in this section, “system” also includes equipment or a process). It is particularly suitable for characterizing the performance spectrum associated with individual component failures within the system. Thus, it is ideal for identifying all potential failure modes for systems of interest typically of moderate complexity. In some cases, the impact may not just be the failure of the system to perform its intended function, but could result in an accident condition of interest, such as an explosion in a process line.

The analysis proceeds as follows:

- Identify the major components (example: detectors);
- Identify the systems using these components (example: ventilation);
- Identify all failure modes for each component (high, low, loss of signal);
- Identify the effects of component failures on the systems.

Finally, for system consequences of interest, such as failure of the system to perform its function or an accident of concern, the controls or safeguards to prevent such failures are identified.

FMEA equipment failures. As indicated, FMEAs are ideal for evaluating system failure modes, but are not well-suited to supporting the identification of process hazard scenarios. FMEAs also lack the structure to examine process upsets (e.g., reverse flow, process chemistry deviations) as initiators. Inexperience with using the method can also lead to an excessively narrow focus on individual failures as opposed to integrated process behavior. Therefore, because the FMEA is narrowly focused, it is usually applied in combination with other techniques such as fault tree analysis to provide a more detailed understanding on how a system could fail.

Table 2-6 shows an application of the FMEA method to the Metal Dissolution Process evaluated in Table 2-5 for flow from the heat exchanger to the spray chamber through a pipe. The component and the failure modes of interest within this process is those associated with the hydrogen detector.

Table 2-6. FMEA Example.

Process: Metal Dissolution Line Component: Hydrogen Detector

Failure Mode	Effect	Safeguards	Comments/Actions
Fails high	Generates premature process shutdown for low H_2 concentration. Fails safe	Indication on operational console, Shutdown interlock.	Fail safe: None
Fails low	Failure to generate process shutdown, when required, leading to unsafe conditions (e.g., a potential for exothermic reaction and hydrogen explosion)	Indication on operational console, Spray chamber temperature sensor (also feeds shutdown interlock), Temperature indications on operational console	Potential accident of concern Increased hydrogen concentrations are generally accompanied by higher temperatures. A runaway exothermic reaction would still yield a shutdown. However, conditions short of that could yield H_2 concentrations in excess of the shutdown limit.
Fail as is	Failure to generate process shutdown when required See “Low Failure Mode”	See “Low Failure Mode”	Potential accident of concern See “Low Failure Mode” comments/actions
Loss of Power	Triggers shutdown interlock	Indication on operational console, Shutdown interlock.	Fail safe: None
Signal to Interlock, Mode A	Triggers shutdown interlock	Indication on operational console, Shutdown interlock.	Fail safe: None
Signal to interlock, Mode B	Failure to generate process shutdown when required See “Low Failure Mode” Effects	See “Low Failure Mode” safeguards	Potential accident of concern See “Low Failure Mode” comments/actions

2.4.5 METHOD #4: EVENT TREES AND FAULT TREES

Event trees and fault trees are formal logic constructs designed to document progression paths for an event. Event trees utilize inductive reasoning while fault trees utilize deductive reasoning. These two tools can be combined in a formal quantitative or probabilistic risk assessment, but such an assessment for an entire facility or process is not typical when evaluating DOE nonreactor nuclear facilities. Event trees and fault trees are normally used in DSAs as support tools to illuminate a specific issue of interest.

Inductive reasoning is often characterized as a “bottom-up” analysis since it starts with a specific premise and moves toward a general conclusion. An event tree correspondingly starts with a specific initiating event and moves toward a broad collection of potential outcomes. Regarding DSA hazard analysis, this approach results in event sequences with varying consequences in terms of radiological release potentials, based on the success and failure of any preventive controls that may terminate the event or mitigative controls that may reduce the consequences. A simple example of an initiating event might be “loss of cooling water to a furnace.” Every action that can result from that event then forms a decision point from which multiple possible outcomes branch. For example, suppose Alarm A is supposed to sound to generate an operator response if cooling flow is lost. The first decision point is therefore “Alarm A functions.” Two branches stem from that point: (a) if alarm A functions, the progression moves to a decision point labeled “Operator responds;” (b) if Alarm A does not function, operator response is initially bypassed and the resulting branch moves to a different decision point. The end result is a complete spectrum of outcomes, from successful to unsuccessful to catastrophic, which are characterized in terms of actions and controls associated with their progression. Each individual path through this event tree represents a separate event sequence. Thus, the minimum cut sets that yield failure of the system or its safety function can be defined. Event trees graphically depict the relationship between an initiating event and controls; thus, defining ranges of potential scenarios, their frequencies, and potential consequences based on the response of credited controls. Event trees, as well as fault trees, are typically used to support accident analyses and are not necessarily elevated to the DSA.

Deductive reasoning is often characterized as a "top-down" analysis since it uses general premises to arrive at a specific conclusion. A fault tree thus begins with the undesired end state as the top event such as a specified consequence of a potential accident and analyzes equipment failures and human errors that cause the top event. Such end states have often been identified by application of other hazard evaluation methods. For demonstration purposes, a simple example of an undesired end state is "the car does not start." The next step down in the fault tree lists the immediate causes such as starter motor failure, spark plug failure, and lack of gas in the cylinder. The next step down lists all the potential causes for each immediate cause: no gas in supply tank, failure of the fuel pump, fuel line leak. These potential failure mechanisms are joined by "AND" or "OR" gates depending on whether multiple mechanisms (A "AND" B) are needed to cause the failure above or if a single mechanism (A "OR" B) suffices. This process ends either in basic occurrences that cannot be subdivided further or at a predetermined evaluation boundary. Again, the minimum cut sets that yield failure of the system or its safety function can be defined.

The strengths of this approach includes logical rigor, recording of results in a branch structure as the evaluation occurs, and direct support of numerical estimation of likelihood of the postulated significant consequences. Weaknesses include a tendency toward tunnel vision if the failure mode or safety function of interest is not precisely defined, as well as a significant resource and time investment to generate integrated results.

2.5 INITIAL DEVELOPMENT OF A DSA HAZARD EVALUATION TABLE

The commercial industry hazard evaluation methods previously discussed evaluated process upsets, equipment failures, human errors, and potential safety features. Table 2-7 shows how similar hazard studies can be used to start development of a hazard evaluation table for the DSA, based on an example of a vehicle collision plus fire involving TRU waste containers which has often been evaluated using the "What-If" method.

Table 2-7. Initial Development of Hazard Evaluation Table.

Event No.	Event Description	Initiators	Preventive Features	Mitigative Features
FR-1	Fuel powered vehicle suffers a fuel leak due to an impact with TRU waste drums in the Shipping/Receiving Area and is ignited. A forklift carrying a single pallet with four drums impacts a stack (two high) of palletized drums with moderate to severe stress causing breach with material spill of 12 drums and ensuing pool fire that involves 88 additional drums in the Shipping/ Receiving Area. MAR: xx alpha curies in 100 drums (DOE-STD-5506-2007 statistical MAR distribution for Waste Isolation Pilot Plant complaint containers applied, see Table yy) INITIAL CONDITIONS: Staging area inventory limit; TRU waste in metal containers; Metal pallets.	• Operator error • Equipment malfunction • Vehicle impact with fuel spill • Ignition of combustible and/or flammable materials • Lightning • Wildland fire	SSCs: Concrete vehicle barriers. Waste staging building foundation. ADMINISTRATIVE: Procedures and Training Program (Forklift Operator training); Vehicle maintenance program; Fire Protection Program: • Combustible controls Waste handling operations curtailed outdoors during inclement weather; Movement of waste is to be accomplished using electric or manual powered equipment; Fuel exclusion zone in the Shipping/Receiving Area.	SSCs: None ADMINISTRATIVE Procedures and Training Program (workers trained to evacuate); Emergency Preparedness Program (emergency response activities).

Control identification occurs as part of the initial hazard evaluation development and is recorded in the hazard evaluation table as shown in Table 2-7. At this stage of developing the hazard evaluation table, all preventive and mitigative controls are listed that are available, or can be readily implemented, to demonstrate defense in depth as described in DOE-STD-3009.

2.6 LIKELIHOOD, CONSEQUENCE, AND RISK METHODS

The next step of the DSA hazard evaluation is to perform a qualitative estimate of the unmitigated consequences, likelihood, and optionally, risk ranking of the hazard scenarios. The following subsections present methods for these evaluations.

2.6.1 QUALITATIVE CONSEQUENCES

2.6.1.1 RECEPTOR CONSEQUENCE LEVELS

Table 2-8, reproduced from DOE-STD-3009-2014, Table 1, provides three qualitative consequence thresholds (bins) to estimate potential effects on facility workers, CWs, and the public (i.e., MOI).[13] High, moderate, and low consequence levels are quantitatively defined for the offsite public and CWs. High consequence levels are qualitatively established for facility workers consistent with DOE-STD-3009

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[13] These bins are similar to consequence level thresholds defined in DOE-STD-3009-94, CN3.

guidelines for a significant worker consequence. Moderate and low consequence levels are not defined for facility workers, because qualitative analysis would not yield results that provide a meaningful comparison to a distinguishable threshold.[14]

Table 2-8. Consequence Thresholds.

Consequence Level	Public[1,4]	Co-located Worker[2,4]	Facility Worker[3]
High	≥25 rem TED[5] or ≥PAC[6]-2	≥100 rem TED or ≥PAC/TEEL-3	Prompt death, serious injury, or significant radiological and chemical exposure.
Moderate	≥5 rem TED or ≥PAC/TEEL-1	≥25 rem TED or ≥PAC/TEEL-2	No distinguishable threshold
Low	<5 rem TED or <PAC/TEEL-1	<25 rem TED or <PAC/TEEL-2	No distinguishable threshold

[1] MOI - A hypothetical individual defined to allow dose or dosage comparison with numerical criteria for the public. This individual is located at the point of maximum exposure on the DOE site boundary nearest to the facility in question (ground level release), or may be located at some farther distance where an elevated or buoyant radioactive plume is expected to cause the highest exposure (airborne release).

[2] A CW at a distance of 100 m from a facility (building perimeter) or estimated release point.

[3] A worker within the facility boundary and located less than 100 m from the release point.

[4] Although quantitative thresholds are provided for the MOI and CW consequences, the consequences may be estimated using qualitative and/or semi-quantitative techniques.

[5] Total Effective Dose (TED), 50-yr commitment.

[6] DOE's PAC - see Chapter 9.

High consequence thresholds identified in Table 2-7 do not represent acceptable exposure levels to the public or workers; they are merely criteria used to identify safety class and safety significant controls.

Qualitative judgment is inevitable in hazard evaluation. It is routinely utilized in industries outside DOE. *Guidelines for Hazard Evaluation Procedures* (CCPS, 2008, Pg. 22), notes the following:

> The subjective nature of these deliberations may trouble some people who use the results of these studies because this subjectivity creates a lack of confidence in the results. Some people incorrectly believe that if the analyst uses quantitative methods to express the significance of a problem, then the limitation of subjectivity will simply fade away. However, this is not the case. The apparent numerical precision of a QRA ["quantitative risk analysis" or "quantitative risk assessment"] can mask (1) a great deal of the judgment that influenced the selection of accident models and (2) large uncertainties associated with the data used to estimate risk.

Estimating consequences qualitatively requires consistent assignments of the high, moderate, and low consequence levels for similar scenarios. This may require "normalizing" hazard scenarios by comparing against one another for consistent assignment of a severity level and to verify no outliers exist absent a sound explanation. In addition, for those hazard scenarios that were selected as representative or unique design basis accidents/evaluation basis accidents (DBA/EBAs) for further quantitative accident analysis, insights from that quantitative analysis should be used to verify the qualitative consequence assignments for the hazard evaluation (i.e., an iterative process between the hazard evaluation and the accident

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[14] Mitigated analysis that credits controls to reduce unmitigated high consequences to the facility worker generally show mitigated low consequences on the DSA hazard evaluation table.

analysis).

Assigning qualitative consequence levels may be informed by use of quantitative scoping estimates of effects on facility workers, CWs, and the MOI. Consequence estimation is performed differently for facility workers that may be near the source of the event or other areas within the facility where exposure may occur, as opposed to CWs or the public located at a distance from the facility. The latter often has a simplified quantitative basis. That is, it is a straightforward exercise to identify radioactive materials of greatest concern downwind using specific activity and dose equivalents that also incorporate the dispersion analysis. Likewise, chemicals that combine significant volatility and toxicity are easily identified. The safety analyst therefore starts with a short list of materials and release scenarios that are bounding. Bounding is intended to refer to the accident with the highest consequences among a group of similar accidents.

It is a simple matter to calculate “unit release” consequences at any distance of concern (within the capabilities of atmospheric dispersion tools being used) to yield “rules of thumb” for screening calculations such as rem/Curie released or concentration/mass released. These in turn are used to qualitatively scale given events into qualitative consequence bins or levels of severity (high, moderate, low) for the CW and MOI.

The CW scoping calculations may also provide the technical basis to meet the following requirement from DOE-STD-3009-2014, Section 3.1.3.1:

> Consequence determinations used for co-located workers in the hazard evaluation shall be supported by an adequate technical basis such as scoping calculations consistent with Section 3.2.4. Alternately, the quantitative evaluation of co-located worker consequences used to compare to Table 1 thresholds may be performed in the accident analysis and reported in the DSA Section [3.4].

2.6.1.2 FACILITY WORKER CONSEQUENCES

Given the qualitative nature of the consequence thresholds for facility workers in Table 2-8; the designation of facility worker consequences is based on first understanding how these type of consequence thresholds can be triggered by common hazards found in the DOE complex, or what these consequence thresholds mean in relation to radiological or hazardous chemical worker exposures. That is, facility worker consequences in many cases are based on accepted past-experience or consensus judgments from previous hazard evaluations throughout the DOE Complex, and not on quantitative calculations with their associated hard-to-defend assumptions and uncertainties. Thus, the following are recommendations and best practices to determine facility worker consequences.

Past experience and consensus judgments indicate that prompt death can only occur by a limited set of hazards and scenarios such as:

- nuclear criticalities,
- exposures at levels over 400 rads to penetrating radiation such as gamma or X-rays, and
- energetic releases of extremely hazardous chemicals.

Exposure to airborne (non-penetrating) radioactive material such as plutonium and uranium due to a wide range of accident scenarios such as fires or spills are unlikely to result in prompt death. However, these could result in significant radiological exposures depending on several factors associated with the hazard (e.g., inventory, form of material) and the scenario themselves; as discussed in more detail below.

DOE has no simple numerical consequence metric to assess threshold consequences for facility workers. Because of the location of the postulated facility workers inside a facility or very near the source of a release, downwind considerations such as X/Q are not applicable. Therefore, the determination of facility worker consequences is usually based on judgment, and not quantitative calculations.

In order to use a quantitative metric, one would have to equate a "serious injury or significant exposure" to a mutually-accepted quantitative exposure level (either radiation dose or toxic concentration) to define a threshold numerical value that is equivalent to a high consequence as defined on Table 2-8. This has been accomplished in DOE-STD-3009-2014 for the co-located worker and public, but not for the facility worker. Some previous DSAs have been based on a metric that radiation exposures due to accident conditions that could lead to exceeding emergency planning threshold or process safety management levels may be considered significant, since the selected level implies the onset for potential long-term health effects. Nevertheless, if a quantitative approach is desired, agreement on what constitutes a significant exposure should be reached with the DOE Approval Authority before any quantification is performed in support of determining the facility worker consequences.

A quantitative analysis may not be necessary where insights from past industrial accidents are available, as may be the case for large-scale releases of toxic substances such as hydrogen fluoride. Local facility worker consequences should be evaluated with some sense of perspective and historical experience, as it is possible to conceive extreme events immune to any possible set of controls.

The analyst should focus on the work areas in which accidents may result in a release of radioactive or hazardous material. If quantitative analyses are to be performed to support facility worker consequences, the associated concentrations of such releases are typically evaluated without reliance on specific assumptions about worker placement and hypothetical work area volumes for mixing of the release. However, a conservative but reasonable period of exposure could be assumed. Further guidance on these issues is provided later in this section.

The unmitigated consequence potential should not be underestimated, nor should unmitigated consequences be exaggerated (relative to historical experience) to a point where every exposure to the local facility worker is a high consequence event. DOE-STD-3009-2014 states:

> To ensure an informed and defensible qualitative evaluation, the determination of facility worker consequences should be based on a combination of the following:
>
> - Magnitude, type, and form of radioactive and hazardous materials involved in a hazard scenario;
> - Type and magnitude of energy sources involved in a hazard scenario;
> - Characteristics of the hazard scenario such as duration and the location where it may occur (e.g., in unmanned areas such as tank vaults); and
> - Potential for a hazard to impact workers' mobility or ability to react to hazardous conditions.

Some additional discussion of the fourth bullet is warranted. DOE-STD-3009-2014, Section 3.1.3.1 states that "the facility worker's mobility or ability to react to hazardous conditions should not be used as the sole or primary basis for determining facility worker impacts." This means that all four of the factors listed above ought to be considered collectively, not individually. A "see and flee" approach that results in unmitigated low consequences should not be used without due consideration of the accident characteristics. The last bullet, therefore, injects some realism into the event scenario for a "reasonable" unmitigated estimate of potential consequences to the facility worker. As an example, an assumption that a worker within a building is unaffected by a release from a building fire (based on hazard recognition and timely evacuation) would have to be justified by considering the location and characteristics of the fire relative to radioactive or hazardous material.

Although unmitigated analysis may not take credit for administrative controls or active engineered features, it is reasonable to assume that facility workers have some knowledge of the facility hazards and adequate training to react to hazardous situations. This assumption, however, is valid only when the accident is not disabling, provides obvious warning signs, and is slow-developing. However, care should be taken not to rely excessively on crediting this type of condition as defaults for unmitigated analysis. Any credit of this nature needs to be justified in the evaluation of the unmitigated consequences for facility workers, based on the contributing elements discussed in this section.

In evaluating the unmitigated consequences associated with a postulated hazard scenario, the following considerations may be important in assigning facility worker consequences:

1. Timing of radiological release: Hazard scenarios involving fires can develop quickly, but not so rapidly as to preclude evacuation in a reasonable period of time. Other scenarios, like criticality accident, explosion, and instantaneous release from confinement enclosures or containers can entail significantly more rapid radiological exposure. Another example is a long duration release such as during a spill of a radioactive or hazardous chemical liquid where a worker in the vicinity of the spill would not be expected to stand in the spilled liquid for an extended period of time. Therefore, though some exposure might occur, a conservative but reasonable time of exposure should be assumed.
2. Hazard warning: The availability of an obvious hazard warning and its timing relative to significant radiological or toxic chemical exposure may impact facility worker consequences. Warning may be provided by the event itself, as in smoke from a fire. However, engineered detection and notification systems such as air monitors are not credited for the unmitigated analysis. It is not reasonable to assume that a worker would remain in a room subject to flashover or toxic concentrations from a major fire in order to receive a significant radiological or toxic

chemical exposure. A conservative but reasonable period of exposure should be assumed, including whether the workers may choose to respond to the event.[15]

These points should also be considered:

- If the facility worker would reasonably be aware of the event's occurrence, and could take self-protective actions after the event occurs to protect themselves from a fatality or serious injuries from the non-radiological or non-hazardous material consequences, assume that the facility worker will be exposed for a conservative, but reasonable period of time even when warning is provided by the event itself.
- In cases where the facility worker would not be reasonably aware of the event's occurrence (e.g., characteristics of the release such as no odors, no visibility of plumes or smoke, occurrence in areas that could mask the release), there is no specified period of exposure, such as two hours. Consider reasonable lengths of time the facility worker would normally be present based on the nature of planned activities.

3. Scenario effect on protective action capability: Hazard scenarios involving explosions and NPH-initiated failure of buildings or equipment can cause damage to structures or injury to personnel impeding egress, thus increasing potential radiological or toxic chemical consequences. The potential for human errors or equipment malfunctions, in response to mitigating or evacuation actions following the accident, should be considered. Such an error might be putting the ventilation system in an operational mode that will worsen the consequences due to smoke generation. Also of importance is the impact of a toxic chemical release on potential worker ability to take protective actions.
4. Potential exposure magnitude: Severity of radiological uptakes or chemical exposures is a function of the magnitude of the energy associated with the accident scenario, the quantity and specific activity or toxicity of the material estimated to be released, and the pathways for transport to and absorption by workers. Inhalation is most often the dominant exposure pathway for airborne radioactive material releases, though skin exposures to small quantities of some chemicals such as aqueous hydrofluoric acid can be fatal.
5. Location: The impact to facility workers could be affected by the location of the worker with respect to the location of the postulated scenario; or whether the accident being evaluated occurs inside or outside of structures. For releases outside of structures, consider the qualitative impacts on dose of the plume moving past the facility worker. For releases inside a nuclear facility, consider whether the release is being mixed within a relatively small work area volume, such as with glovebox operations or into a large open area such as waste container staging buildings. Also, for releases within the facility, consider facility layout and unique non-ideal conditions such as mining operations or areas of limited visibility that can make evacuation difficult to achieve quickly.

As a general rule-of-thumb application of the above considerations, examples of high unmitigated radiological or toxic chemical consequences to the facility worker are: (1) explosions, pressurized powders or high-concentration liquid sprays, and other energetic events that impact large quantities of radioactive material are considered to cause significant radiological exposure to the facility worker due to the rapid nature of the event, the resulting source term, and the inability of the worker to take protective action prior to receiving a substantial dose[16]; and (2) the prompt dose received from a criticality accident. Other types of events such as fires, spills, or dropping of a container require more careful evaluation of

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[15] Workers may respond to incipient stage fires only with portable fire extinguishers, if they have been trained to use the extinguishers and feel safe in doing so.

[16] This also apples to the consequences of exposure to hazardous chemicals.

the characteristics of the actual accident event (e.g., time to develop) before credit can be given for the elements identified in this section. Any credit taken in the potential unmitigated consequences for facility workers needs to be justified.

2.6.1.3 STANDARD INDUSTRIAL HAZARD CONSEQUENCES TO FACILITY WORKER

Consequences to facility workers due to SIHs are included in the DSA when radiological or hazardous materials are involved and the SIHs are not screened out. These consequences are addressed in DOE-STD-3009-2014, Section 3.1.3.1 as follows:

> Facility worker consequences, due solely to a standard industrial hazard, do not need to be categorized in the hazard evaluation if screened out per Section 3.1.1. However, the evaluation of radiological or chemical hazards that result in a prompt death or serious injury should be assigned a high consequence per Table 1. Examples of such hazards might include the generation of flammable/explosive hydrogen gas by electrolysis of uranium in water or a spill of sodium hydroxide used in radioactive waste processing.[17]

For potentially serious injuries or fatalities, the event is assessed to determine whether the physical hazard associated with initiating or worsening a radiological or other hazardous material accident is a SIH or if it should be assigned a high consequence level. The primary consideration in determining whether the physical hazard is a SIH is if the regulated material (i.e., radioactive or other hazardous material) is not a primary cause or major contributor to the hazardous event, and that it is adequately addressed by 10 CFR Part 851 (and its adoption of OSHA and industry standards), 10 CFR Part 835, *Occupational Radiation Protection*, and Integrated Safety Management System HA requirements. These regulations and safety management programs are committed to in the DSA/TSRs. Examples of SIH accident initiators of a radioactive or other hazardous material release that may also cause physical injuries/fatalities are provided below to clarify that the unmitigated consequences do not include those SIH physical considerations. They illustrate that the unmitigated consequences do not include those SIH physical considerations, unless these could potentially affect their ability to safely manage the facility or respond to an accident condition. In that situation, the SIH should be considered for further analysis:

- **Thermal hazards** to the worker are due to welding equipment and combustible or flammable material fires ignited by typical ignition sources (e.g., electrical or thermal). The welding torch is a common SIH throughout various industries. The fires with typical ignition sources are also SIHs because the hazard and potential physical consequences are due to common types of equipment found throughout various industries. Both of these events are adequately regulated by 10 CFR Part 851, OSHA, NFPA, and national consensus standards.
- **Explosions** may involve ignition of flammable gases used with welding equipment; battery and fuel vapors; or offgasing from waste containers. The welding and equipment explosion and potential physical consequences are considered a SIH because these events commonly occur in general industry and are adequately regulated by 10 CFR Part 851, OSHA, and national consensus standards.
- **Missiles** are caused by an equipment explosion, failure of pressurized or mechanical system (e.g., air compressor or gas bottle), compressed gas cylinder failures, over-pressurization or deflagration of a hazardous (i.e., non-TRU) waste container, or from extreme straight-line winds, hurricanes and tornadoes. Missiles are considered an SIH because these events commonly occur in general industry and are adequately regulated by 10 CFR Part 851, OSHA, and national

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[17] The above reference to Section 3.1.1 of DOE-STD-3009-2014 is located in Section 2.2.4 of this Handbook. Table 1 of the Standard is reproduced as Table 2-8 in this Handbook.

consensus standards, or by the DOE NPH directives. However, if the missile physical consequence to the worker is due to the primary hazard being the regulated material, then those physical hazards are considered along with the radiological or other hazardous material consequences in assigning unmitigated consequences.

- **Equipment-related events** including vehicle/equipment load drops are SIHs because the hazards are presented by the equipment used in the work process, and the events are not caused by the regulated material. These events are adequately regulated by 10 CFR Part 851, OSHA, and national consensus standards.
- **Material and equipment movement** is a hazard presented by moving, lifting, dropping, vehicle-impact-induced movement, collapse due to corrosion/degradation, or movement due to a seismic event. The hazard is due to the size and mass of the object being moved and is not a hazard presented by the regulated material. The same hazard exists in various industries, such as construction. These events are adequately regulated by 10 CFR Part 851, OSHA, and national consensus standards.
- **Asphyxiant hazards** are presented by the use of small quantities of nitrogen and P-10 gas associated with loading or unloading shipping casks; acetylene or other compressed gases for maintenance activities and liquid nitrogen dewers for assaying waste containers; and exhaust buildup from material handling vehicles inside a facility. These hazards are common in various industries, and are adequately regulated by 10 CFR Part 851, OSHA, and national consensus standards. Smaller amounts of gases (i.e., nitrogen or argon) present for equipment calibration are in quantities that do not present an asphyxiation hazard. However, a large, rapid release of a nitrogen or argon from glovebox inerting systems for a nuclear process into a small confined occupied area that has an asphyxiation potential should be considered in assigning unmitigated consequences if the system has unique hazards requiring special design and controls that are not addressed by industry codes and standards.
- **Other impacts** encompass collisions from vehicles such as trucks traveling on the site, vehicles external to the site, and potential site aircraft crashes. These hazards exist in everyday life and are accepted by the public. Although no specific controls may be identified for these SIHs, the safety management programs, as committed to by the DSA/TSRs, which govern the conduct of activities involving various industrial hazards, will provide protection to the worker for these occupational hazards.

The qualitative evaluation for the facility worker may be supported by conservative quantitative scoping calculations, engineering judgment, and acquired knowledge. This qualitative approach is used because quantitative estimates are sensitive to a variety of possible assumptions such as facility worker position, circumstance, and close proximity to the point of release. Consequence estimates can rely on historical accident data or can be determined from: (1) simple bounding source term calculations, (2) existing safety documentation, and/or (3) qualitative assessment supported by calculations.

2.6.2 QUALITATIVE LIKELIHOOD

Likelihood of a hazard or accident scenario is assigned to qualitative bins defined by guidelines, which offer numerical ranges of two orders of magnitude or more. Table 2-9, reproduced from DOE-STD-3009-2014, Table 2, defines the qualitative likelihood bins.

Table 2-9. Qualitative Likelihood Classification.

Description	Likelihood Range (/year)	Definition
Anticipated	Likelihood $>10^{-2}$	Events that may occur several times during the lifetime of the facility (incidents that commonly occur).
Unlikely	10^{-2}>likelihood $>10^{-4}$	Events that are not anticipated to occur during the lifetime of the facility. Natural phenomena of this likelihood class include: International Building Code-level earthquake, 100-year flood, maximum wind gust.
Extremely Unlikely	10^{-4}>likelihood $>10^{-6}$	Events that will probably not occur during the lifetime of the facility.
Beyond Extremely Unlikely	Likelihood $<10^{-6}$	All other accidents.

Although the exercise of determining accident likelihood is qualitative, safety analysts often develop a numerical basis for judgments to provide consistency. An example is provided in DOE-STD-3009 that a simple methodology for unmitigated likelihood assignment could be to assign a probability of “1” to non-independent events, “0.1” to human errors, and “0.01” to genuinely independent SSC failures that would be used to establish the initiating event likelihood[8] as described on Table 2-9. For the unmitigated analysis, these human errors and equipment failures cannot represent the failure probability of a preventive control that would otherwise provide a SC or SS safety function. To determine the likelihood of an accident scenario, only initiating events are expressed as rate of occurrence with the units of inverse time (i.e., per year), and other enabling events are expressed in terms of dimensionless failure probabilities.

Another methodology for unmitigated initiating event likelihood classification would be to use a summary of historical data. Historical accident data may be used as long as this data represents the frequency of initiating events for such type of scenarios, and not the frequency of the entire scenario. Thus, caution is necessary in using historical data to support unmitigated frequency estimates for hazard scenarios, since it may not result in conservative frequency estimates for such scenarios.

Conservative values are chosen to accommodate uncertainties in frequency levels used in Table 2-9. A conservative choice is particularly important when an event frequency is at the borderline, just below the next highest frequency level. For example, 9.7E-3/year is at the upper limit of the unlikely frequency level. Thus, considering the sources, methods, and uncertainty associated with this value, this event may be better assigned to a frequency level of anticipated. For initiating events at the borderline of frequency ranges, for the general rule is to assign to the next bin unless it can be justified based on the conservatism of the analysis. For example, an event just below a frequency of 10^{-2}/year may be conservatively considered assigned to the anticipated frequency level. The same applies for scenarios with frequencies slightly less than 10^{-4}/yr and 10^{-6}/year, i.e., may be assigned to the next higher frequency level of Unlikely and Extremely Unlikely, respectively. The exception for this is for Beyond Extremely Unlikely scenarios for external events only, which by default have always being defined as scenarios with a likelihood below 10^{-6}/yr.

The mitigated frequency of occurrence when crediting preventive controls could also apply simple numerical estimates to assign a lower frequency bin. For example, a 0.01 failure probability could be assigned to a preventive engineered control or a SAC based on the technical justification in DSA Chapter 4.

Estimating likelihoods qualitatively requires consistent assignments of the likelihood bins for similar scenarios. To achieve consistency, hazard scenarios should be "normalized" by comparison to one another.

2.6.3 QUALITATIVE RISK

The primary purpose of risk ranking is to support the selection of bounding DBA/EBAs for further quantitative accident analysis and determination of SC controls that are based on consequences, not risk rankings. However, risk rankings may also be used to support the hazard evaluation and SS control selection. Combining a likelihood and a consequence level leads to defining a qualitative risk level, sometimes called Risk Category or Risk Class. Table 2-10, reproduced from DOE-STD-3009-2014 Table A-1, provides an example of a risk ranking table that combines likelihood and consequence, which is based on using the consequence and likelihood thresholds in Table 2-8 and Table 2-9, respectively.

Table 2-10. Qualitative Risk Ranking Bins.

Consequence Level	Beyond[18] Extremely Unlikely Below 10^{-6}/yr	Extremely Unlikely 10^{-4} to 10^{-6}/yr	Unlikely 10^{-2} to 10^{-4}/yr	Anticipated Above 10^{-2}/yr
High Consequence	III	II	I	I
Moderate Consequence	IV	III	II	II
Low Consequence	IV	IV	III	III
Risk Category I = Combination of conclusions from risk analysis that identify situations of major concern Risk Category II = Combination of conclusions from risk analysis that identify situations of concern Risk Category III = Combination of conclusions from risk analysis that identify situations of minor concern Risk Category IV = Combination of conclusions from risk analysis that identify situations of minimal concern				

Beyond the qualitative application of consequences and likelihoods (or supplemented with quantitative perspectives) for the hazard evaluation, risk ranking serves the broader purpose of confirming for the DOE approval authority that the overall mitigated risk of facility operation is low. Risk ranking can also highlight a given scenario whose mitigated risk remains significant. Additional guidance on use of unmitigated risk estimates for control selection is provided in Chapter 10.

2.7 UNMITIGATED AND MITIGATED HAZARD EVALUATIONS

The DSA hazard evaluation is based on unmitigated and mitigated analyses that derive the selection of hazard controls. The guidance from Section 2.6 is applied to assign qualitative estimates of the unmitigated and mitigated consequences, likelihood, and optionally, risk rankings of the hazard scenarios.

An unmitigated hazard scenario is evaluated for each initiating event by assuming the absence of preventive and mitigative controls. Unmitigated likelihood and consequence estimates assume that active engineered and administrative controls are not available to reduce either the consequence or likelihood of the hazard scenario. However, the unmitigated analysis does assume that passive design features exist and provide their safety function if these features are not affected by the accident scenario, or these features are affected by the accident scenario and a separate assessment determines that they will survive accident conditions.

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[18] For external events, likelihood below 10^{-6}/yr conservatively calculated is "beyond extremely unlikely."

Passive features assumed to perform their safety functions are evaluated per DOE-STD-3009 for potential designation as SC or SS SSCs and protection as TSR Design Features. In addition, the unmitigated analysis considers facility geometry and physical plausibility, and evaluates the unmitigated likelihood and consequence accordingly. For example, in an explosion scenario, the unmitigated likelihood would not be reduced by an engineered control, such as a vessel purge. However, the unmitigated likelihood of the explosion could be reduced based on physical realities of the facility, activity, or operation that will cause the explosion-initiating condition to occur (accumulation of minimum explosive concentration); no credit is allowed in the reduction of the likelihood for subsequent enabling conditions that will result in the explosion itself (e.g., presence of an ignition and/or oxygen). Thus, the likelihood of the scenarios should be based only the likelihood of the conditions leading to a physically meaningful initiating event, and not on the subsequence engineering or administrative controls that maybe available to prevent the explosion. Additional requirements and guidance on unmitigated analysis are provided in DOE-STD-3009-2014, Section 3.2.2.

Initial conditions may be necessary to define the unmitigated evaluation and are identified as shown on Table 2-7 and another example is provided later in Table 2-11. Credit for the initial condition is factored into the unmitigated likelihood or consequence assignments, and that initial condition is evaluated per DOE-STD-3009 for potential designation as a TSR control (e.g., MAR inventory-specific administrative control). Additional guidance is provided in DOE-STD-3009-2014, Section A.3, and is further discussed in Section 3.3 of this Handbook.

A mitigated analysis is performed to determine the effectiveness of SS and SC controls to protect CWs and the public. This analysis should be the same as the unmitigated analysis except that event likelihood is estimated with preventive controls available, and consequences are estimated with mitigative controls available. The selection of preventive and mitigative controls is a judgment-based iterative process to credit sufficient controls that provide confidence that the accident or release is prevented, or if not prevented, the consequences will be reduced to below thresholds of concern. Additional requirements and guidance on mitigated analysis are provided in DOE-STD-3009-2014, Section 3.2.3. The selection and classification of the hazard controls for the mitigated analysis are discussed in Chapter 10 of this Handbook.

2.8 HAZARD EVALUATION PRESENTATION IN DSA

Results for the unmitigated and mitigated hazard analyses are presented in the DSA hazard evaluation section as discussed in a DSA Section [3.3.2.3], Hazard Evaluation Results (see DOE-STD-3009-2014, Section 4.0). The DSA hazard evaluation table, or alternate hazard evaluation data sheet as described in DOE-STD-3009-2014, has certain essential characteristics:

- If multiple types of operations are being analyzed, the table is broken into separate sections where each section presents results for one specific type of operation.
- Specific hazard scenarios are described in terms of well-defined events. For example, a HAZOP may have dozens of entries for parameter-guide word combinations. These need to be turned into discrete events. A HAZOP may note that low flow caused by incorrect positioning of valves upstream has no major effect on a process other than operational disruption, while low flow due to a large leak represents a significant operator hazard. Those are two entirely different events.
- Initial conditions and assumptions are identified.
- Potential preventive or mitigative controls are identified.
- Unmitigated and mitigated consequences and likelihoods, and optionally, risk estimates, are identified to support control selection and classification. Source term parameters such as MAR,

Damage Ratio (DR), Airborne Release Fraction (ARF), and Respirable Fraction (RF) may optionally be listed.

Table 2-11 presents an example hazard evaluation table for presentation in the DSA, which builds upon the example provided in Table 2-7. This table includes both the unmitigated and mitigated analysis. There are many different formats that can be used to present this data, bearing in mind that the purpose is to achieve a comprehensive hazard evaluation and an unmitigated analysis of hazard scenarios in terms of potential consequences, their likelihoods, and identification of preventive and mitigative controls. The hazard evaluation table, in whatever format is chosen, should also present the mitigated analysis that credits safety controls, or this could be described in the DSA hazard evaluation results section. The mitigated hazard evaluation can be included as additional columns as shown on Table 2-11, or another convention is to use separate rows for the unmitigated and mitigated evaluations.

Appendix A provides another example of a hazard evaluation table for safety design basis documents, as part of the process to perform a Preliminary Hazard Analysis required by DOE-STD-1189-2016, *Integration of Safety into the Design Process*. Some additional data are included such as methods of detection and more emphasis on further planned improvements and investigations as the design matures.

Table 2-11. DSA Hazard Evaluation Table Example.

			Unmitigated Analysis					Mitigated Analysis		
Event	**Event Description**	**Event Causes**	**Freq. Level**	**Consequence Level**	**Risk Category**	**Preventive Features**	**Mitigative Features**	**Freq. Level**	**Consequence Level**	**Risk Category**
x	Fuel-powered vehicle suffers a fuel leak due to an impact with TRU waste drums in the Shipping/Receiving Area and is ignited. A forklift carrying a single pallet with four drums impacts a stack (two high) of palletized drums with moderate to severe stress causing breach with material spill of 12 drums and ensuing pool fire that involves 88 additional drums in the Shipping/ Receiving Area. MAR: xx alpha curies in 100 drums (DOE-STD-5506-2007 statistical MAR distribution for Waste Isolation Pilot Plant compliant containers applied, see Table yy) INITIAL CONDITIONS: **Staging area inventory limit;** **TRU waste in metal containers;** **Metal pallets.**	• Operator error • Equipment malfunction • Vehicle impact with fuel spill • Ignition of combustible and/or flammable materials • Lightning • Wildland fire	U	Radiological FW – High CW – Moderate MOI – Low Hazardous Chemical FW – Low CW – Low MOI – Low RELEASE MECHANISM: Impact + fire – 12 drums, 10% DR, 1E-3/0.1 spill ARF/RF plus unconfined burning 1E-2 ARF/RF and 90% confined burning 5E-4 ARF/RF. Pool fire – Conservatively modeled in a single layer of drums with no stacking. Unconfined burning 1E-2/0.1 ARF/RF of 25% of drums that experience lid loss (22 drums) that eject 33% contents and have confined burning 5E-4 ARF/RF of remaining contents in those drums, plus confined burning of 66 drums that experience seal failures (0.5 DR).	 I II III III III III	SSCs: **Concrete vehicle barriers.** **Waste staging building foundation.** ADMINISTRATIVE: Procedures and Training Program (Forklift Operator training); Vehicle maintenance program; Fire Protection Program: • Combustible controls Waste handling operations curtailed outdoors during inclement weather; **Movement of waste is to be accomplished using electric or manual powered equipment (SAC);** **Fuel exclusion zone in the Shipping/Receiving Area (SAC).**	SSCs: None ADMINISTRATIVE: Procedures and Training Program (workers trained to evacuate); Emergency Preparedness Program (emergency response activities).	BEU	Radiological FW – High CW – Moderate MOI – Low Chemical FW – Low CW – Low MOI – Low	 III IV IV IV IV IV

Notes:
1. Likelihood: A = Anticipated U = Unlikely EU = Extremely Unlikely BEU = Beyond Extremely Unlikely
2. Consequences: H = High M = Moderate L = Low
3. FW = Facility Worker CW= Co-located Worker at 100 m MOI = Maximally-exposed Offsite Individual at 2.9 km
4. Risk Classes: I = Combination of conclusions from risk analysis that identify situations of major concern
   II = Combination of conclusions from risk analysis that identify situations of concern
   III = Combination of conclusions from risk analysis that identify situations of minor concern
   IV = Combination of conclusions from risk analysis that identify situations of minimal concern

Bold/Underlined controls are credited in the mitigated analysis to reduce frequency, consequences, and Risk Class, or as Initial Condition

3 ACCIDENT ANALYSIS

This chapter provides an introduction to the accident analysis process. The starting point is a review of the hazard scenarios that were identified in the hazard evaluation table as discussed in Chapter 2 of this Handbook. Specific events are selected for further quantitative accident analysis. This particular chapter also addresses assumption and initial conditions, beyond DBAs/EBAs, and software quality assurance (SQA).

In general, formal accident analysis is performed for HC-2 facilities, and may or may not be necessary for HC-3 facilities. Accident analysis is the formal quantification of a subset of accidents, termed DBAs or EBAs by DOE-STD-3009. These accidents represent a complete set of bounding conditions. The basic components of accident analysis are accident type selection, accident scenario development, source term analysis, consequence analysis and control selection. This process is highly iterative to ensure accident scenarios are adequately developed, source term and consequence analysis is bounding, the suite of controls are comprehensive and tailored to reflect accident conditions, and all identified facility hazards are understood and properly controlled.

3.1 ACCIDENT TYPE SELECTION

It is expected that only a subsect of the total hazard scenarios identified in the hazard analysis will be evaluated as potential DBAs or EBAs in the accident analysis. The predominant purpose of accident analysis is to evaluate the need for SC controls to protect the public from radiological accidents. However, it may also be used to evaluate the need for defense in depth SS controls for protection of the public from radiological or toxic chemical accidents, or for protection of the CWs. The facility worker is not included in the scope of the DSA accident analysis and instead is addressed by the qualitative hazard evaluation discussed in Chapter 2 of this Handbook.

DBAs are accidents to be analyzed in a DSA for the design of a new nuclear facility and major modifications to an existing facility. The DSA will also include accident scenarios established during the design of an existing facility. DOE-STD-1189-2008 provides guidance for selecting and analyzing facility-level radiological and/or toxic chemical release events in the DBAs.

EBAs are postulated for existing facilities where DBAs were not identified as part of the design. The term EBA recognizes that an existing facility was not *designed* to DBAs to prevent or mitigate the accident, but rather is *evaluated* to ensure that it could do so with existing systems or added systems/controls. When an adequate set of DBAs does not exist, EBAs are selected from the following types of events:

- Operational accidents — process deviations (such as high temperatures and high pressures) and initiating events internal to the facility (such as fires, explosions, and loss of power resulting in release of radioactive or hazardous materials);
- NPH events such as earthquakes, floods, tornadoes, and wildland fires; and,
- Man-made external events such as an aircraft crash, external vehicular accident, or gas pipeline break.

Two types of EBAs, representative and unique, are defined in DOE-STD-3009-2014 for further quantitative accident analysis.

DBAs/EBAs are derived from the spectrum of hazard evaluation scenarios. Three screening steps convert the spectrum of hazard evaluation scenarios into the selected DBAs/EBAs:

- The first screening identifies potential consequences by population in relative bins of increasing severity. This step will discard scenarios whose higher consequence potential relates only to in-facility workers, because accident analysis focuses on consequences at a distance from the facility.

- The second screening looks at accident types. It is necessary for DSA documentation purposes to include at least one hazard and its consequence of each major accident type (e.g., fire, explosion, spill, NPH), unless the scoping calculations for the hazard evaluation demonstrate low consequences that do not have the potential to challenge the offsite Evaluation Guideline (EG) (DOE-STD-3009). These are called representative scenarios with similar preventive and mitigative control sets that bound the collective scenarios for that type.

- The final screening consists of looking at the remaining scenarios within a selected accident type to see if any would warrant safety SSC designation to protect the public (and CW if included in the DSA accident analysis, as mentioned above), but involve a different control set than the representative accident already chosen for that type. These are called unique accidents.

As an aid in screening the many hazard scenarios identified in the hazard evaluation, representative or unique EBAs may be selected based on organization by accident category (operational, NPH, man-made external event), accident type, and magnitude. Other means of grouping accidents may also be used, especially for complex facilities that may require a broad suite of hazard controls. The selected representative and unique scenarios are designed to bound all other postulated hazard scenarios, including high risk scenarios that still may challenge the EG (as determined during the hazard analysis process using the qualitative risk matrix in Section 2.6.3), or that may have high risk to the co-located worker if that is being evaluated in the accident analysis.

An example of an aid to screen hazard scenarios is provided in DOE-STD-5506-2007, Table 3.3-1, Minimum TRU Waste Activity/Hazard Evaluation Event Matrix. This table correlates 25 hazard scenarios or accidents by TRU waste processing activities for use in the hazard evaluation, or as EBAs. The minimum set of events addresses those with the potential for consequences that could be significant enough to warrant crediting preventive or mitigative controls, safety classifications of those controls, and explicit TSRs. Another example aid in screening hazard scenarios for EBA selection is NUREG/CR-6410, *Nuclear Fuel Cycle Facility Accident Analysis Handbook,* Table 2-2, Methods of Release of Radioactive Materials Anticipated for Nuclear Process Facilities.

3.2 ACCIDENT ANALYSIS PROCESS

The accident analysis process consists of the following sequence of steps intended to document numerical estimates of radiological and toxic chemical consequences to the public (or CW as needed for the DSA hazard evaluation):

1. Define the postulated accident scenario that releases radioactive material or toxic chemicals from the facility.
2. Estimate the damage to the facility to the extent it affects the potential MAR and source term released from the facility, e.g., loss of confinement areas.
3. Identify types and quantities of material involved in the accident MAR.
4. Determine the accident source term.
5. Conduct a dispersion analysis to determine the potential radiological dose or toxic chemical consequences.

Chapter 4 addresses steps 1-3 for potential accidents at DOE nuclear facilities. Chapter 5 addresses step 4. Chapters 6, 7, and 8 address step 5 for radiological releases, while Chapter 9 addresses step 5 for toxic chemical releases.

The potential controls identified in the hazard evaluation are further evaluated in the mitigated accident analysis, using the control selection and classification process described in Chapter 10.

3.3 ANALYSIS INPUTS AND ASSUMPTIONS

For most DOE accident analyses, the phenomena being examined have aleatory and systemic uncertainties. Most often it is not possible to derive precise and absolute conclusions from first engineering principles. Therefore, it is important to document the inputs, frame of reference, initial conditions, and assumptions of the accident analysis to ensure that these are not only defensible but conservative. This applies to all elements of the accident analysis process from accident selection, to frequency estimates, and source term and consequence analyses. The focus in this section is on the analysis of inputs and assumptions related to defining scenarios and their frequencies. Section 5.4.1 addresses the use of technically justified input and assumptions related to source term and consequence calculations.

Both hazard and accident analyses make use of initial conditions (ICs) to define hazard or accident scenarios to be evaluated. Initial conditions are specific assumptions regarding a facility and its operations that are used to define these scenarios. When not referring to physical facility features, these are sometimes called “initial assumptions,” which creates confusion regarding the need for TSR controls to protect these assumptions. The use of “IC” in this Handbook refers to *initial conditions*.

As discussed in DOE-STD-3009-2014, Sections 3.2.2 and 3.2.3, facilities are analyzed as they exist, or are designed, when quantifying meaningful release mechanisms. For design of new facilities, the unmitigated analysis may need to assume failure of the SSC to determine the potential consequences for safety classifications of SSCs and their appropriate design requirements, for example, design criteria for the selected NPH Design Category.

Accident scenario description includes, as appropriate, the operating mode of the system, all pertinent aspects of the physical configuration of the system and its environment, and relevant operating parameters, such as temperature, pressure, material inventories, and confinement, at the time the accident is postulated to begin. Not all of these assumptions are ICs. Where a range of possible ICs, physical properties, or environmental conditions exists, the range is specified, and the most conservative physically credible combination of normal operating conditions is chosen, and an explanation of why the choices are considered conservative should be provided.

As stated in Chapter 2, significant assumptions in hazard scenarios should be identified and justified, and this also applies to the accident analysis. Specific examples of ICs include:

- A vault or building can withstand NPH events according to its NPH Design Category.
- Facility geometry or layout limits accident progression or release with respect to in-facility transport.
- Solid TRU waste is contained in a certified Department of Transportation (DOT) Type-A drum (i.e., an additional barrier).
- A certain material is present only within a certified DOT Type B shipping container.
- Facility and process inventories are limited to those identified.
- A passive engineered SSC prevents significant consequences.

ICs should not include administrative controls, except those necessary to limit the inventory of radioactive or toxic chemical materials, or as specified by the analyst and/or regulator. Controls should be selected to protect assumptions such as MAR critical to the consequence analysis. ICs, and in some cases the associated administrative control associated with the ICs, should warrant some level of Safety SSC designation or SAC to ensure that the assumptions remain valid throughout the operating life of the facility. Defining and documenting ICs and associated administrative controls ensures that they are appropriately controlled, classified as SC or SS, and preserved via TSR operating limits, design features, or SACs.

Initial conditions that clearly prevent an accident and are part of the facility design basis (e.g., the structure is designed to withstand vehicle impact) are encouraged. Other safety controls are discouraged from being used since they may skew the unmitigated risk levels and result in unanalyzed or inadequately controlled hazards. For example, a fire door may be improperly credited as an IC for preventing fire propagation. This control may fail (blocked open door) so it does not completely prevent the event, but only reduces the likelihood. If the likelihood reduction “moves” the event risk to a level that does not require further analysis, then the adequacy of the control is not evaluated and the safety functions of the door may not be properly determined. Additionally, this may lead to a larger control set since controls identified for other fire events (e.g., combustible loading limits) may be adequate to protect against this event.

Spreadsheet calculation and computer modeling of accident sequences can provide valuable insights on the sensitivity of parameters, as well as indicating what reasonably lower and upper limits of response might be expected so that an overall conservative consequence is estimated (see Section 5.4, Appropriateness of Source Terms). The foundation of any accident analysis can be reduced to a set of inputs and assumptions. An input can be defined as a value feeding into the analyses that can be measured confidently and is readily obtainable. It could, for instance, be the internal freeboard volume of a tank, the specific gravity of a solution, or the metal skin thickness of a 55-gallon drum. An input value would not be expected to change as more information relative to it is obtained. An assumption, on the other hand, is a value feeding into the analyses that is not known with reliability and accuracy. Significant judgment therefore enters into the process of selecting the value or parameter of interest.

To address the uncertainty associated with the impact of assumptions and input variables, the default values in DOE-STD-3009 and DOE-HDBK-3010 are to be used to ensure an overall conservative analysis, and an analysis that is conservative to the extent envisioned when the Evaluation Guideline was established. Section 5.4.1 provides additional guidance on the use of non-default values or values that depart from the default values in the above-mentioned standard or handbook.

Examples of assumptions would be the rate of in-facility dispersion of a flammable gas leaked into a ventilated volume, the degree to which two spilled chemicals that react together might intermingle (synergism), or the nature of the physical interactions occurring in a structural collapse. The flammable gas leak example can be calculated, but the means of calculation itself introduces an implicit set of theoretical assumptions and uncertainties. The other two examples intrinsically involve making judgments about what is likely to occur. Analysts should strive to use as few assumptions in the accident analysis as possible, but their presence to some degree is inevitable. This point is specifically emphasized in *Guidelines for Hazard Evaluation Procedures* (CCPS, 2008):

> Because many of the events considered by the team may never have happened before, the team must use their creativity and judgment to decide whether the potential causes and effects of the accident pose a significant risk. The subjective nature of these deliberations may trouble some people who use the results of these studies because this subjectivity creates a lack of confidence

> in the results. Some people incorrectly believe that if an analyst uses quantitative measures to express the significance of a problem, then the limitation of subjectivity will simply fade away. However, this is not the case.

Another consideration is that there may be a difference between the level of conservatism of methods used to derive input parameters used for unmitigated dose consequence calculations and input parameters used to show that the design withstands physical stresses from the accident scenario. For example, dose consequence calculations may use an extremely conservative value or method to calculate aerosol generation for the purpose of determining the source terms and ultimately supporting classifying controls. However, these conservative values or methods may not be appropriate for design basis calculations.

3.4 BEYOND DESIGN/EVALUATION BASIS ACCIDENTS

The DSA [Section 3.4] Accident Analysis (see DOE-STD-3009-2014, Section 4.0) evaluates DBAs/EBAs for control selection and classification purposes. Section 3.5 of DOE-STD-3009-2014 provides guidance on the consideration of the need for analysis of accidents, which may be beyond the design basis of the facility. This section addresses accident analysis of these extreme events.

The purpose of an analysis of accidents beyond the design or evaluation basis of the facility is to provide (1) a perspective of the residual risk associated with the operation of the facility, and (2) additional perspectives for accident mitigation. That standard describes that Beyond Design Basis Accidents/Beyond Evaluation Basis Accidents (BDBAs/BEBAs) need not be analyzed to the same degree of detail as DBAs/EBAs. The analysis is intended to provide insight into the magnitude of consequences of such events and to identify potential facility vulnerabilities. The analysis has the potential, therefore, for identifying additional facility features that could prevent or reduce severe accident consequences. Unlike the unmitigated conservative analysis for DBAs/EBAs, a realistic analysis of potential BDBA/BEBA consequences may be performed to determine whether accidents have a much larger consequence (a “cliff edge effect”) than the largest DBA/EBA.

After the March 11, 2011 Fukushima Dai-Ichi nuclear plant accident in Japan, DOE embarked upon several initiatives to investigate the safety posture of its nuclear facilities relative to Beyond Design Basis Events (BDBEs). These initiatives included issuing Health, Safety and Security (HSS) Safety Bulletin 2011-01, “Events Beyond Design Safety Basis Analysis,” conducting pilot evaluations to refine possible process improvements, and conducting two DOE nuclear safety workshops. DOE issued two reports documenting the results of these initiatives: *Review of Requirements and Capabilities for Analyzing and Responding to BDBEs* (DOE, 2011); and *A Report to the Secretary of Energy: Beyond Design Basis Event Pilot Evaluations, Results and Recommendations for Improvements to Enhance Nuclear Safety at DOE Nuclear Facilities* (DOE, 2013). A summary description of the pilot evaluation process and results is provided in the HSS Operating Experience Level 1 notice (DOE HSS OE-1, 2013), “Improving Department of Energy Capabilities for Mitigating Beyond Design Basis Events.” Additional details of the pilot activities are provided in a companion technical report, *Technical Details on Beyond Design Basis Event Pilot Evaluations* (DOE Technical Report, 2013).

The focus of the pilot evaluations was the review of BDBEs and response capabilities at four DOE nuclear facilities representing a range of DOE sites, nuclear facility types and activities, and responsible program offices. The pilot evaluations looked at (1) how BDBEs were evaluated and documented in each facility’s DSA, (2) potential BDBE vulnerabilities and margins to failure of facility safety features as obtained from general area and specific system walkdowns and design documents reviews, and (3) preparations made in facility and site emergency management programs to respond to severe accidents. It also evaluated whether draft BDBE guidance on safety analysis and emergency management could be used to improve the analysis of and preparations for mitigating severe accidents (including BDBEs), which were updated and provided as Attachments 1 and 2, respectively, to the DOE HSS OE-1 (2013). The Attachment 2 safety analysis guidance may be used in annual updates to DSAs, and is reproduced here:

> Attachment 2 - Documented Safety Analysis (DSA) Guidance
>
> The purpose of this guide is to provide expectations for performing an enhanced evaluation of beyond design basis events (BDBEs) as a part of the annual DSA updates. It is generally expected that existing DSAs subject to the criteria of Action 2 already include an evaluation of BDBEs as required by DOE-STD-3009. The enhanced evaluation incorporates an analytical approach that was developed during the BDBE pilots, but documents the results of the analysis in the same manner as described in STD-3009. The enhanced evaluation process should incorporate lessons learned as described in "A Report to the Secretary of Energy: Beyond Design Basis Event Pilot Evaluations, Results and Recommendations for Improvements to Enhance Nuclear Safety at Department of Energy Nuclear Facilities," January 2013.
>
> As with any DSA preparation and update activity, the BDBE evaluation should be conducted by a qualified team leader and a multidisciplinary team consisting of experts in the areas of facility operations, facility safety analysis, structural/mechanical engineering, NPH, and emergency management, the last of which is particularly relevant to the objective of this evaluation. The intent is to perform an expert-based and qualitative evaluation.
>
> The facility's DSA should serve as a starting point for the evaluation of BDBEs. The DSA is expected to include a discussion of the BDBEs considered, and may include a discussion of analyses or enhancements made to the facility to meet DOE Order O 420.1 C, *Facility Safety*, requirement to evaluate the impact of changes in NPH data and/or analysis methodologies every ten years. The new analyses and enhancements should identify how the design has "evolved" to provide assurance of safety under events that are beyond the original design basis. As described in the HSS report to the Secretary referenced above, it is prudent for the team to perform a walkdown of the facility to support a qualitative evaluation of how a BDBE may impact the facility (the qualitative evaluation is discussed in the next section of this attachment) and to look for potentially unknown vulnerabilities to BDBEs (e.g., unsealed penetrations or low-lying electrical equipment in the case of flooding accidents).[19] This walkdown also ensures the reviewers are familiar with facility's size, key features and distances to other structures, and potential temporary service connections (like fire hydrants or well water sources).
>
> This enhanced BDBE evaluation is intended to identify BDBEs that may cause a release of radioactive material beyond that analyzed in the unmitigated accident analysis in the DSA and/or to disable important controls relied on to mitigate the release of radioactive material. The types of BDBEs that should be evaluated include:
>
> - Seismic events
> - Floods
> - Fires
> - Lightning
> - Wind and tornadoes
> - Snow and ice

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[19] An example might be unsealed penetrations or low-lying electrical equipment in flooding events.

- Ash fall
- Accidental aircraft crash
- Station blackout, as an initiating event or as a consequence from any of the above events
- Cascading effects of design basis events analyzed in the DSA that were previously ruled out because of the low likelihood of associated multiple failures.

If BDBE's from the above list are excluded, the rationale for exclusion should be documented. The general categories of failures to be considered for each BDBE listed above include:

- Collapse of building structure and interior walls
- Breach of water storage pools or collapse of storage racks
- Loss of electrical power and emergency power equipment (e.g., transformers, switchgear, or motor control centers)
- Loss of electrical distribution systems (e.g., conduit or cable trays)
- Operational failure of active mechanical equipment (e.g., pumps, compressors, or fans)
- Loss of pressure boundary of static equipment (e.g., tanks, vessels, or gloveboxes)
- Failure of distribution systems (e.g., piping, tubing, or ducts)
- Failure of alarms
- Loss of an emergency response center.
- Adverse spatial seismic interaction (e.g., failure of adjacent buildings or failure of adjacent stacks)
- Adverse flood-inducing interaction (e.g., failure of an adjacent water tank)

The enhanced BDBE evaluation should provide a gross estimate of the bounding impacts associated with BDBEs. It is qualitative in that it relies on a simple "what if?" type of hazard evaluation technique where a multidiscipline team participates in a brainstorming session to methodically evaluate the potential failures in facility systems, structures, and components (SSCs) that could be caused by each type of BDBE. The evaluation should estimate the consequences associated with failures of SSCs that provide safety functions such as confinement, energy removal (e.g., decay heat removal or fire suppression), or prevention of energetic reaction (e.g., explosion). The evaluation may draw upon existing unmitigated accident analysis performed in the DSA.

This qualitative evaluation process is applied to each type of BDBE so different failure modes and associated effects can be understood. Although a seismic event will typically present the worst-case consequences, it is important to step through all applicable BDBEs using the same structured "what if?" brainstorming technique. This information can be important when considering potential mitigation strategies.

SSCs identified as mitigating BDBE consequences should be subjected to a margins assessment (MA) to provide insights into their margin-to-failure. This should be a qualitative assessment based upon expert judgment. Civil/structural engineers should perform the MA by reviewing existing design basis analyses and supporting calculations for SSCs. This information should then be used as a baseline to compare against a SSC's expected response to higher level stresses. A MA can be difficult to accomplish if facility design information is not available, i.e., for older DOE facilities. In this case, the MA may have to rely on bounding, simplified assumptions, and judgments by subject matter experts, supported by the results of structured walkdowns. For NPH events, the margins assessment should be accomplished by analyzing the facility for higher stress levels than the systems' design (for example, the next higher seismic performance or design category) based on qualitative expert judgment.

> Descriptions of performance capabilities of the existing SSCs should also be added to or referenced in the DSA, as new and relevant information is learned from above BDBE evaluation. SSCs that provide protection against BDBEs are typically SC controls, or a subset of these controls, credited in the DSA for design basis events. If the BDBE evaluation identifies non-credited SSCs, it is not expected that these SSCs would be classified as SC or SS based solely on BDBE consequences, and, therefore, additional TSRs for these SSCs would not be created. These may include facility features such as temporary utility connections (power or water) and critical parameter instrumentation readings that permit monitoring after a BDBE occurs. The DSA should identify these SSCs as important for providing additional mitigation of BDBEs, and these SSCs should be maintained within the facility configuration management and maintenance programs in the same manner that other non-SC and SS DSA controls are treated to preserve their safety function. PSOs should establish for their facilities whether the Unreviewed Safety Question program should be used to determine the approval authority for changes to BDBE controls, or whether more general provisions of maintenance and configuration control should be relied upon.
>
> Based on the results of the enhanced BDBE evaluation, existing DSA descriptions of BDBE accident scenarios should be updated as necessary to clarify important assumptions needed to develop abnormal or emergency operating procedures. This may include details such as potential accident conditions associated with the range of BDBEs, cascading effects of certain scenarios, time-frames associated with scenario development, and time-critical mitigative actions. Additionally, emergency management plans for responding to BDBEs (updated using the guidance in Attachment I) could also identify potential facility design changes for consideration. An example would be the addition of standardized connections, outside the facility, that could be used to supply cooling water, deliver fire suppression water, or provide electrical power using resources obtained through emergency management mutual aid agreements. These improvements should also be conveyed as part of the DSA annual update.

Note that this guidance includes a BDBA/BEBA evaluation of accidental aircraft crashes. This is not specifically required by DOE-STD-3009-2014, or DOE-STD-3009-94, CN3, if less than a likelihood screening threshold. The most recent guidance on BDBA/BEBA evaluations provided in DOE-STD-3009-2014 states:

> Operational BDBAs/BEBAs are operational accidents with more severe conditions or equipment failures than are estimated for the corresponding DBA/EBA identified in the unmitigated analysis, or with likelihood of beyond extremely unlikely based on PRA results as described in Section 3.2.1. NPH BDBAs/BEBAs are defined by the initiating likelihood of the natural event itself (i.e., return period greater than the DBA/EBA return period for the next higher level as defined in DOE-STD-1020-2012). Man-made external events determined to be less than 10^{-6}/yr, conservatively calculated, do not require further evaluation in the DSA.

3.5 SOFTWARE QUALITY ASSURANCE

Software used in support of (a) DSA hazard and accident analysis calculations and (b) TSR implementation of SC and SS safety functions or SAC inventory control, is subject to the quality assurance requirements of 10 CFR Part 830 Subpart A, such as the DOE software quality assurance (SQA) guidance and applicable national consensus standards. SQA criteria for safety software are discussed in DOE O 414.1D, Chg. 1, *Quality Assurance*, and DOE G 414.1-4, *Safety Software Guide for* *use with 10 CFR 830 Subpart A, Quality Assurance Requirement.*[20] The analyst is encouraged to become familiar with these documents and the processes contained therein.

There are three subcategories of "safety software": (1) Safety System Software, (2) Safety and Hazard Analysis Software and Design Software, and (3) Safety Management and Administrative Controls Software. The Safety and Hazard Analysis Software is of primary concern to the DSA analyst. Software developers have the responsibility for ensuring that their software code has undergone appropriate SQA evaluation before it is distributed to the end users. Moreover, the software user has the responsibility of ensuring that the safety software to be used has successfully met all SQA processes prior to adopting it for any DSA analysis. As part of the SQA process, software developers should also provide technical manuals and user guides to assist the analyst in assessing appropriate application domains for the software to ensure its proper implementation. This documentation should address system requirements and their technical bases and describe default parameter values and default computational modes. The methodology for modifying these default values and modes should also be documented.

There are ten SQA requirements that need to be satisfied, but the heart of the SQA process is the verification and validation requirement. A comprehensive definition of verification and validation is provided in draft DOE G 414.1-4A, *Safety Software Guide for Use with DOE O 414.1D, Quality Assurance*. A simplified distinction between verification and validation is:

- Verification: The detailed examination of the code to ensure that the coding precisely and accurately reproduces the mathematical model approximations in its algorithms.
- Validation: Entails a comparison of the software model results to actual test or physical data through scientific assessment and benchmarking against other models.

Scientific assessment involves examination of encoded algorithms against theoretical principles and ground-truth data, where available, to assess the ability of those algorithms to accurately model the phenomena of interest. Benchmarking involves comparing the output of one software code with the output of similar code, or the results of a hand calculation or spreadsheet that serves as a baseline. This type of comparison does not necessarily constitute validation, but has merit as part of a validation procedure to the extent the baseline model is generally accepted as a reasonably accurate predictor for the phenomena of interest. Benchmarking can also provide insight into model limits of applicability, computing expense, input requirements, and important sensitivities or uncertainties. Ideally, computer code results should be compared against experimental results that were obtained in environments that mimic those to which the model will be applied. However, due to the expense associated with large-scale field tests or experiments, this type of data is generally very limited.

Parametric studies can uncover the sensitivity of a model to its various inputs. This can be extremely useful if it can be determined that the model is insensitive to certain parameters, such that validation does not need to overly concern itself with those parameters. Parametric studies can also be useful in situations in which there is a large variability or uncertainty associated with a particular input parameter. The results can be used in these cases to define parametric specifications that can establish conservative model predictions. The results of any sensitivity analyses should always be fully documented, as they are part of the framework that puts specific model results in proper perspective.

The capabilities of the techniques selected to perform the analysis should also be commensurate with the levels of detail required. This capability should be consistent with the "graded approach," which directs (among other criteria) that effort should be proportional to the complexity of the facility and the safety

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[20] DOE G 414.1-4 was written for DOE O 414.1C and is currently being revised as DOE G 414.1-4A to conform to DOE O 414.1D.

systems relied upon to maintain an acceptable level of risk. For a more comprehensive discussion of graded approach, see DOE-STD-3009-2014, Section 2.2. Accordingly, assessment of the possible consequences of an accidental release of radiological or toxic chemical substances into the atmosphere requires computations that could range from developing estimates on a spreadsheet to applying advanced computer codes that address source term phenomenology and atmospheric transport and diffusion. These are listed below:

Several national consensus standards provide guidelines on verification and validation activities for scientific and engineering computer programs for use in the nuclear industry:

- ANSI/ANS-10.7-2013, *Non-Real Time, High Integrity Software for the Nuclear Industry – Developer Requirements*;
- ANSI/ANS-10.4-2008 (R2016), *Verification and Validation of Non-Safety Related Scientific and Engineering Computer Programs for the Nuclear Industry*
- ASME/NQA-1-2008, *Quality Assurance Requirements for Nuclear Facility Applications, Subpart 2.7*; and
- IEEE 1012-2004, *IEEE Standard for Software Verification and Validation*.

Safety analysis calculations in many cases are completed without the need to resort to DOE software toolbox codes, such as Hotspot, ALOHA, and MACCS2. Calculations that may fall into this category include:

- Hand calculations;
- Commercial software package, such as Excel and Mathcad, where the primary use of the software is ease of implementation in automating arithmetic operations;[21] and
- Non-DOE toolbox codes, such as MCNP, KENO VI, and other government or industrial codes that are widely accepted and meet the requirements of DOE O 414.1D or ASME NQA-1.

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[21] These calculations (e.g., spreadsheets) also are subject to 10 CFR Part 830 Subpart A quality assurance requirements if the DSA relies on them. One of these requirements is that the technical reviewer have no active involvement in the development of the calculation.

4 EVALUATION OF EFFECTS OF MAJOR ACCIDENT TYPES

4.1 INTRODUCTION

This chapter describes methods for developing information on accident progression and the effect of the accident on radioactive and hazardous material and SSCs. The following types of accidents will be considered in separate subsections:

- Fires (Section 4.2);
- Explosions (Section 4.3);
- Loss of confinement/spills (Section 4.4);
- Chemical reactions (Section 4.5);
- NPH events (Section 4.6); and
- Man-made external events (Section 4.7).

The information developed in these analyses, in conjunction with data and information in DOE-HDBK-3010-94, is used to determine the source term, which will be addressed in Chapter 5 of this Handbook. This information will provide the basis for:

- Identifying physical insults and stresses associated with the scenario that can impact SSCs and hazardous material;
- Establishing the MAR and DR for the scenario;
- Establishing the ARFs and RFs for the scenario;[22]
- Providing insights to establish an LPF for a mitigated analysis; and
- Determining release effects on the atmospheric dispersion analysis (such as buoyancy from energy of the release).

This information also assists in evaluating the effectiveness of the control set chosen to prevent or mitigate the accident as described in Chapter 2, *Hazard Analysis*, to determine whether the control can be credited to provide the safety function under the accident conditions. Regarding the methods, models, and input data presented in this chapter:

- There may be additional models available other than those presented;
- Other models may be more appropriate to use for certain conditions;
- Viability and applicability of a model should be evaluated by the analyst before using; and
- Use of the model needs to be justified in the accident analysis write-up.

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[22] The convention “ARF/RF” is used throughout this Handbook. This term is adopted from DOE-HDBK-3010-94. The term represents the pair of recommended bounding values that are multiplied together to determine the airborne source term, and does not represent dividing the ARF by the RF.

4.1.1 INFORMATION FROM ACCIDENT ANALYSIS TO INCLUDE IN THE DSA

DOE-STD-3009 specifies the format and content of the accident analysis information to be presented in the DSA. Regarding the effects of accidents, Section 3.4.2 of the DSA should contain:

- For each operational DBA or EBA, a description of the unmitigated and mitigated scenarios, sufficiently documented to reveal the thought process used for the analysis. This description should include: (a) the initiating event and progression of the accident; (b) the amount of material release and magnitude of the energy release; (c) the physical conditions (such as temperature or pressure) relevant to accident progression; and (d) effects on SSCs and MAR.

- For each DBA or EBA caused by an NPH, a description of: (a) the unmitigated consequence assessment utilized to determine the NDC; (b) the return period of the resulting design basis NPH event; and (c) the magnitude of the design basis event.

- For each external-event DBA or EBA, a description of the external event likelihood along with its technical basis.

Taking fire events as an example, the DSA should qualitatively summarize the fire initiator, describe the event progression from fire initiation, to fire growth (including flashover if possible) through extinguishment without external intervention (such as fire suppression system or fire department response) for the unmitigated analysis, describe expected damages to SSCs, and ultimately define the impacts on the radiological or hazardous chemical MAR, including estimates of ARF, RF, and DRs. All important assumptions should be identified. Reference should be made to the engineering calculations that include the details of the analysis.

For all events (operational, NPH, and external man-made), the impact of the events on SSCs and their ability to function should be included. In such cases, this subsection should reference the analysis or facility documentation, summarize relevant assumptions, and discuss the degree of conservatism in the evaluation. For example, the fire accident summary in the DSA should provide the key inputs and assumptions used in the analysis, such as combustible loading assumptions, facility fire hazard analysis conclusions on adequacy of fire barriers, and physical design features such as rated barriers. Of particular importance are those assumptions that, if not protected by a TSR, would potentially increase the severity or impact of scenarios.

4.2 FIRE SCENARIO ANALYSIS

Quantitative analysis of fires may range from relatively simple to very complex calculations, depending on the fire hazards, facility design and features, and a variety of other considerations. The simple evaluations apply the five-factor source term formula from Chapter 5 along with dispersion and consequence analysis described in Chapters 6, 7, 8, or 9. More complex fire analyses include application of fire models, such as computer codes or hand calculations as presented in this section to determine the magnitude of the fire and its damage potential, to provide input to in-facility transport modeling, and/or buoyant plume modeling.

The majority of fires analyzed for the DSA are referred to as *compartment fires* (i.e., fires in enclosed spaces such as gloveboxes or process rooms). However, fires may also occur outside the facility's confinement features.[23] Knowledge of the effect of the fire on radioactive material or hazardous chemicals and SSCs response to fires will be useful in determining the source term (MAR, DR, ARF/RF,

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[23] Examples: loading dock with doors open, outside staged waste containers, or wildfire.

LPF) and whether the release may be a lofted plume due to buoyancy from the sensible heat of the fire. Maximizing heat rates is not always conservative when plume rise is taken into account due to increased lofting associated with higher heat plumes.

The fire phenomena also affects evaluation of the effectiveness of the control set and evaluation of fire effects on safety SSCs, for example, heat, smoke, and water impingement.

This section presents summary information needed to understand and evaluate the progression and severity of fire events. The following subsections describe the phenomenology of fire initiation, growth, and propagation. Analytical solutions are based on empirical correlations that have been shown to provide reasonable engineering predictions. References to publicly available methodology guides, manuals, standards, or codes are provided where applicable.

4.2.1 FIRE SCENARIOS

The DSA fire assessment should be performed in coordination with a designated fire protection engineer. Credible fire scenarios evaluated in the DSA hazard evaluation and the accident analysis should be consistent with the Fire Hazard Analysis (FHA) (See Section 4.2.2).

For all DBA/EBA scenarios, it is a best practice to include all details that have an effect on the analysis. These details may include room dimensions, contents, and materials of construction; combustible loading; arrangement of rooms in the building; sources of combustion air; position of doors and airlocks; and numbers, locations, and characteristics of occupants. All assumptions that may have a significant effect on the analysis should be listed. Details of the analysis are either presented in the DSA, or are documented in the FHA or in a supporting calculation that is then summarized and referenced in the DSA.

Typically, fire scenarios selected for analysis will include those which can result in significant release of radioactive material affecting workers or the public. Scenarios that result in similar consequences and controls (preventive and mitigative) may be analyzed as a group using the most limiting/severe conditions for that group. Fires can be further categorized as to the location and/or MAR involved in order to develop representative events to address the nature of fire hazards within a glovebox, within the facility areas serviced by the confinement ventilation, and external to facilities serviced by the confinement ventilation system.

The selected fire scenarios should consider:

- Configuration of the fire area and characteristics of the associated fire barriers;
- MAR quantities that could be involved in an accident;
- Presence, location and type of ignition sources;
- Combustible loading; and
- Specific hazards that necessitate unique controls to prevent or mitigate a fire accident.[24]

Application of these considerations should be documented and evaluated for the need to protect any assumptions as applicable. For example, an ignition source is generally assumed to exist; deviation from this accepted approach would require sufficient justification. Combustible loading is another area that requires significant attention to the assumptions made. Combustible loading assumptions should remain physically meaningful with respect to the facility operations while also being significantly conservative. It

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[24] Materials of construction that are radioactive (considered as MAR) and are involved in the fire, and the chemical form of the radioactive material as different materials with separate chemical forms, may have a different ARF and RF.

may not be appropriate, for example, to assume a large fuel spill near a glovebox line where vehicles cannot access but considerable ordinary combustible inventory may be possible in off-normal conditions such as recovery from a contamination event or construction activities. Where a fire scenario is particularly sensitive to the assumed combustible loading, a credited control is typically appropriate.

Scenarios that are analyzed as a group should be evaluated to ensure that the control set is effective for all scenarios in that group. For example, if a fire suppression system is a control for a group of scenarios, the fire suppression system needs to be evaluated to ensure that the system will actuate under all the scenarios.

4.2.2 FIRE ANALYSIS

Fires have four stages or distinct regimes: (1) ignition, (2) growth, (3) fully developed, and (4) decay. Ignition can occur when flammable vapors are present in sufficient quantity to be ignited. Vapors may result from release of a flammable gas, spillage of a flammable liquid, or the heating of a combustible liquid or solid material (i.e., pyrolysis). Following ignition of the initial fuel source, neighboring materials can be heated through direct flame impingement and/or heat transfer, causing propagation and overall growth of the fire.

A fire can become fully developed when it reaches either a fuel-limited or a ventilation-limited state. Scenarios, such as an outdoor pool fire, reach a fuel-limited state when the entire surface area becomes involved and sufficient oxidant, usually air, is available for combustion. Ventilation-limited fires occur in enclosures where sufficient openings and/or supply air are not available to provide enough air for combustion. A fire can remain in a fully-developed state until all available combustibles are burned or intervention takes place (e.g., fire-fighting response). Intervention of the fire can result in extinguishment or control. Figure 4-1 shows a conceptual model of the four fire regimes of fire growth without intervention as a function of Heat Release Rate (HRR) and time as presented in the fire science literature. That figure also conceptually shows the effects of intervention to extinguish or control the fire.

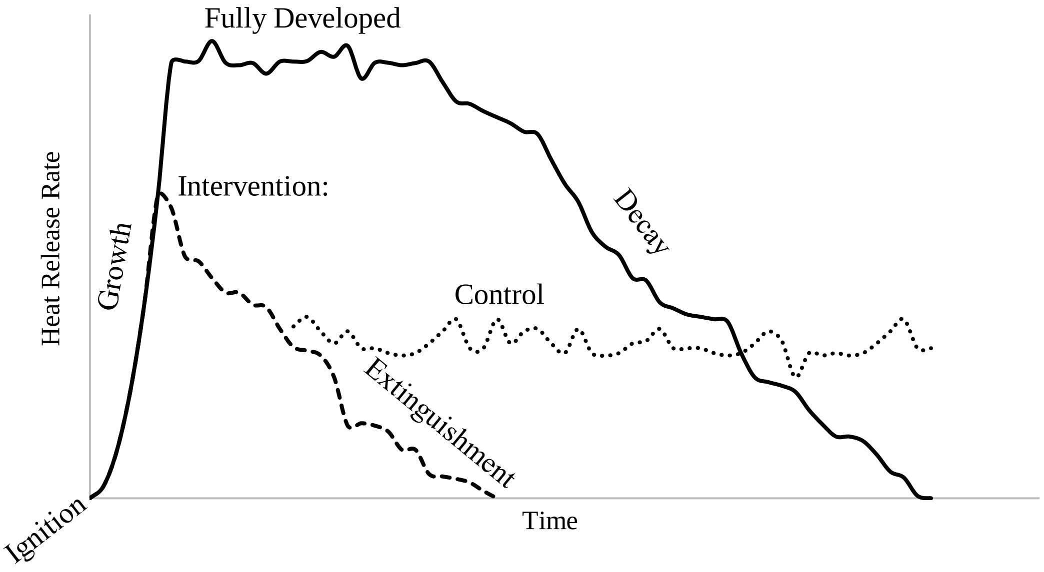

Figure 4-1. Fire Growth Model.

The facility FHA should serve as the basic input to the DSA fire scenario development and any fire analysis performed to support the DSA. As directed by DOE O 420.1C, Chg. 1, *Facility Safety*, the FHA "… must be integrated into safety basis documentation." Integration of the FHA and DSA can be achieved through various approaches with the primary objective being the consistency of similar fire analyses, credited controls, and conclusions.

In general, the FHA will describe and assess various postulated fires with primary quantitative focus placed on the maximum possible fire loss, the maximum credible fire loss, and the fires selected as DBA/EBAs for the DSA.[25] Additional analysis beyond that performed in the FHA may be necessary to serve the purpose of evaluating the effect on MAR, equipment, structures, and safety SSCs. Input to DBA/EBAs taken from the FHA should be reviewed closely to ensure consistency with DSA principles (e.g., use of unmitigated scenarios) and for assumptions requiring protection.

It is beneficial to have the assumptions, analytical methods, and conclusions be closely related when these fires are described and analyzed in both the FHA and the fire analysis document supporting the DSA. Execution of the integration between the FHA and DSA has been continually improving in the DOE complex for many years. Detailed discussion of important concepts, approaches, and recommendations has been developed by the EFCOG/SAWG, *Fire Analysis for DOE Nuclear Facilities* (2008), which further evolved and updated the guidance in Appendix B, White Paper on Fire Hazards Analysis, in DOE-HDBK-1163-2003, *Integration of Multiple Hazard Analysis Requirements and Activities.*

Correlations based on experiments and testing for numerous phenomena related to fire have been developed and have been proven to be reasonable estimates for modeling and analysis. Much of these can be applied as hand calculations. The following introduces some basic calculation methods commonly used for accident analysis. In addition to governmental resources such as the U.S. National Institute of Standards and Technology (NIST) and the NRC, the Society of Fire Protection Engineers (SFPE) and National Fire Protection Association (NFPA) also provide numerous publications detailing quantitative fire analysis methodologies.

Extensive analysis techniques are documented and available in various NFPA standards, in the NFPA's *Fire Protection Handbook* (NFPA, 2008), in the SFPE's *Handbook of Fire Protection Engineering* (SPFE, 2008), and in other fire protection engineering references. Another useful reference document is NRC's NUREG-1805, *Fire Dynamics Tools (FDT*^{s}*): Quantitative Fire Hazard Analysis Methods for the U.S. Nuclear Regulatory Commission Fire Protection Inspection Program.* FDT^{s} was developed using state-of-the-art fire dynamics equations and correlations, many of which were derived from the principles presented in the SFPE and NFPA handbooks and other fire science literature. The hand calculations that follow are primarily from NUREG-1805. In addition, there are spreadsheets associated with NUREG-1805, available for download from the NRC (http://www.nrc.gov/reading-rm/doc-collections/nuregs/staff/sr1805/), that allow the user to input heat, diameter and fuel type, and the spreadsheet performs the calculation and provides a text listing of the equation being solved.[26]

The level of detail in the fire analyses should be performed using a graded approach, depending on the potential consequences of the DBA/EBA fire event. DBA/EBAs that do not challenge established thresholds generally do not require exhaustive analysis for a scoping assessment, and the level of detail for DBA/EBAs that greatly exceed the consequence thresholds of concern would have much greater

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[25] The maximum possible fire loss and maximum credible fire loss scenarios are evaluated to meet fire protection program requirements based on other considerations such as property damage and economic loss, and may not be the bounding scenarios for release of radioactive or hazardous materials for the DSA evaluations.

[26] Applications of these spreadsheets and any other fire codes are subject to the DOE SQA requirements as discussed in Section 3.5 of this Handbook.

expectations.

4.2.2.1 EXAMPLE ANALYTICAL METHODS

The following presents information to assist in understanding and evaluating the progression and severity of fire events. The analytical methods presented focus on simple fire phenomena that can be analyzed with a hand calculation. Multiple methods of calculation for fire dynamics phenomena may be available, each with varying applicability for specific scenarios. Understanding the limitations, uncertainties, and background of the chosen analytical method is essential to ensure proper application. The analyst should refer to NUREG-1805, the SFPE and NFPA handbooks, or other applicable fire science references for specific applications.

Complex models involving multiple rooms and openings or the need to understand detailed heat transfer characteristics can be more effectively modeled using computer-based analysis. The Consolidated Model of Fire and Smoke Transport (CFAST) Versions 3.1.7 and 5.1.1 is a Central Registry Toolbox Code approved by DOE for use in safety basis and FHA development. Further guidance on CFAST can be found in DOE-EH-4.2.1.4, *CFAST Computer Code Application Guidance for Documented Safety Analysis*. Another available code is Fire Dynamics Simulator, a computational fluid dynamics model of fire-driven fluid flow managed by NIST.

4.2.2.1.1 HEAT RELEASE RATE

In order to evaluate a fire scenario, the combustible loading and configuration need to be established (see Section 4.2.1 for additional guidance on initial conditions). It is usually necessary to first understand the unmitigated fire potential in terms of HRR. The two examples that follow detail common methods for determining the potential HRR for a fire involving liquids and solids. To determine the maximum potential HRR, the fires are assumed to be fuel-limited with adequate oxygen to support full involvement of the fuel. Note that this assumption will produce higher mass-loss rates, and thus shorter durations, than a ventilation-limited fire.

4.2.2.1.2 POOL FIRE HEAT RELEASE RATE

Liquid pool fires can occur following a spill or leak of flammable or combustible liquid. Common scenarios include:

- A confined spill into a diked area or sump followed by ignition;
- An unconfined spill onto a hard surface followed by ignition;
- An unconfined spill onto a permeable surface such as loose soil followed by ignition; and
- A flowing spill that is ignited.

Methods to establish the HRR for these scenarios are described in the SFPE Handbook. Contained spills are covered in the SPFE Handbook Section 3, Chapter 1, Heat Release Rates, and in NUREG-1805 Chapter 3, Estimating Burning Characteristics of Liquid Pool Fire, Heat Release Rate, Burning Duration, and Flame Height. Both of these references were used for the example provided below. The other three scenarios listed above are described in the SFPE Handbook Section 2, Chapter 15, “Liquid Fuel Fires.”

Typically, pool fires are assumed to be circular. It is common practice to estimate arbitrarily shaped fires using an equivalent area circle (see NUREG-1805, Section 5.3.1). Highly elongated shapes are not applicable to the methods described below (SFPE, 2008).

Example: A 100 gal (0.38 m^3) kerosene spill, which is contained by a 3 m by 5 m diked area, is ignited. The objective is to estimate the HRR from the burning pool. Because the diked area is rectangular, an effective pool diameter needs to be estimated.

$$D_{eff} = \sqrt{\frac{4A}{\pi}} = \sqrt{\frac{4(3m)(5m)}{\pi}} = 4.4m \qquad \textbf{Equation 4-1}$$

Where:

D_{eff}	effective pool diameter (m)
A	pool fire area (m^2)

The HRR for a pool fire burning in still open air, is estimated using (from SFPE 2008):

$$\dot{Q} = \Delta h_c \dot{m}''_{\infty}\left(1 - e^{-k\beta Deff}\right) \times A \qquad \textbf{Equation 4-2}$$

Where:

$\dot{Q}$	HRR (MW)
Δh_c	net heat of combustion (MJ/kg)
$\dot{m}''_{\infty}$	mass loss rate per unit area (kg m^{-2} s^{-1})
$k\beta$	extinction absorption coefficient and beam length correction (m^{-1})

For kerosene, Equation 4-2 becomes:

$$\dot{Q} = \left(\frac{43.7MJ}{kg}\right)\left(\frac{0.039kg}{m^2 s}\right)\left(1 - e^{-(3.5m^{-1})(4.4m)}\right)[(3m)(5m)] = 25.6MW \qquad \textbf{Equation 4-3}$$

For a uniform pool depth, the approximate burn duration for the fire is (SFPE, 2008)[27]:

$$t = \frac{\rho V}{\dot{m}''_{\infty}(1-e^{-k\beta D)} \times A} \qquad \textbf{Equation 4-4}$$

Where:

t	fire duration (s)
ρ	liquid density (kg/m^3)
V	spill volume (m^3)

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[27] NUREG-1805, Section 3.3.1 provides another equation for the burning duration as {V / [A * regression rate]} or {(ρV) / [A * $\dot{Q}$ per unit area]}.

For the postulated 100 gal spill, the fire duration from Equation 4-4 is:

$$\boldsymbol{t = \frac{\left(820\frac{kg}{m^3}\right)(0.38m^3)}{\left(0.039\frac{kg}{m^2s}\right)\left(1-e^{-\left(3.5\frac{1}{m}\right)(4.4m)}\right)[(3m)(5m)]} = 533\,sec = 8.9min}$$ **Equation 4-5**

Note that this analytical method is limited to pool fires with diameters between 0.2 m and 50 m (SFPE, 2008).

4.2.2.1.3 PALLET FIRE HEAT RELEASE RATE

Wooden pallets are common in many facilities and can produce a high HRR. NUREG-1805, Table 2-8 provides HRR per unit area for various heights of stacked pallets, while SFPE Handbook Section 3, Chapter 1 provides a correlation to estimate the HRR from a stack of wood pallets based on height.

Example: For a 5 ft high pallet stack with a nominal area of 4 ft x 4 ft (1.2m x 1.2m), referencing NUREG-1805, Table 2-8, the HRR per unit area is 3,970 kW/m^2. The total HRR would be:

$$\boldsymbol{\dot{Q} = A\,\dot{Q}'' = (1.2m)^2\left(3,970\frac{kW}{m^2}\right) = 5,717kW = 5.7M}$$ **Equation 4-6**

4.2.2.1.4 FLAME HEIGHT

Determination of a fire’s flame height can be helpful in order to estimate the likelihood of further propagation or structural impacts. Flame height at sea level of a fire may be predicted using Equation 4-6, based on the 1995 Heskestad method (NUREG-1805 Section 3.4, Flame Height [which also includes the 1962 Thomas method], SFPE 2008). Flame height corrections at elevations significantly above sea level can be found in Section 2, Chapter 1 of the SFPE Handbook. Equation 4-7 represents the height of the flames above the base of the fire and is based on empirical test data.

$$H = 0.235\,\dot{Q}^{2/5} - 1.02D$$ **Equation 4-7**

Where:

H	flame height above base of fire (m)
$\dot{Q}$	HRR (kW)
D	flame diameter (m), i.e., the diameter of the burning area as described in NUREG-1805.

Example: This equation can be applied to fires reasonably approximated by a circle. For this example, the flame height for the pallet fire discussed in Section 4.2.2.1.2 will be found (5 ft stack of 4x4 ft pallets).

The effective diameter from Equation 4-1 is:

$$D_{eff} = \sqrt{\frac{4A}{\pi}} = \sqrt{\frac{4(1.2m)(1.2m)}{\pi}} = 1.4m$$ **Equation 4-8**

The flame height from Equation 4-7 is:

$$H = 0.235(3{,}010\ kW)^{2/5} - 1.02(1.4m) = 4.4m$$ **Equation 4-9**

4.2.2.1.5 ENCLOSURE FIRE DYNAMICS

Fires within an enclosure, such as a glovebox or a room in a building, exhibit distinct behavior that differs from well-ventilated fires. There are two primary differences when considering an enclosure fire: (1) interaction with the enclosure boundary; and (2) the development of an upper layer (hot, gaseous products) of the fire that collect in the compartment. In both cases, the enclosure boundary and the upper layer have the ability to reflect and radiate heat within the enclosure. Heat and mass transfer effects out of the boundary may also affect the behavior of the fire.

Flashover is a phenomenon of importance when analyzing enclosure fires. Flashover is "the rapid transition to a state of total surface involvement in a fire of combustible materials within an enclosure" (ASTM E176). The occurrence of flashover is dependent on many variables such as available vent area, heat transfer from the enclosure boundary, and HRR of the fire. Flashover occurs when the temperature of the enclosure, with consideration given to the radiative effects of the upper layer, is sufficient to effectively ignite all combustibles in the enclosure. Upon transition to flashover, the fire is in a ventilation-limited state.

4.2.2.1.5.1 PRE-FLASHOVER

Pre-flashover room temperatures can be estimated for simple geometries using energy balance techniques. NUREG-1805, Section 2.6 and the SFPE Fire Protection Handbook, Section 3, Chapter 6 (SFPE, 2008) describes methods that can be applied to

- Small to medium size room with natural ventilation such as a single open door or window; or
- Small to medium size room with forced ventilation.

The following analytical method predicts the temperature of the upper layer as a function of HRR. This methodology can be used to estimate the onset of flashover and can also be used as input to sprinkler or heat detector activation. This method is primarily applicable to thin walled, ventilated enclosures with high heat conductive boundaries.

Example: Room Fire with Forced Ventilation. A 500 kW fire occurs in a ventilated steel box. The box is 2.4 m wide, 6.0 m long, and 2.3 m high with 16 mm thick walls. The ventilation flow rate is 1,000 cfm (0.57 kg/s for air at standard temperature and pressure). Predict the upper layer temperature at 5.0 minutes.

The upper layer temperature is (Section 2.64.4 of SFPE, 2008):

$$\boldsymbol{T_g = \frac{\dot{Q}}{\dot{m}_g c_p + h_k A_T} + T_\infty}$$ **Equation 4-10**

Where:

T_g	upper layer gas temperature (°K)
T_∞	ambient air temperature (°K)
$\dot{Q}$	HRR of the fire (kW)
$\dot{m}_g$	ventilation mass flow (kg/s)
c_p	specific heat of air (kJ/kg °K)
h_k	effective heat transfer coefficient (kW/m^2 °K)
A_T	compartment surface area (m^2)

The compartment surface area is:

$$A_T = 2(2.3m)[(6.0m) + (2.4m)] + 2(6.0m)(2.4m) = 67m^2$$

Equation 4-11

The effective heat transfer coefficient for a thin-walled compartment will range from 0.012 to 0.03 kW/m^2·K, calculated from the following (SFPE, 2008):

$$\boldsymbol{h_k = 30 - 18\left[1 - e^{\left(-\frac{50t}{p\delta c}\right)}\right]}$$

Equation 4-12

Where:

h_k	heat transfer coefficient [W/m^2 °K]
t	exposure time (s)
ρ	compartment boundary density (kg/m^3)
δ	compartment boundary thickness (m)
c	specific heat of compartment boundary (J/kg °K)

Using commonly available material properties for steel, at 5 minutes (300 seconds) the effective heat transfer coefficient is:

$$h_k = 30 - 18\left[1 - e^{\left(-\frac{\left(50\frac{W}{m^2{}^\circ K}\right)(300s)}{\left(7833\frac{kg}{m^3}\right)(0.0016m)\left(465\frac{J}{kg\,{}^\circ K}\right)}\right)}\right] = 13.4\ \frac{W}{m^2{}^\circ K}$$

Equation 4-13

The upper layer temperature is:

$$T_g = \frac{500kW}{\left(0.57\frac{kg}{s}\right)\left(1.01\frac{kJ}{kg\,{}^\circ K}\right)+\left(0.0134\frac{kW}{m^2\,{}^\circ K}\right)(67m^2)} + 293^\circ K = 623^\circ K = 360℃$$

Equation 4-14

4.2.2.1.5.2 FLASHOVER

Upper layer temperatures, such as those found using methods discussed above, can be used to predict flashover. Upper layer temperatures of 500°C to 600°C are widely considered to be associated with the onset of flashover (NUREG-1805, SFPE 2008, NFPA 2008). More rigorous flashover prediction can be performed using methods from NFPA 555, *Guide on Methods for Evaluating Potential for Room Flashover*, or NUREG-1805 Chapter 13, which applies different correlations.

A common screening criterion for predicting flashover in a compartment with a single vent opening is detailed in the example below, based on the Thomas method (NUREG-1805 Chapter 13, SFPE 2008 Section 3 Chapter 6, NFPA 555) using the empirical formula presented in Equation 4-15. This example estimates the HRR necessary to achieve flashover; this can be compared to the HRR for the postulated fire as found using methods such as those presented in 4.2.2.1.

Example: Estimate the HRR required to cause flashover in a room 2.4 m deep, 6.0 m long, and 2.3 m high. The door is 2.36 m high and 1.19 m wide.

$$\dot{Q} = 7.8A_{room} + 378A_{vent}\sqrt{H_{vent}}$$ **Equation 4-15**

Where:

$\dot{Q}$	HRR required for flashover (kW)
A_{room}	total area of walls, floor, and ceiling, less the vent area (m^2)
A_{vent}	total vent area (m^2)
H_{vent}	height of vent (m)

The vent area associated with the door would be:

$$\boldsymbol{A_{vent} = (2.36m)(1.19m) = 2.81m^2}$$ **Equation 4-16**

The surface area of the compartment would be:

$$\boldsymbol{A_T = 2(6.0m)(2.4m) + (2.3m)[2(6.0m) + 2(2.4m)] - (2.81m^2) = 64.6m^2}$$ **Equation 4-17**

The HRR needed to create flashover with the door fully open is:

$$\boldsymbol{\dot{Q} = 7.8(64.6m^2) + 378(2.81m^2)\sqrt{(2.36m)} = 2,100kW}$$ **Equation 4-18**

4.2.2.1.6 SOLID FUEL IGNITION AND RADIANT HEATING

Describing the progression of a postulated fire requires analysis of potential propagation. Specifically, co-located combustible materials can be ignited by a fire. Determining if these combustibles will ignite in a given fire or determining the minimum separation distance to prevent ignition is an important consideration.

There are two basic ignition metrics: (1) heat flux; and (2) surface temperature. Both metrics may be used, but heat flux is the more common method to predict solid fuel ignition. There are multiple test methods be used to measure ignition heat flux. Results will vary with the test method. In general ignition heat fluxes will be lower for piloted tests than for autoignition tests (i.e., piloted tests include a flame or spark; autoignition tests do not). Ignition heat fluxes will also vary with the duration of the exposure. Lower fluxes require longer exposures to cause ignition. A commonly accepted default ignition heat flux used for cellulosic materials is 12.5 kW/m^2. For additional ignition flux data, see the *Ignition Handbook* (Babrauskas, 2003).

One methodology to estimate the heat flux imposed on a target is based on Beyler's 2002 equation as presented in NFPA 555, SFPE 2008, and NUREG-1805 (Section 5.3.2 Solid Flame Radiation Model with Target At and Above Ground Level):

$$\dot{q}'' = F_{f-t}E_f \qquad \textbf{Equation 4-19}$$

Where:

$\dot{q}''$	heat flux at the target fuel package (kW/m^2)
F_{f-t}	view factor between the flames and a differential area on the target fuel package (dimensionless)
E_f	emissive power of the flames (kW/m^2)

When using the fire flame height estimation in Equation 4-7, the corresponding emissive power correlation is based on the Shokri and Beyler 1989 empirical correlation from experimental data as presented in NFPA 555, SFPE 2008, and NUREG-1805 Section 5.3.2:

$$E_f = 58(10^{-0.00823D}) \qquad \textbf{Equation 4-20}$$

Where:

E_f	emissive power of the fire (kW/m^2)
D	fire diameter (m)

Figure 4-2 shows the view factor for a differential planar element (dA$_1$) of an object at a specified distance (h) to a finite-length right circular cylinder, where the normal to the element passes through the one end of the cylinder and is perpendicular to the cylinder axis. The view factor (F) is calculated using the following equation (Siegel & Howell, 1992; NUREG-1805 Section 5.3.2.2, Configuration Factor F$_{1-2}$ under Wind-Free Conditions, has different view factor equations from Beyler in 2002 for vertical and horizontal targets at ground level and above ground level):

$$F = \frac{1}{\pi H} tan^{-1}\left(\frac{L}{\sqrt{H^2-1}}\right) + \frac{L}{\pi}\left(\frac{(X-2H)}{H\sqrt{HY}}\right) tan^{-1}\left(\sqrt{\frac{X(H-1)}{Y(H+1)}}\right) - \frac{1}{H} tan^{-1}\left(\sqrt{\frac{(H-1)}{(H+1)}}\right) \qquad \textbf{Equation 4-21}$$

Where:

F	view factor (dimensionless)
h	distance from the object to the centerline of the cylinder (m)
l	height of the cylinder (m)
r	radius of the cylinder (m)
H	distance from the object to cylinder radius ratio (h/r) (dimensionless)
L	cylinder height to radius ratio (l/r) (dimensionless)
X	$(1+H)^2+L^2$ (dimensionless)
Y	$(1-H)^2+L^2$ (dimensionless)

Since the above solution is for a right circular cylinder with the differential area at the base of the cylinder (i.e., fire), to obtain the peak heat flux, which occurs at the mid-height of the cylinder, the actual view factor is twice the value calculated using Equation 4-21, if the cylinder height is taken as half the fire height.

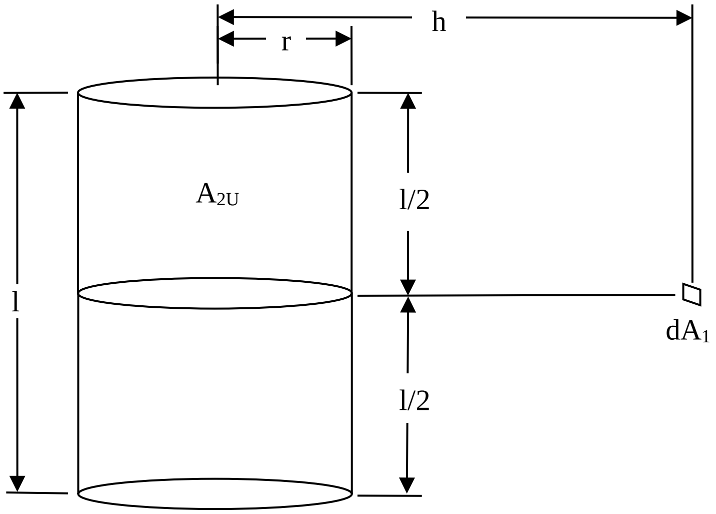

Figure 4-2. Adaptation of View Factor Geometry for a Fire Model.

Example: For a 2 MW fire with a base diameter of 1.2 meters, estimate the heat flux 0.5 meters from the fire at the mid-height of the flames.

The emissive power from Equation 4-20 would be:

$$\boldsymbol{E_f = 58\left(10^{-0.00823D}\right) = 57\,\frac{kW}{m^2}} \qquad \textbf{Equation 4-22}$$

From Equation 4-7 the flame height would be:

$$\boldsymbol{H = 0.235\,(2{,}000kW)^{2/5} - 1.02(1.2m) = 3.69m} \qquad \textbf{Equation 4-23}$$

The view factor for a fire to object separation of 0.5 m is presented below:

l = 3.69 m/2 m=1.845 m

r = 1.2 m/2 m=0.6 m

h =0.5 m + 0.6 m = 1.1 m

H = h/r = 1.1 m/0.6 m = 1.833 m

L = l/r = 1.845 m/0.6 m = 3.075 m

X = $(1+H)^2+L^2 = (1+1.833)^2+(3.075)^2 = 17.48$

Y = $(1-H)^2+ L^2 = (1-1.833)^2+(3.075)^2 = 10.15$

$$\begin{aligned} F = {} & \frac{\tan^{-1}\left(\frac{3.075}{\sqrt{(1.833)^2-1}}\right)}{\pi(1.833)} \\ & + \frac{3.075}{\pi}\left(\frac{\left((17.48)-2(1.833)\right)}{(1.833)\sqrt{17.48(10.15)}}\right)\ \tan^{-1}\left(\sqrt{\frac{(17.48)\left((1.833)-1\right)}{(10.15)\left((1.833)+1\right)}}\right) \\ & - \frac{\tan^{-1}\left(\sqrt{\frac{\left((1.833)-1\right)}{\left((1.833)+1\right)}}\right)}{1.833} = 0.26 \end{aligned}$$

As discussed previously this view factor is for a half-cylinder. The effective view factor is thus twice this value, or 0.52. The heat flux would thus be:

$$\dot{q}'' = (0.52)\left(57\,\frac{kW}{m^2}\right) = 30\,\frac{kW}{m^2} \qquad \textbf{Equation 4-24}$$

Note that when using this method, the SFPE Handbook Section 3, Chapter 10, recommends a safety factor of 2 for heat fluxes in excess of 5 kW/m^2. Application of this safety factor would, thus, increase the prediction of heat flux in Equation 4-24 to 60 kW/m^2. Additionally, this methodology is based on data of pool fires; NFPA 555 endorses the use of this methodology when considering fuel packages but care should be taken when considering the flame height and emissive power of the postulated fire. It should be noted that applying the NUREG-1805 methodology does not include this doubling factor as it sums the horizontal and vertical view factors.

4.2.3 SOURCE TERM CALCULATION FOR FIRE SCENARIOS

DOE-HDBK-3010-94 (page 1-11) describes how a fire can cause an airborne release as follows:

> [Fire] generates heat and combustion gases that may destroy/stress the radioactive material and/or the substrate upon which radioactive materials may be deposited, compromise barriers, and/or pressurize containers/enclosure that may lead to the airborne release of contained radioactive materials. Mass flux of vapors from the reacting surfaces suspend material in air. This material is then entrained in general convective currents that provide transport for particulate materials.

The following discusses the effect of a fire on radiological and hazardous material in terms of parameters important to the source term calculations, thermal effects on SSCs, and smoke damage.

4.2.3.1 EFFECT ON HAZARDOUS MATERIAL

4.2.3.1.1 DETERMINING MAR FOR THE FIRE EVENT

One of the principal outputs of fire analysis is the determination of the affected MAR. In addition, the fire analysis provides information used in conjunction with DOE-HDBK-3010-94 to determine the DR and ARF/RF of the event.

The amount of MAR involved in the event may be the material within the area affected by the fire. For example, the analysis of a small fire within a glovebox that is shown to not propagate beyond the enclosure would consider only the MAR within the glovebox. For large fires, all hazardous material in areas potentially affected by the thermal energy or structural impacts of the fire should be included in the MAR. Therefore, establishing the boundary of the fire's impact area, for example, a rated fire barrier, is important when specifying each component of the MAR.

The determination of a bounding MAR that may be involved in a fire may need to include MAR in adjacent structures. Spatial separation between buildings is evaluated in the FHA and usually evaluated using NFPA 80A, *Recommended Practice for Protection of Buildings from Exterior Fire Exposures*. This code provides information on the role of building type and the impact of distance between buildings on fire propagation. FM 1-20, *Protection Against Exterior Fire Exposure* (2016), may also be consulted. NFPA 80A separation values assume that fire department response will be timely. If an unmitigated separation evaluation is necessary, NFPA 80A recommends that the separation value be increased by a factor of three.

4.2.3.1.2 DETERMINING DR AND ARF/RF FOR THE FIRE EVENT

As further discussed in Chapter 5, DOE-HDBK-3010-94, states the following important consideration regarding MAR and DR:

> The damage ratio is the fraction of the MAR actually impacted by the accident-generated conditions. A degree of interdependence exists between the definitions of MAR and DR. If it is predetermined that certain types of material would not be affected by a given accident, some analysts will exclude this material from the MAR.

Justification of DRs for a fire scenario is generally a function of the size of the fire and facility configuration, as well as how the MAR is being defined due to its interdependence with the DR (see above MAR discussion and Section 5.2.2, Damage Ratio). For example, MAR for a single glovebox operation is normally associated with a 1.0 DR for a fire inside the glovebox, while MAR for a process area could have lower DRs as determined by the fire analysis. Including DRs <1.0 will require refined analysis to justify that the equipment and containers affected by the fire scenario act to limit interaction with the MAR.

Where test data or other criteria are established, DRs for containers can be based on calculations of heat fluxes to targets, sizes of fuel pool fires, and other factors. (see Section 4.2.2, Fire Analysis Methods). For example, the performance of standard 55 gallon drums in fire conditions have been studied in depth; using analytical methods to determine the fire scenario's interaction with a storage array, in concert with the published testing data, can be used as a basis for a DR < 1.0.

For more comprehensive analyses, CFAST or other fire modeling software, such as Fire Dynamics Stimulator, can be used to model the potential damages from fires. These damage estimates can then be used to assess appropriate DRs (see Section 4.2.2.3).

For TRU waste operations, DOE-STD-5506-2007 provides guidance for selection of DRs associated with fire events based upon the type of metal waste container involved and whether a fuel pool fire or an exposure fire is being evaluated. WCH-SD-SQA-ANAL-501, *Fire Protection Guide for Waste Drum Arrays* (Beyler and Guttok, 1996), is a source of experimental data regarding how waste drum arrays responded to pool fires.

Generally, DRs < 0.01 require extensive justification. Consideration needs to be given to describing scenarios, which attempt to use very small DRs to ensure that the bounding event is being described. If there is the potential for another scenario with a higher DR to occur, the differences between the scenarios needs to be clearly outlined in the DBA/EBA section.

The fire analysis should define the scenario progression adequately in order to determine the DR, and the ARF/RF using DOE-HDBK-3010-94. DOE-HDBK-3010-94 provides data on the ARF/RF for the following types of fire-related stresses affecting radioactive material that generate airborne releases:

- Heating of aqueous solution in flowing air without surface rupture of bubbles.
- Boiling (bubbles continuously breaking the surface of the bulk liquid with <30% of the volume of the liquid as bubbles).
- Volatiles such as iodine, under all conditions.
- Quiescent burning, small surface area pools, or small solvent layer over large aqueous layer burning to self-extinguishment.
- Vigorous burning large pools or solvent layer burning over limited aqueous layer with sufficient turbulence to disrupt bulk of aqueous layer.
- Large, vigorously burning organic fire that burns to complete dryness or burning solvent over aqueous phase burning to complete dryness for both phases (requires external heat source).
- Aqueous solution or air-dried salts under gasoline fire on a porous or otherwise absorbing surface.
- Airborne release of particulates formed by oxidation at elevated temperature, greater than room temperature but less than self-sustained oxidation (ignition).
- Airborne release of particulates formed by self-sustained oxidation.
- Airborne release of particulates during complete oxidation of metal mass.
- Airborne release during free-fall of molten metal drops.
- Plutonium compounds subjected to thermal stress (temperature <1000º C, natural convection).
- Contaminated combustible materials heated/burned in packages.
- Dispersed ash dropped into airstream or forced draft air.

Selection and development of ARF/RF is further discussed in Chapter 5.

4.2.3.2 THERMAL EFFECTS

Another output of the fire analysis is information useful in determining the environmental stressors on SSCs, in particular safety SSCs relied on to mitigate the event.

Failure of structural members can have a major impact on the accident progression; the fire analysis should consider structural members located near postulated fires. The strength and stiffness of structural steel begins to worsen when heated leading to possible deformation and failure. Structural, reinforced concrete also may begin to degrade when subjected to extreme temperatures. Building codes generally provide prescriptive fire ratings for structural members; however, detailed analytical methods can be used for design of critical structural components and should include heat transfer analysis and consideration of steel properties at elevated temperatures (Buchanan, 2001).

Radiant heating, direct flame impingement, and hot gas layers can cause the failure of both passive and active mechanical SSCs. Temperature limits of valves, motors, and sensors should be considered in conjunction with radiant heating models when reviewing effects to SSCs from postulated fires. Radiant heating and hot gas layer temperature models were presented in Section 4.2.2. Although most fire analysis relates to the direct release of hazardous material due to the effect of the fire itself, fire in control systems in adjacent areas could indirectly cause a release of MAR.

Accordingly, the best practice is to calculate the potential thermal effects of the fire events to determine what SSCs would be available for both the unmitigated and mitigated consequence calculations.

4.2.3.3 SMOKE DAMAGE

The intent of this section is not to look at the effects of smoke on the workers or members of the public, but on equipment integrity. Smoke can damage equipment and render active SSCs either inoperable or behaving in an unpredictable manner. Sensitive electrical components such as programmable logic controllers used in safety-instrumented systems could fail due to smoke conductivity or corrosivity. Circuit bridging has been observed in testing of electrical components subjected to heavy smoke environments (NUREG/CR-7123, *A Literature Review of the Effects of Smoke From a Fire on Electrical Equipment*); consideration may need to be given to the failure state of electronics. Longer-term degradation effects of smoke (days to months) are also important considerations upon restart following a fire.

Smoke can also affect nuclear ventilation system High Efficiency Particulate Air (HEPA) filters causing them to clog. There are two main failure mechanisms for HEPA filter failure from smoke generated by a fire; plugging and blowout/media failure. Plugging occurs when the filter media becomes saturated with particles and prevents adequate airflow. Blowout/media failure occurs when holes or other openings in the media occur and allow particulate matter to pass through the HEPA filter. Both of these mechanisms are important, since they both will create unfiltered leakage paths, which increase the LPF, thus contributing to the amount of released material. The effect of HEPA filter failure needs to be included in assessment of radioactive releases in the FHA and DSA. In the case of plugging, the fire generates hot gases, which pushes smoke and contamination outward in the absence of adequate HEPA filter flows. With HEPA media failure the ventilation system flows are no longer effectively filtered. Filter clogging occurs before blowout/media failure, and therefore, has been used to determine when loss of confinement occurs.

Correlations have been developed by researchers and the fire protection industry and used in FHAs and DSAs to estimate the rate of smoke loadings on HEPA filters; however, there is no one universally accepted model, nor universally accepted criteria recommended for determining when plugging causes loss of confinement or filter blow-through. An example of one model is provided in *Analysis of Filter System Soot Loading for Postulated Fires in the K-Area Complex Container Surveillance and Storage Capability Project (U)* (Sprankle, 2007). Another example of smoke loadings on HEPA filters is in WIPP-058 (Revision 2), *DSA Supporting Calculation, Fuel Spill, HEPA filter Plugging, Fire Compartment Over-Pressurization, Facility Pallet Survivability, Lube Truck Standoff Distance, Waste Array Fire Spread, and Internal Drum Event Fire in CH Bay and Along Waste Transport*.

A good summary of performance of HEPA filters under accident conditions in terms of filter efficiencies and pressure differentials is provided in Appendix F, Filtration, of NUREG/CR-6410. Regarding smoke modeling and confinement ventilation systems, DOE-HDBK-1169-2003, *Nuclear Air Cleaning Handbook,* provides discussions in Sections 10.4 and 10.5. Section 10.4 provides these cautions on the use of modeling:

> Fire models for FHAs range from simple algorithms that predict thermodynamic changes in enclosures to complex programs that can account for heat, mass transfer, and smoke production in multiple enclosures. Many mathematical models have been installed in software codes and are available on the Internet bulletin boards of various government agencies. These codes can predict the development and spread of fire and smoke conditions through multiple rooms, and can account for changes in the structure and composition of enclosures. Application of these models requires considerable understanding of their use and limitations, statements of which are usually included in the instructional

> text published with the software codes. Reduction of complex models to simple terms supported by empirical data is often useful in predicting uncomplicated systems.

4.3 EXPLOSION SCENARIO ANALYSIS

The DSA analyzes explosion scenarios developed from hazardous or upset conditions that challenge the material at risk in non-reactor nuclear facilities involving tanks, pipes, vessels and/or containers, filled with flammable or non-flammable, gases or liquids, pressurized or not. Explosion events are assessed inside or outside the facility. An explosion scenario can arise from a wide spectrum of hazards, operational conditions, and from deviations in the safety requirements in the facility or its production process.

The quantitative analysis of the effects of an explosion on the SSCs establishes the basis to identify safety controls for preventive or mitigative considerations. The explosion scenarios, analyzed for the facility DSA, are used to demonstrate the effectiveness of the control strategy such as the ability of explosion barriers, efficient implementation of hazardous material protection, testing, surveillance and maintenance.

Explosion models using hand calculations are presented in this section to aid in the assessment of the explosion magnitude, and its damage potential, such as blast (overpressures), fragmentation, and thermal damages.

Explosion accidents that have unique dispersion characteristics may be modeled using phenomenon-specific codes more accurately representing the release conditions. Areal Locations of Hazardous Atmospheres (ALOHA) Version 5.4.6 is a chemical consequence code (see Section 9.7) that is capable of calculating consequences for Boiling Liquid Expanding Vapor Explosions (BLEVE), explosions due to delayed ignition and radiant heat from fires resulting from explosions.

The intention of this chapter is to provide basic insights and formulas for the various calculations presented with the expectation that further insight and clarification can be attained by consulting the referenced literature. Subsections 4.3.1 and 4.3.2 describe how an explosion event can be defined and analyzed. Subsection 4.3.3 briefly describes the damages to receptors and SSCs in terms of potential consequences and subsection 4.3.4 presents a brief assessment for the source term estimation for explosion scenarios. A specific case of a hydrogen explosion is presented in subsection 4.3.5.

4.3.1 EXPLOSION EVENT TYPES AND SCENARIOS

Explosions can be defined in a variety of ways. In the textbook *Explosion Hazards and Evaluation* (Baker et al., 1983), one finds the following general definition of an explosion:[28]

> In general, an explosion is said to have occurred in the atmosphere if energy is released over a sufficiently small time in a sufficiently small volume so as to generate a pressure wave of finite amplitude traveling away from the source. This energy may have originally been stored in the system in a variety of forms; these include nuclear, chemical, electrical or pressure energy, for example. However the release is not considered to be explosive unless it is rapid enough and concentrated enough to produce a pressure wave that one can hear. Even though many explosions damage their surroundings, it is not necessary that an explosion produce external damage. All that is necessary is that the explosion is capable of being heard.

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[28] This reference is also cited in NUREG/CR-6410 and NUREG-1805.

NUREG-1805 states that “An explosion is defined as a sudden and violent release of high-pressure gases into the environment” and that “In its most widely accepted sense, the term ‘explosion’ means a bursting associated with a loud, sharp noise and an expanding pressure front, varying from a supersonic shock wave to a relatively mild wind.” The NUREG also offers several other definitions and concepts of an explosion from the literature.

The word “explosion” thus applies to a variety of phenomena that can cause a range of damage from mild to severe. Generally, there are two categories of explosions 1) the result of purely physical phenomena such as the rupture of a high pressure air tank, or 2) as the result of a chemical reaction. Figure 4-3 provides a simplified explosion categorization for likely scenarios at DOE facilities. This section does not addresses natural explosions (lighting, volcanoes, meteors, atmospheric pressure change from tornado or hurricane), intentional explosions (nuclear, high explosives, firearms), dust explosions, runaway reactions, neither does it cover the toxicity and asphyxiation effects (see Chapter 9) as consequence of explosions since these events are subject to more detailed evaluations that are beyond the scope of this handbook.

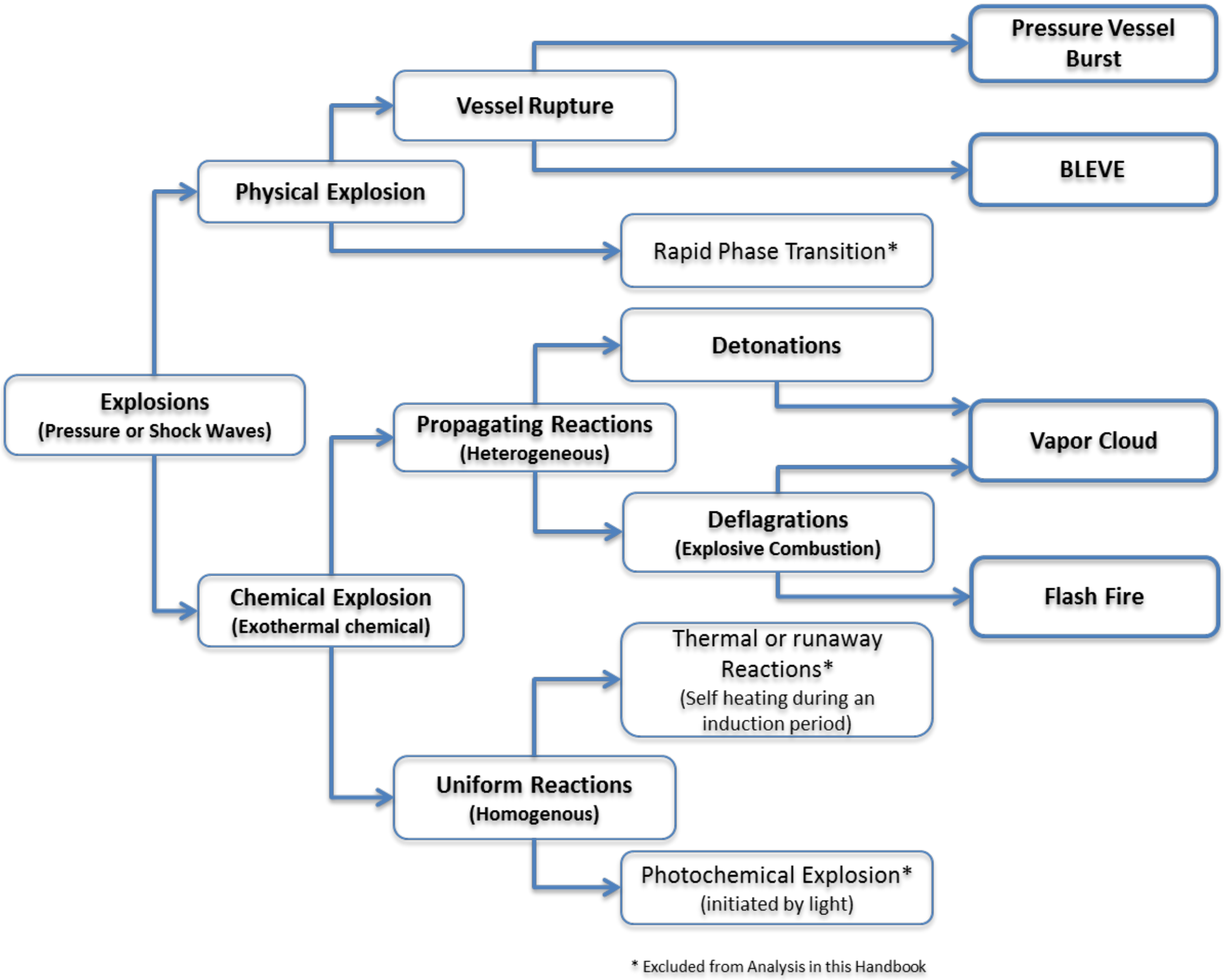


Figure 4-3. Simplified Explosion Categorization.

Special terminology associated with explosions is explained below.

Physical Explosion: Those caused when the high-pressure gas is generated only by mechanical means without any chemical change as in the following types of explosions:

- external heating of a tank resulting in increased internal pressure and resultant failure of the tank; and
- sudden release of super-heated liquid which flash-evaporates, causing a rapid explosion.(NUREG-1805, page 15-2)

Chemical Explosion: Caused when high-pressure gas is generated by a chemical reaction. The generation of high pressure gas is the result of exothermic reactions where the fundamental chemical nature of the fuel is changed. Chemical reactions of the type involved in an explosion usually propagate in a reaction front away from the point of initiation. NFPA 921, *Guide for Fire and Explosion Investigations,* states they "can involve solid combustibles or explosive mixtures of fuel and oxidizer, but more common will be the propagating reactions involving gases, vapors, or dust mixed with air. Such combustion reactions are called propagation reactions because they occur progressively through the reactant (fuel), with a definable flame front separating the reacted and unreacted fuel."

In a confined environment, a hydrogen explosion or other flammable gases released in the waste from the decomposition of water and other organics (via radiolysis, catalytic and other mechanisms) is also considered a chemical explosion. Dissolved hydrogen and small quantities of flammable organics may also be released from the waste. Since the waste tanks have an air atmosphere, quantities of oxygen sufficient to allow an explosion are assumed available. For the purpose of an unmitigated scenario, it is assumed that an ignition source is present." (WSRC-TR-2005-00467)

This type of explosion is commonly considered in the hazard and accident analysis for facilities where radiolysis is a hazard, such as high level waste facilities.

While fragmentation is also a concern, a major consequence of these explosions is the airborne release of the hazardous material that was in the vessel or pipe. Such airborne release can occur even if the vessel does not rupture. (see Section 4.3.5 Case: Source Term Calculation for Hydrogen Explosion) Basic "detonation" and "deflagration" descriptions are provided below:

Detonation: The literature offers several definitions, for example:

- A detonation is a propagating chemical reaction of a substance in which the reaction front advances into the unreacted substance at or greater than sonic velocity in the unreacted material. (*Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs* [CCPS, 1994]).
- "Propagation of a combustion zone at a velocity that is greater than the speed of sound in the unreacted medium." (NFPA 68, Definitions).
- In a detonation, the flame or combustion wave propagates through the reactants at supersonic speeds, typically on the order of 2,000 m/sec (6,562 ft/sec). (NUREG-1805, page 15-3).

Deflagration: Again, the literature offers several definitions, for example:

- A propagating chemical reaction of a substance in which the reaction front advances into the unreacted substance rapidly but less than sonic velocity. (CCPS, 1994).
- "Propagation of a combustion zone at a velocity that is less than the speed of sound in the unreacted medium." (NFPA 68, Definitions).

- In a deflagration, the rate of propagation is below the speed of sound in air at 20 °C (68 °F), which is approximately 330 m/sec (1,082 ft/sec). (NUREG-1805, page 15-3).

A brief description for each type of explosion, an associated scenario, and an example are provided in Table 4-1.

The DBA/EBA explosion outlined in the facility's DSA may be a single event consisting of any combination of the explosion types as listed in Table 4-1 and Figure 4-3. The DBA/EBA explosion event needs to identify the bounding explosion analyzed and any other explosion phenomena that are considered credible and bounded by the DBA/EBA selection. In the hazard evaluation, each explosion scenario needs to define the physical boundaries and the associated MAR so that the accident analysis can group the events into similar types to determine the appropriate control sets.

Table 4-1. Types of Explosions Descriptions.

EXPLOSION TYPE	DESCRIPTION	SCENARIOS	EXAMPLES	EFFECTS OF CONCERN
Pressure Vessel Burst	The explosive rupture of a pressure vessel, where the stored energy is released instantaneously, creates a blast wave (i.e., shockwave) in the surrounding air and propels fragments. The shockwave and fragment characteristics depend on vessel contents, pressure, vessel geometry and mode of vessel failure. (Cain, 1996)	An air compressor, during an highly hypothetical event in which all the safety controls fail (relief valves, automatic controls, sensors, instrumentation), continues to run until the internal pressure of the vessel increases and ruptures the vessel. The rupture can occur at a substandard weld, a partial through-wall crack, fatigue from pressurization cycles, and corrosion resulting in wall thinning.	Pressure Vessel Explosion in Houston, TX at the Marcus Oil Facility in December 2004; no fatalities; significant material and structural damages in the neighborhood; Cause: faulty welds in a steel process pressure vessel https://www3.epa.gov/region10/pdf/rmp/cepp_newsletter_0308.pdf	• Overpressure, burst, shock, and/or blast effects • Fragmentation • Thermal effects (if the content in the pressurized vessel is a flammable liquid/gas)
Boiling Liquid Expanding Vapor Explosion (BLEVE)	The explosively rapid vaporization and corresponding release of energy of a liquid, flammable or otherwise, upon its sudden release from containment under greater-than-atmospheric pressure at a temperature above its atmospheric boiling point. A BLEVE is often accompanied by a fireball if the suddenly depressurized liquid is flammable and its release results from vessel failure caused by an external fire. The energy released during flashing vaporization may contribute to a shock wave. (CCPS, 1994)	An ammonia tank, during an highly hypothetical event in which all the safety controls fail (relief valves, automatic controls, sensors, instrumentation) and the tank is punctured by forklift tines at the time a fire in the vicinity exposes the vessel to high temperatures.	BLEVE explosion in Toronto, Canada at the Sunrise Propane Industrial Gases in August 2008; 6 people hospitalized; more than $1.8M in cleanup efforts; various causes: one is attributed to illegal transfer between vessels of liquid propane.	• Overpressure, burst, shock, and/or blast effects • Fragmentation • Thermal effects (if the content in the pressurized vessel is a flammable liquid/gas)
Vapor Cloud	The explosion resulting from the ignition of a cloud of flammable vapor, gas, or mist in which flame speeds accelerate to sufficiently high velocities to produce significant overpressure. (CCPS, 1994)	A flammable gas escapes from its containment and mixes with air to form a flammable mixture, and an ignition source causes the gas cloud to explode.	Vapor Cloud explosion in a city block of Allentown, PA in February 2011; 6 fatalities; $500K fine by the natural gas company UGI Utilities, Inc.; plus extensive costs for the infrastructure replacements of gas distribution system; cause: natural gas leak; Vapor cloud explosion in East Harlem neighborhood in Manhattan, New York; March 2014; 8 fatalities; property destruction; cause: natural gas leak	• Overpressure, burst, shock, and/or blast effects • Thermal effects
Flash Fire	A fire that spreads rapidly through a diffuse fuel, such as dust, gas, or the vapors of an ignitable liquid, without the production of damaging pressure. (NFPA 2113, General definitions)	Flash fire has a heat flux of approximately 80 kW/m^2 "for relatively short periods of time, typically less than 3 seconds." (NFPA 2113) "A flash fire requires an ignition source and a hydrocarbon or an atmosphere containing combustible, finely divided particles (e.g., coal dust or grain) having a concentration greater than the lower explosive limit of the chemical. Both hydrocarbon and dust flash fires generate temperatures from 538 °C to 1038 °C (1000 °F to 1900 °F). The intensity of a flash fire depends on the size of the gas or vapor cloud. When ignited, the flame front expands outward in the form of a fireball. The resulting effect of the fireball's energy with respect to radiant heat significantly enlarges the hazard areas around the gas released" (NFPA 2113, Topic A.3.3.16)	A polyethylene dust explosion at West Pharmaceutical Services in Kinston, NC, in Jan. 2003, 6 fatalities and 39 workers injured. Cause: Ignition of a fine plastic powder, which had accumulated above a suspended ceiling over a manufacturing area at the plant.	• Overpressure, burst, shock, and/or blast effects • Thermal effects

4.3.2 EXPLOSIONS ANALYSIS

This section provides basic descriptions and calculation methods associated with the type of explosions and effects that receive the greatest attention for DSA hazard and accident analysis in the DOE Complex. They are:

1. Overpressure, burst, shock, and/or blast effects. Blast calculation assesses the sudden release of a gas into the surrounding area after a functional vessel rupture (argon, nitrogen tanks) or from a vapor cloud explosion. The goal is to calculate the expansion energy, shock wave, or shock effect, using one of the methods presented to the analyst in the following subsections.

2. Fragmentation. All explosion calculations that involve sudden vessel failures, such as Pressure Vessel Ruptures or a BLEVE result in vessel fragmentation and thus invoke fragment release calculations. The nature of this calculation is to assess either analytically or statistically, the distance, velocity, and energy of a fragment that could impact the MAR.

3. Thermal Analysis. Thermal effects from explosions when the mix is combustible are of utmost importance in addition to the overpressure and fragmentation effects, if applicable. The analysis expands to the calculation of damage distances from the heat flux and the thermal radiation of the vaporized mass that could result in a fireball if the liquid in the failure vessel is combustible. There are several alternate correlations in the literature than those presented here that may be conservative for a DSA accident analysis to determine the thermal radiation distance from an explosion (see NUREG-1805; ALOHA, 2013; *EPA Risk Management Program Guidance for Offsite Consequence Analysis* [EPA-550-B-99-005]; and *Handbook of Chemical Hazard Analysis Procedures* [ARCHIE, 1989], and their original sources referenced in those documents).

The following sections provide basic methods to assess the effects of explosions, following the order of types listed in Table 4-1.

4.3.2.1 PRESSURE VESSEL BURST

Catastrophic vessel ruptures can occur due to a variety of initiating events such as external fire, metal fatigue, erosion, corrosion, oxidation, installation violations of the American Society of Mechanical Engineers (ASME) codes and standards, (such as the ASME boiler and pressure code) poor maintenance, excessive internal pressure buildup, deficiencies in the safety management program and/or from physical impacts (vessels punctured by forklift tines, vehicle accident outside the facility).

The DSA hazard and accident analysis evaluates explosive hazard scenario to estimate the effects on surrounding SSCs. Assessment of pressurized vessel burst is performed for the following three main effects:

1. Blast effects. Simple calculation of blast effects from vessel bursts are presented for ideal gases. Particular attention across the DOE complex is given to the potential for explosion events from hydrogen generation.

2. Fragmentation effects from pressure vessel burst could also be calculated with particular emphasis if the MAR is present within nearby locations.

3. Thermal radiation effects (if the content in the pressurized vessel is a flammable liquid/gas) are associated with the fireball and depends on its diameter, height, and the combustion duration.

4.3.2.1.1 BLAST EFFECT FROM PRESSURE VESSEL BURST

Baker et al., 1978 and Baker et al., 1977 present a method for predicting blast effects following the rupture of gas-filled pressure vessels, either spherical or cylindrical. The relevant steps in the calculation from those references are depicted in Figure 4-4.

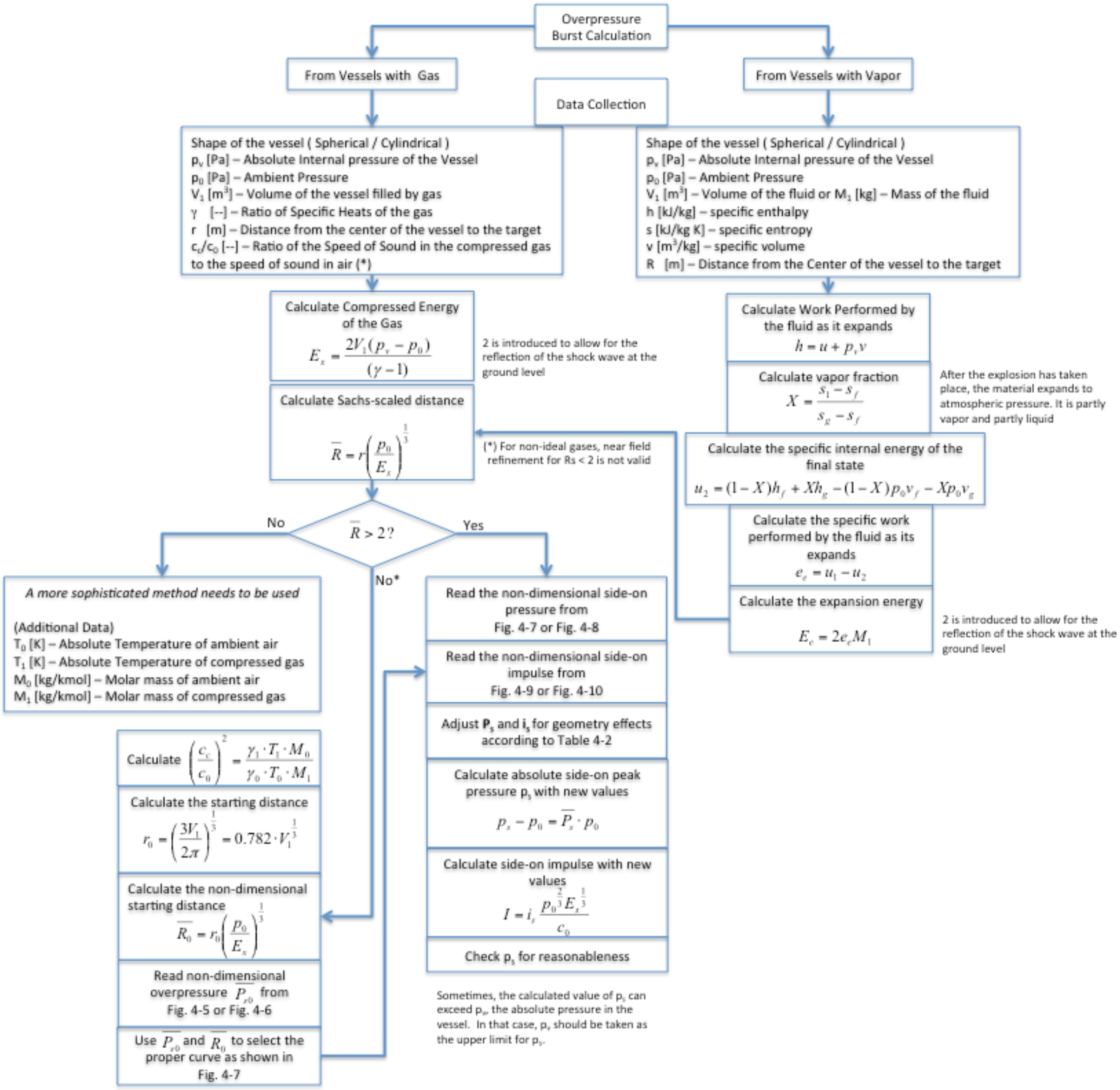


Figure 4-4. A Methodology Example for Calculations of Overpressure Effects.
(Source: Created from discussions in Baker et al., 1977 and Baker et al., 1978)

The method applies to:

1. Gases that can reasonably be approximated as ideal (for example, vessels with hydrogen that rupture); and

2. Non-ideal fluids or superheated liquids (for example, a pressure vessel filled with liquefied propane that ruptures as the result of a fire).

Blast Effects of Gases that can Reasonably be Approximated as Ideal in a Spherical Vessel

The blast effect (overpressure and specific impulse) at a specific distance from a burst vessel is presented with an example as given in Baker et al., 1977. The example uses close to normal temperature and pressure conditions (P=1 atm; T=273.15 K + 20 °C=293.15 K).

- Vessel diameter r_o: 1 m.
- Ratio of specific heats of the gas in the vessel to air ($\gamma = 1.4$)
- Gas pressure in the vessel $P_1 = 1.013\text{x}10^6$ Pa
- Gas temperature in the vessel $T_1 = 273.15$ K + 26.85° C = 300 K
- Ambient pressure $P_a = 1$ atm $= 1.013\text{x}10^5$ Pa

The overpressure versus distance relationship for a bursting gas vessel is strongly dependent upon the pressure, temperature, and ratio of specific heats of the gas in the vessel. For high pressures and temperatures, relative to the air outside the vessel, the overpressure behavior is much like that of a blast wave from a high explosive.

The steps to follow are:

a. Calculate the non-dimensional starting distance R_0

$$R_0 = \frac{1}{\left[\frac{4\pi\left(\frac{P_1}{P_a}-1\right)}{3\ (\gamma-1)}\right]^{1/3}} = \frac{1}{\left[\frac{4\pi\left(\frac{1.013\cdot10^6}{1.013\cdot10^5}-1\right)}{3\ \ (1.4-1)}\right]^{1/3}} = 0.2197$$

Equation 4-25

b. Determine the overpressure at the interested distance (r = 5.0 m)

$$R = \frac{r}{\left[\frac{4\pi r_0{}^3\left(\frac{P_1}{P_a}-1\right)}{3\ (\gamma-1)}\right]^{1/3}} = \frac{\frac{r}{r_0}}{\left[\frac{4\pi\left(\frac{P_1}{P_a}-1\right)}{3\ (\gamma-1)}\right]^{1/3}} = 0.2197\cdot\frac{5.0}{1.0} = 1.099 \sim 1.1$$

Equation 4-26

c. With ($\frac{P_1}{P_a} = 10$ and $\frac{T_1}{T_a} = \frac{300}{300} = 1$) on Figure 4-5 find the non-dimensional starting pressure P_{s0}. This pressure is estimated to be $P_{s0} \sim 1.7$

For gases with $\gamma = 1.667$ use the graphic presented in Figure 4-6.

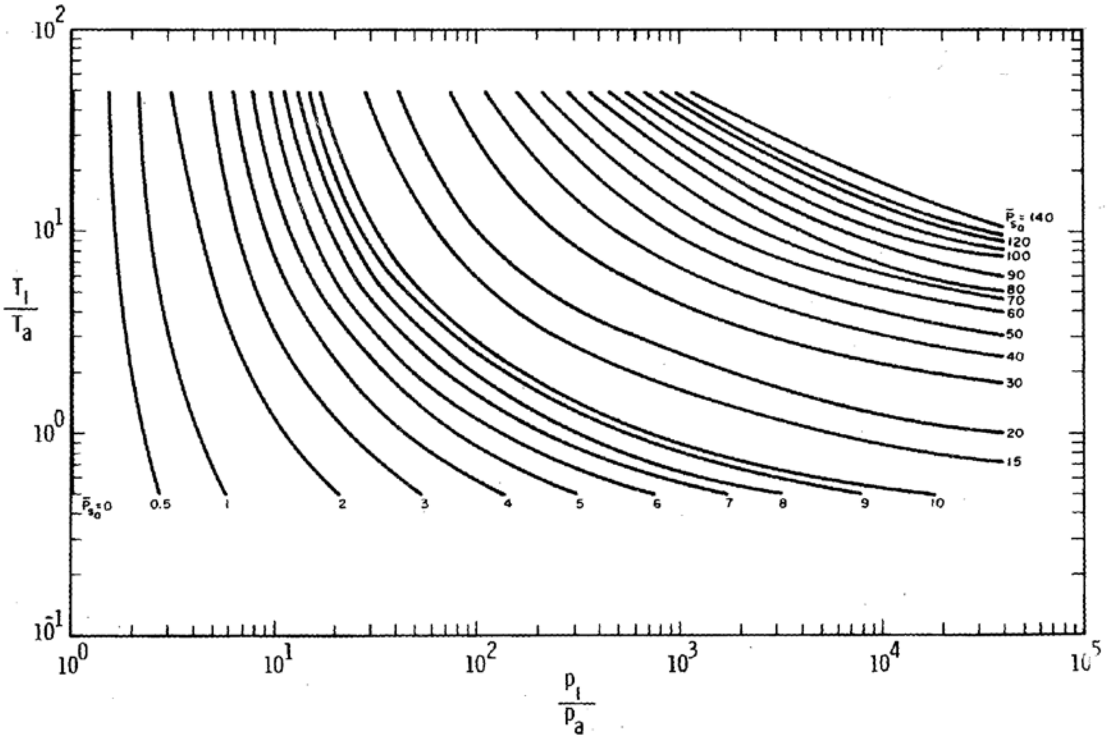


Figure 4-5. Temperature vs. Pressure Ratio for γ = 1.4
(Source: Baker et al., 1978 Figure 2-2; Baker et al., 1977 - Figure 2.20)

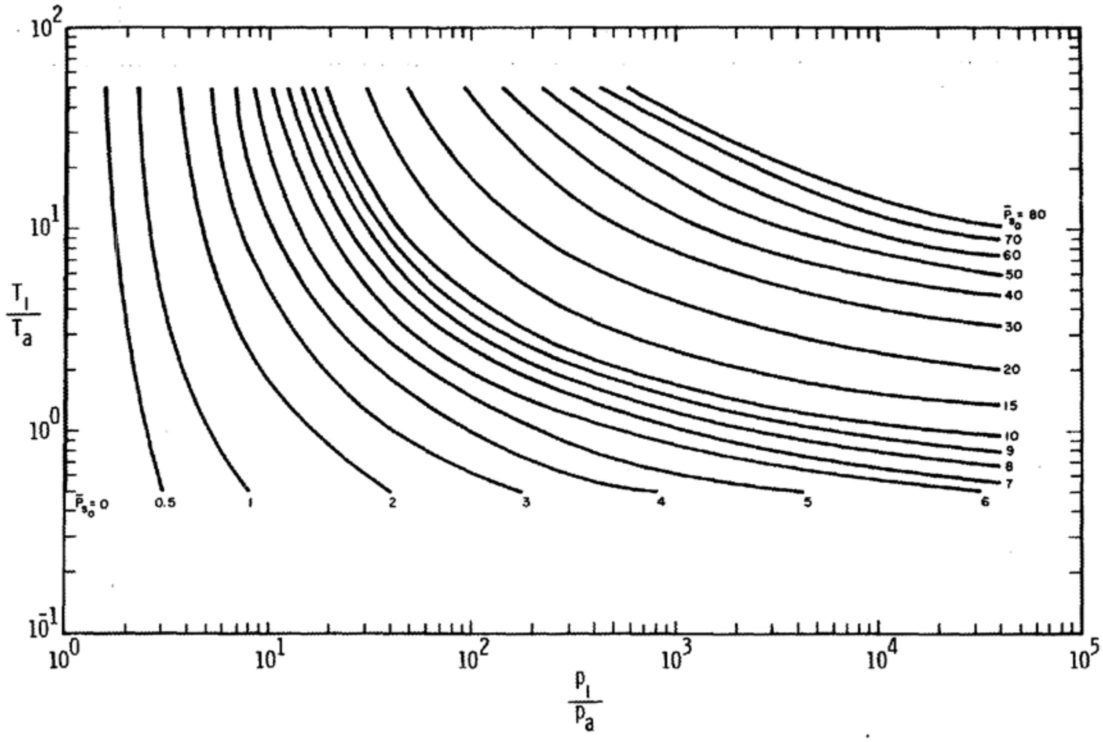


Figure 4-6. Temperature vs. Pressure Ratio for γ = 1.66.
(Source: Baker et al., 1978 Figure 2-3; Baker et al., 1977 Figure 2.21)

d. On Figure 4-7 look for the curve that corresponds to the interception of points $\overline{R_0} = 0.2197$and$\overline{P_{s0}} = \sim 1.7$. Then move on the curve to the point intercepted by $\bar{R}\sim 1.1$ and read on the vertical axis the value that corresponds to the starting the overpressure at 5 m. This is equal to $\bar{P}_s = 0.26$

For values of R>2 use the graphic presented in Figure 4-8.

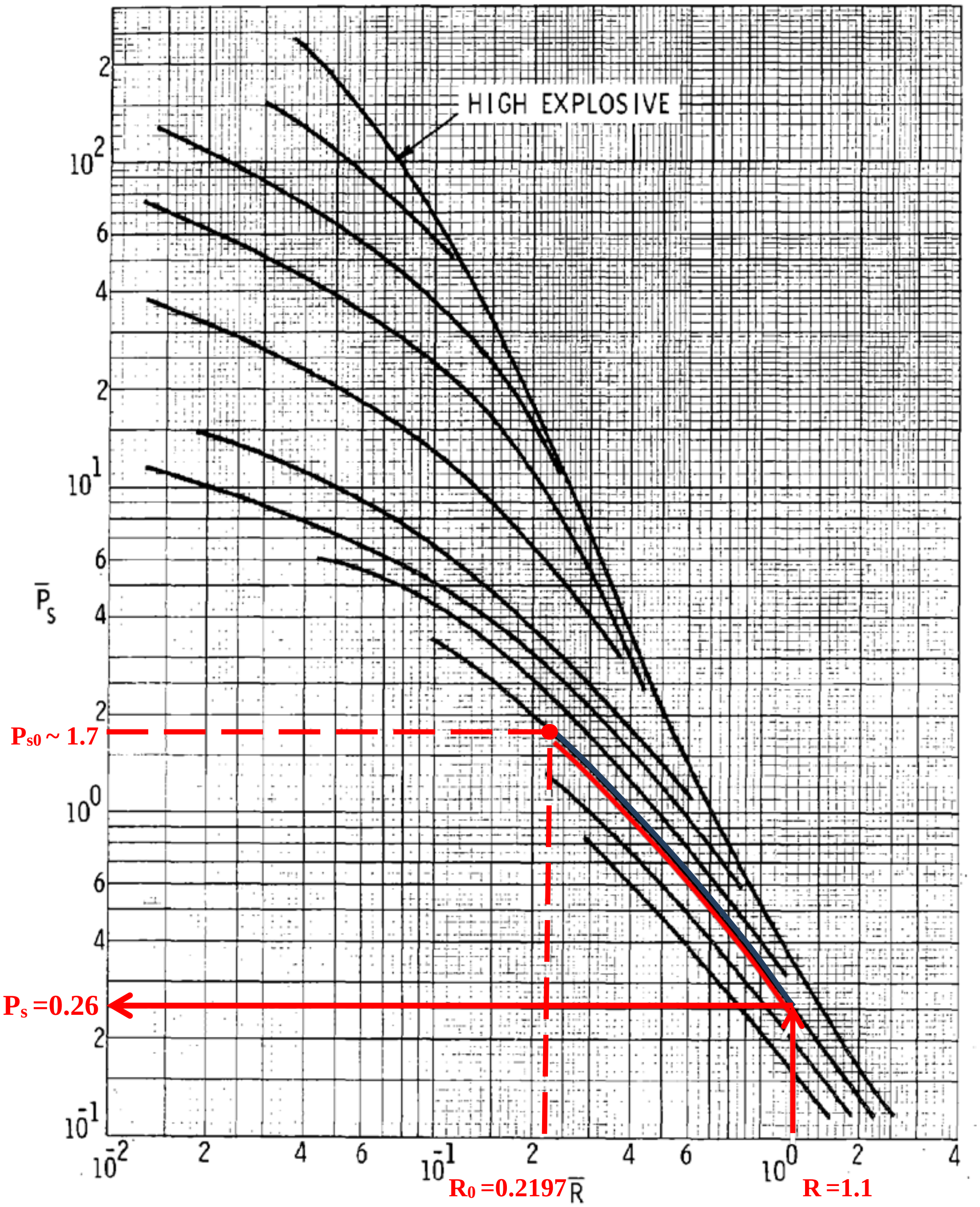


Figure 4-7. P_s vs. R_s for Overpressure Calculations
(Source: Baker et al., 1978 Figure 2-5; Baker et al., 1977 Figure 2.18)

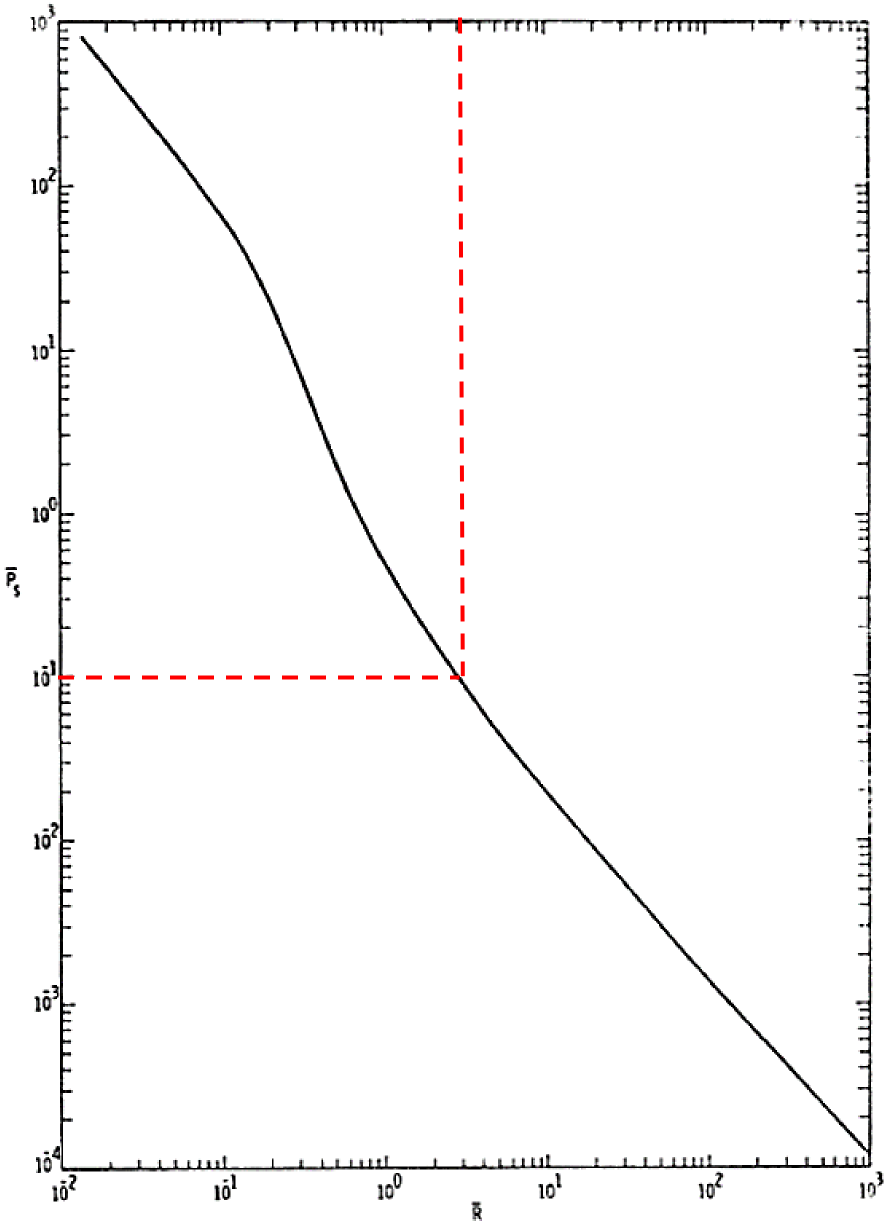


Figure 4-8. Ps vs. Rs for Pentolite
(Source: Baker et al., 1977 Figure 2-19)

To find the specific impulse:

a. Given the calculated $\bar{R} = 1.1$ at the distance of 5.0 m, the non-dimensional, side-on impulse can be found from Figure 4-9 ($\bar{I}$~0.046).

For values of R<1, use the graphic in Figure 4-10.

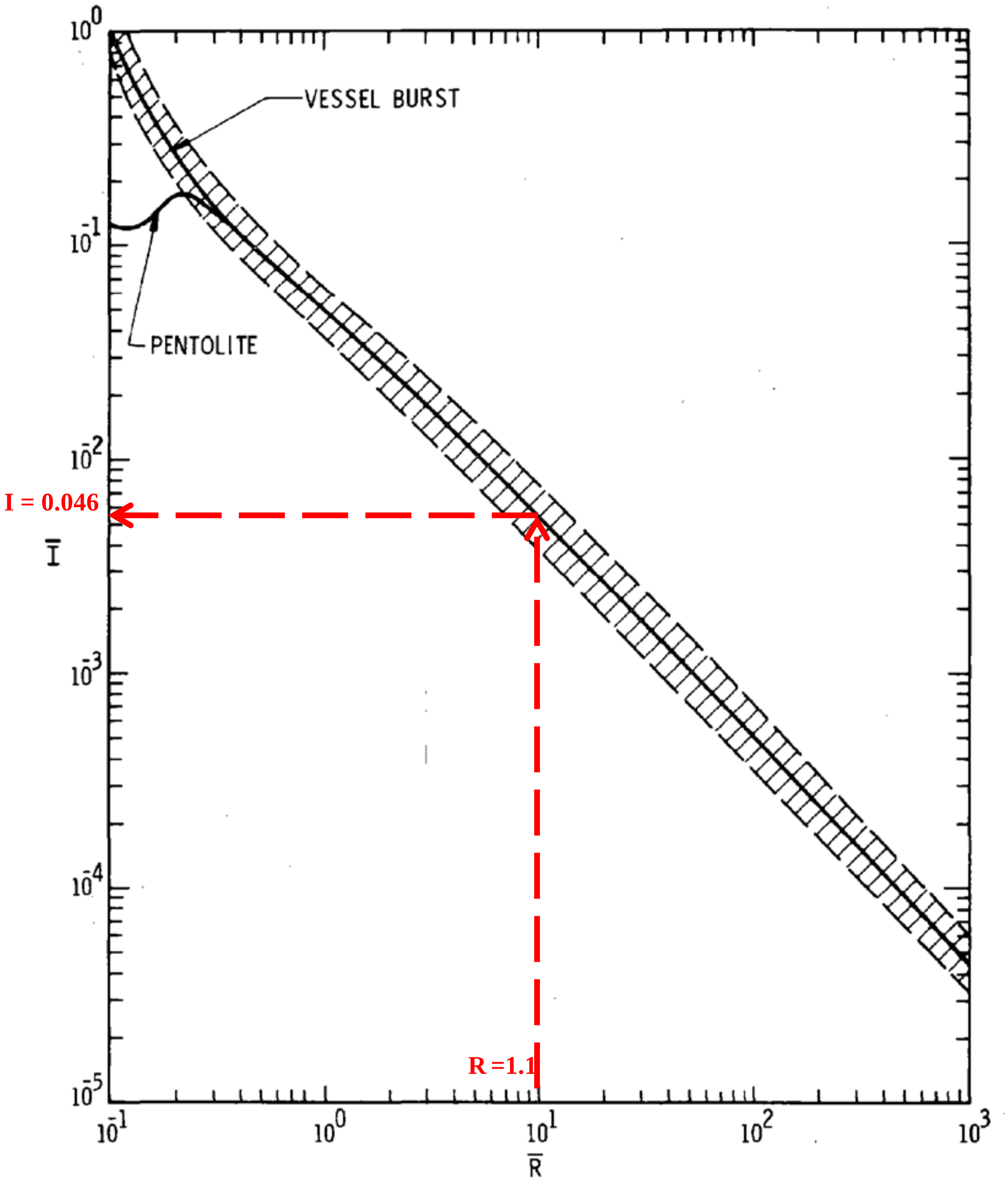


Figure 4-9. I_s vs. R_s for Gas Vessel Bursts and Pentolite
(Source: Baker et al., 1978 Figure 2-6; Baker et al., 1977 Figure 2.23)

b. The energy inside the vessel can be calculated as:

$$E = \frac{4\pi r_o^3}{3}\left(\frac{P_1 - P_a}{\gamma - 1}\right) = \frac{4\pi r_o^3}{3}\frac{(1.013\cdot 10^6 - 1.013\cdot 10^5)}{(1.4-1)} = 9.55 \cdot 10^6\, J$$

Equation 4-27

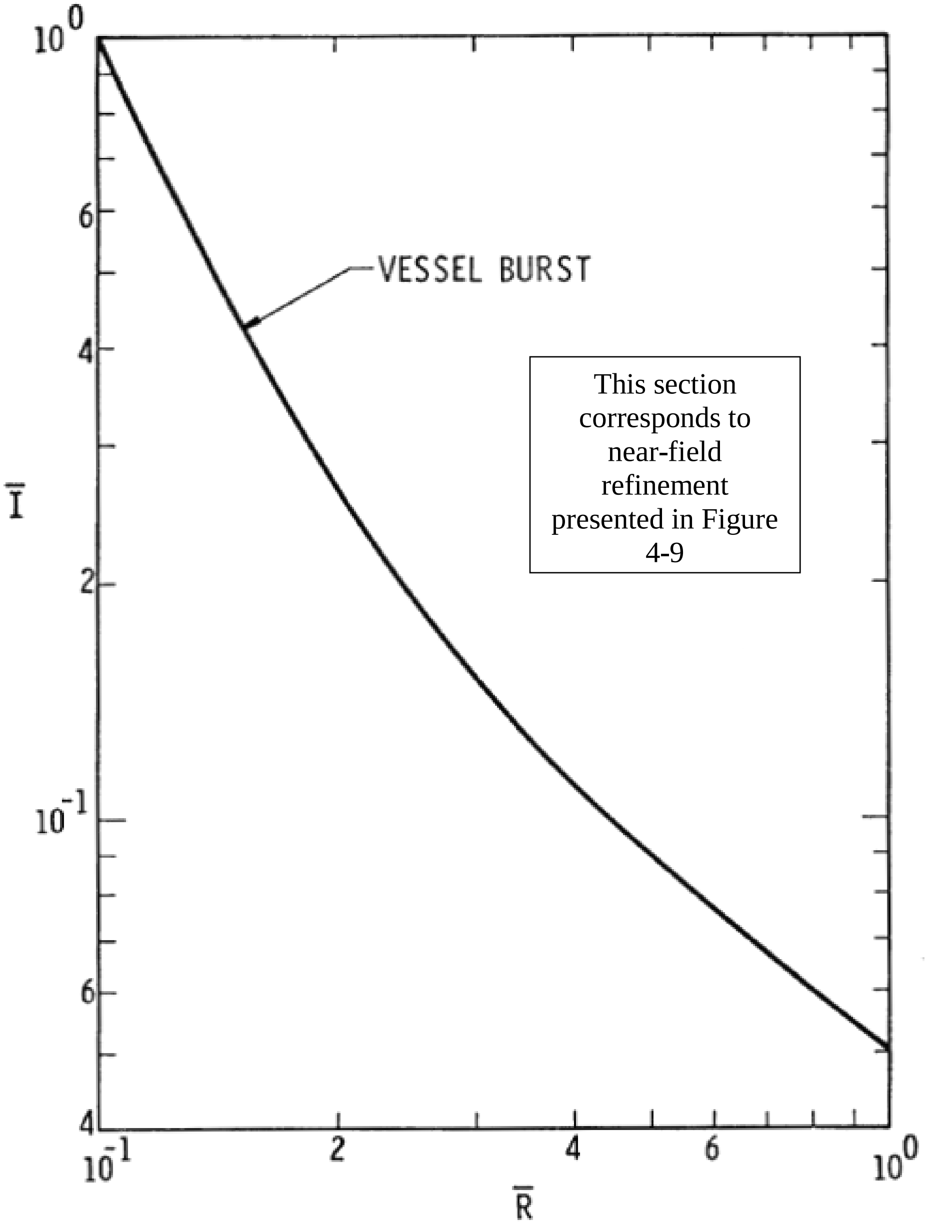
If surface burst is assumed, and a reflected shock wave is considered, then this energy value should be multiplied by 2. NOTE: This is not considered in this example.

c. Impulse (I) is calculated from:

$$\bar{I} = \frac{I \cdot a_a}{P_a{}^{2/3} \cdot E^{1/3}} \Rightarrow I = \bar{I}\,\frac{P_a{}^{2/3} \cdot E^{1/3}}{a_a} =$$ **Equation 4-28**

$$= 0.046\,\frac{(1.013 \cdot 10^5)^{2/3} \cdot (9.55 \cdot 10^6\,)^{1/3}}{331} = 64\,Pa \cdot s$$

Where: a_a is the speed of sound



This section corresponds to near-field refinement presented in Figure 4-9

Figure 4-10. I_s vs. R_s for Gas Vessel Bursts (Small R_s**)**
(Source: Baker et al., 1978 Figure 2-7; Baker et al., 1977 Figure 2.24)

Blast Effects of Gases that can Reasonably be Approximated as Ideal in a Cylindrical Vessel

For a cylindrical vessel, given the length L and the diameter D, use its volume V_v in the equations above, performing the calculations as for a spherical vessel. After P_s and I have been determined, further corrections are necessary according to the following table: Based on text in Baker et al., 1977 (page 67), Table 4-2 summarizes adjustment factors Factors for P_s and I_s for Cylindrical and Spherical Vessels based on R_s.

Table 4-2. Adjustment Factors for P_s and I_s for Cylindrical and Spherical Vessels based on R_s.

Vessel Type	**R_s**	**Multiply for:**	
		P_s	**I_s**
Cylindrical	< 0.3	4	2
	0.3 to 1.6	1.6	1.1
	1.6 to 3.5	1.6	1
	> 3.5	1.4	1
Spherical	< 1	2	1.6
	> 1	1.1	1

(Source: Adapted from Baker et al., 1977 page 67.)

The difference between spherical and cylindrical vessel bursts is only known qualitatively. Therefore, these corrections are very crude.

Blast Effects with Non-ideal Fluids (Vapors)

In practice, most vessels are filled with non-ideal fluids or with superheated liquids. For a pressure vessel filled with propane that ruptures as the result of a fire, the following steps to be followed are similar but not identical to those above.

a. Collect the following data:

- shape of the vessel (spherical or cylindrical).
- absolute internal pressure p_v at the moment of vessel failure;
- ambient pressure p_0
- quantity of the fluid (volume V_c or mass M_c)
- distance R from the center of the vessel to the target;
- specific enthalpy *h*
- specific entropy *s*
- specific volume ν

b. Calculate the work performed by the fluid as it expands

The work done by an expanding fluid is defined by the difference in internal energy between the fluid's initial and final states.

For many situations of interest, for example, a BLEVE from a ruptured propane tank, the values of *h*, *s*, and ν in the initial state are those for saturated vapor or liquid. They can be read from thermodynamic graphs or interpolated from thermodynamic tables given the temperature or pressure in the vessel. Therefore, the specific internal energy of the system immediately prior to the explosion can be calculated. These methods are based on extensive research, experimental work, historical data, and empirical deductions. Equations can be found in thermodynamic textbooks, and physical data for the gas in question can be selected by using a tool such as the one provided in: http://webbook.nist.gov/chemistry/, "Thermophysical Properties of Fluid Systems." An example of selecting these values for evaluating blast effects is provided in CCPS, 1994.

After the explosion has taken place, the material expands to atmospheric pressure p_0. It is partly vapor and partly liquid.

c. Calculate:

- the fraction X that is vapor is given,
- the specific internal energy of the final state u_2,
- the specific work performed by the fluid as it expands e_e
- the expansion energy E_x

The factor of 2 is introduced to allow for the reflection of the shock wave at the ground.

For common fluids, tabulations or graphs exist from which e_e can be directly read.

At this point, the analyst should return to the steps above for ideal gases. Note that the near-field refinement for $R_s < 2$ is not valid for non-ideal gases or flashing liquids. In this case, a conservative estimate of blast effects can be obtained by calculating the energy E_{TNT} presented in the TNT-equivalency method presented in Section 4.3.2.3.4.

4.3.2.1.2 FRAGMENTATION FROM PRESSURE VESSEL BURST

In principle, it is possible to estimate the mass distribution of fragments, their shapes, initial velocity, and its angle of elevation, for any site-specific situation, to determine the SSCs or MAR, struck by the fragment. Quantitatively justifying (demonstrating) for the DSA accident analysis that an operational accident is not plausible per DOE-STD-3009-2014 requires an estimate of the mass distribution of fragments, their shapes, initial velocity, and its angle of elevation.

Two approaches are provided, one analytical and the other statistical.

Analytical Approach

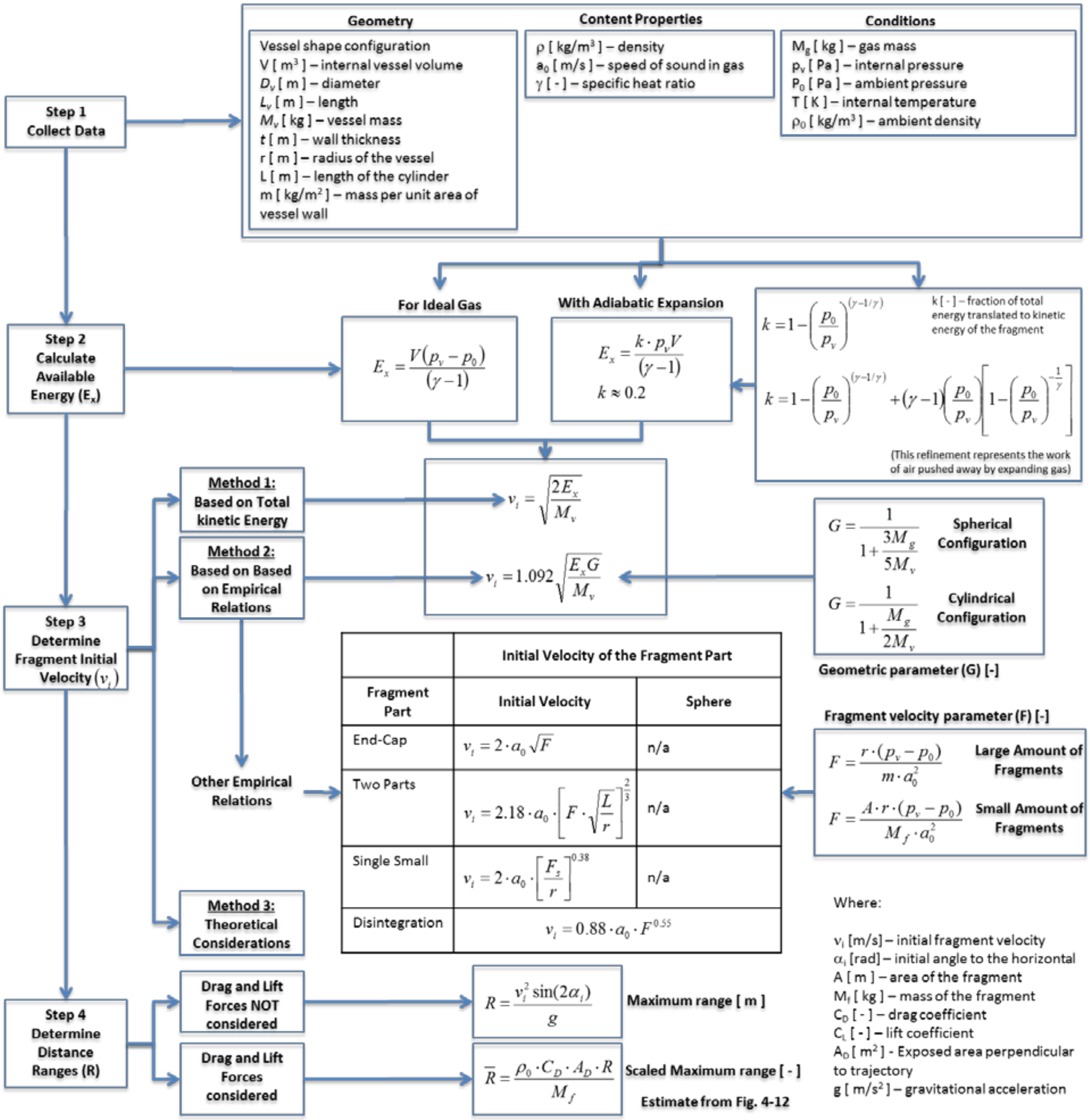
Although it is essentially simple and straightforward, the analytical approach is a highly conservative methodology where consideration should be given to estimating the uncertainties of the results. The relevant steps for the fragmentation effect on adjacent SSCs are depicted in Figure 4-11. These equations can be found in CCPS, 1994. The methodology consists of the following steps:

Step 1. Collect important data related to the vessel in the analysis. This includes design characteristics and vessel configuration as well as the thermodynamic properties of the fluid in the vessel, and operational conditions.

Step 2. Calculate available energy. Calculate the energy of the compressed gas in the vessel, assumed to be converted into kinetic energy of the fragments.

Step 3. Calculate initial velocity of the fragment. Several formulas are represented in the figure from the various methods suggested by the literature to calculate the initial fragment velocity. These methods are based on extensive research, experimental work, historical data, and empirical deductions.

Step 4. Determined the distance ranges, R (Figures 4-11 and 4-12).



	Initial Velocity of the Fragment Part	
Fragment Part	Initial Velocity	Sphere
End-Cap	$v_i = 2 \cdot a_0 \sqrt{F}$	n/a
Two Parts	$v_i = 2.18 \cdot a_0 \cdot \left[F \cdot \sqrt{\frac{L}{r}}\right]^{\frac{2}{3}}$	n/a
Single Small	$v_i = 2 \cdot a_0 \cdot \left[\frac{F_s}{r}\right]^{0.38}$	n/a
Disintegration	$v_i = 0.88 \cdot a_0 \cdot F^{0.55}$	

Figure 4-11. A Methodology Example for Calculations of Fragmentation Effects.
(Source: Adapted from CCPS, 1994)

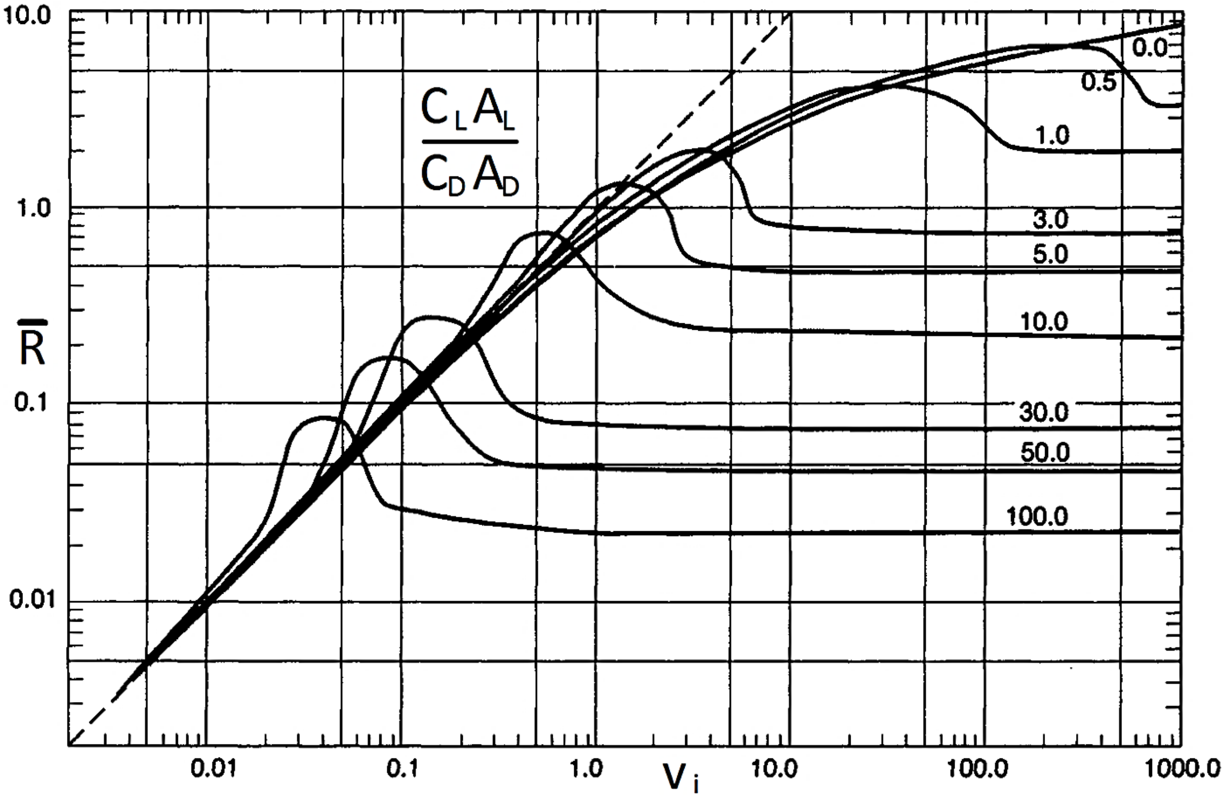


Figure 4-12. Scale Curves for Fragment Range Predictions
(Source: Baker et al., 1978 Figure 4-5; CCPS, 1994 Figure 6.36)

The set of curves in Figure 4-12 above provide predictions of the range distribution from various lift/drag ratio of the fragments based on its velocity. C_D is the dimensionless drag coefficient and A_D is the fragment area perpendicular to the flying trajectory. C_L is the dimensionless lift coefficient and A_L is the fragment area in parallel to trajectory. For fragments where the lift coefficient is zero, the line of importance is denoted by a ratio equal to zero. The higher the drag forces the shorter the distance will be estimated for the fragment in question given its velocity. If a fragment is, for example, a metal plate, then lifting forces will increase the ratio, making the distance prediction shorter as well.

Statistical Analysis

In practice, there is only statistical information on which to base predictions of the fate of any fragments following a pressure vessel burst or a BLEVE.

An analysis in *Workbook for Estimating the Effects of Accidental Explosions in Propellant Ground Handling and Transport Systems* (Baker et al., 1978), considered 20 accidental explosions. The data was organized into six groups, which are summarized in Table 4-3.

Table 4-3. Groups of Like Events—Fragments from Explosions
(Source: Adapted from Baker et al., 1978 Table 4-3).

Group Number	Number of Events	Explosion Material	Source Energy Range (J)	Vessel Shape	Vessel Mass (kg)	Number of Fragments
1	4	Propane, anhydrous ammonia	1.5E+5 to 6E+5	Railroad tank car	25,500 to 83,900	14
2	9	LPG	3,800 to 4,000	Railroad tank car	25,500	28
3	1	Air	5E+11	Cylinder, pipe and spheres	146,000	35
4	2	LPG, propylene	550	Semi-trailer (cylinder)	6,300 to 7,800	31
5	3	Argon	2.4E+9 to 1.1E+10	Sphere	46 to 187	14
6	1	Propane	25	Cylinder	510	11

Statistical analyses were performed on each group to yield estimates of fragment range and mass distributions.

Figure 4-13 and Figure 4-14 can be used to estimate the percentage of fragments which will have a range, $R_{i'}$, equal to or less than a particular range. Figure 4-15 and Figure 4-16 present the fragment mass distributions for groups 2, 3, and 6.

Using this data, the analyst can obtain helpful information; for example:

- For a specific vessel, determine which of the groups 1 through 6 it most closely resembles (Table 4-3).
- Choose a specific percentile (e.g., 50 percent for the median case, 95 percent for a conservative case) and read off the corresponding range from Figure 4-13 or 4-14.
- Within this range, consider whether there are any structures that are particularly vulnerable to missiles, or groups of people who may be within range.
- Consider whether any additional design or procedural measures to reduce the likelihood of the initial explosion or to protect the potential target are necessary. This additional design or procedural measure is necessarily a qualitative analysis.

The reference gives an example on how to use the graphics:

> For example, if we wished to estimate the percentage of fragments which would have a range equal to or less than 600 m for an explosion involving a rail tank car filled with propane (group 1), we would refer to Figure 4-6,[29] and on the range axis (abscissa) at 600 m go upward to the intersection of the group 1 line. Then, at the intersection point read the percentage value from the ordinate, which is 96%. Conversely, if we wanted to know what range 90% of the fragments would not exceed, we would enter the chart on the 90% line, go over to the intersection of the group 1 line and read downward to the range axis the value of 380 m. (Baker et al., 1978)

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[29] Figure 4-6 is Figure 4-13 in this document.

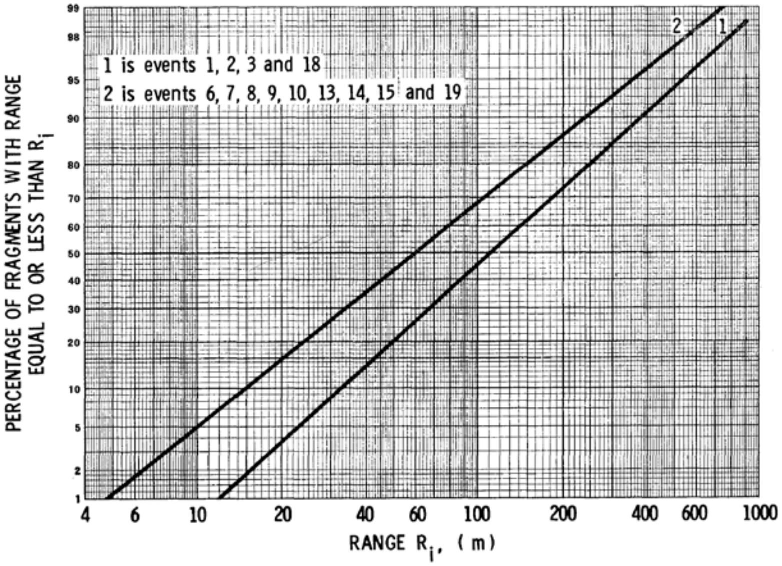


Figure 4-13. Fragment Range Distribution for Event Groups 1 and 2 (Source: Baker et al., 1978 Figure 4-6)

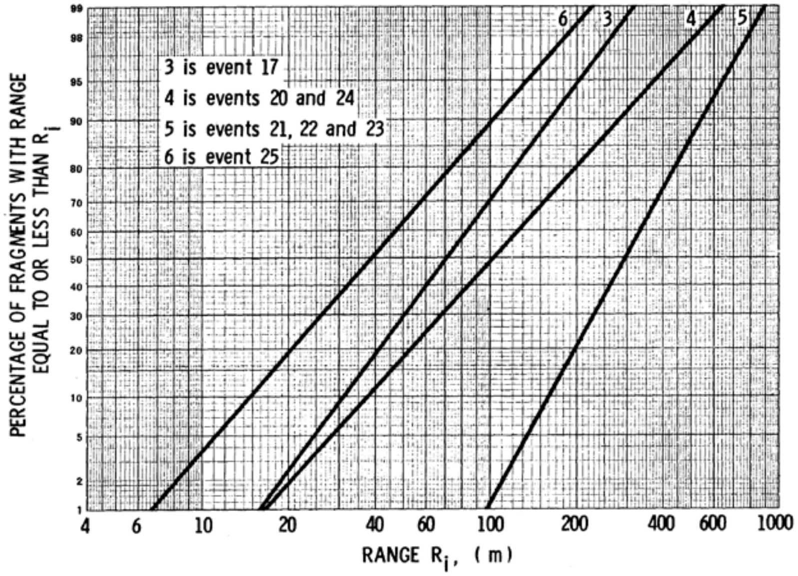


Figure 4-14. Fragment Range Distribution for Event Groups 3, 4, 5 and 6 (Source: Baker et al., 1978 Figure 4-7)

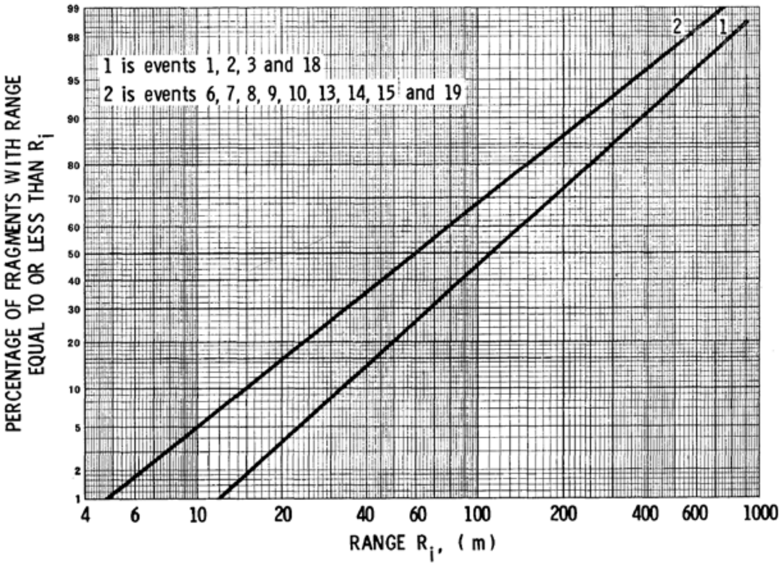


Figure 4-13. Fragment Range Distribution for Event Groups 1 and 2 (Source: Baker et al., 1978 Figure 4-6)

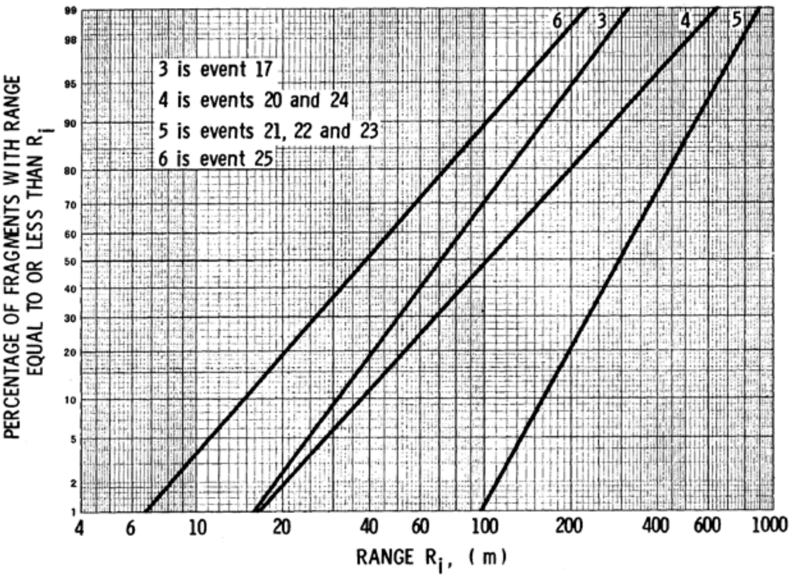


Figure 4-14. Fragment Range Distribution for Event Groups 3, 4, 5 and 6 (Source: Baker et al., 1978 Figure 4-7)

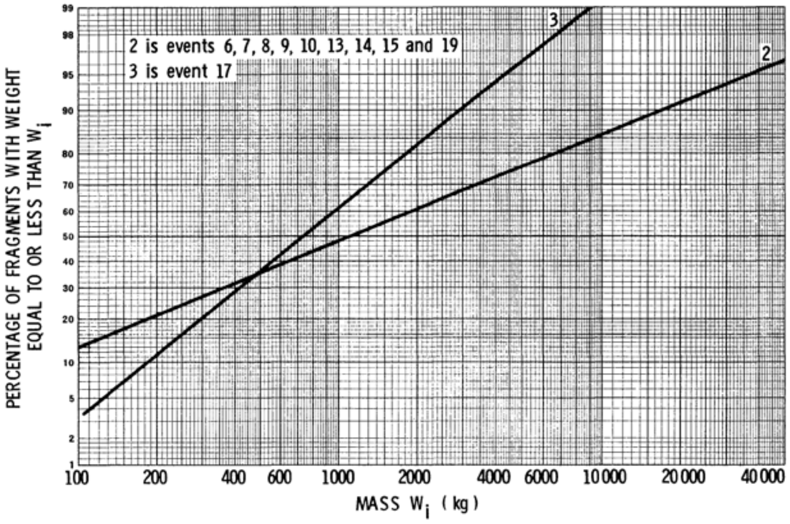


Figure 4-15. Fragment Mass Distribution for Event Groups 2 and 3 (Source: Baker et al., 1978 Figure 4-8).

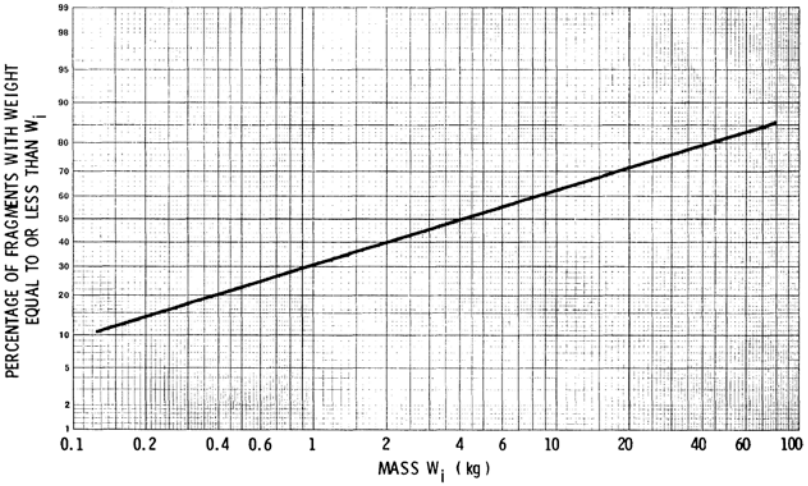


Figure 4-16. Fragment Mass Distribution for Group 6 (Source: Baker et al., 1978 Figure 4-9).

4.3.2.1.3 THERMAL EFFECTS FROM PRESSURE VESSEL BURST

The fire analysis Section 4.2.3.2 of this Handbook provides an explanation of the thermal effects of an unmitigated event that involves a developed fire. The difference between the thermal radiation from a fire and explosion pressure vessel burst with combustion, resides in the conditions capable of sustaining a prolonged fire versus a relatively short amount of time that the fireball lasts during an explosion. Nevertheless, formulations from the literature are presented to the analyst in Section 4.3.2.2.3 in this Handbook that is also applicable to a pressure vessel burst fireball.

4.3.2.2 BLEVE

NUREG-1805 defines a BLEVE as follows:

> … a catastrophic rupture of a pressurized vessel containing a liquid at a temperature above its normal boiling point with the simultaneous ignition of the vaporizing fluid. A short-duration, intense fireball occurs if the liquid is flammable. During the rupture of the vessel, a pressure wave may be produced and fragments of the containment vessel will be thrown considerable distances.

In other words, to consider an explosion of a vessel containing pressurized liquid a BLEVE, conditions, such as instantaneous depressurization and significant superheating of the liquid, need to be met to cause a near instantaneous evaporation.

A common misconception is that the BLEVE produces the pressure that results in a catastrophic vessel failure. Vessels may experience any number of insults, but not all of them result in a BLEVE, which occurs independently of a vessel failure. That is, the explosion does not cause the vessel to fail, it is the failure of a vessel that leads to a sudden depressurization of superheated liquid.

Sudden vessel depressurization of superheated liquid leading to a BLEVE may result from:

1) Failure of equipment such as valves and vaporizers.
2) Human errors made by operators, maintenance, or delivery personnel.
3) External impacts (such as pipe whip) where vessel integrity has already been compromised by heating and internal boiling.
4) Other causal chains such as extensive corrosion and extreme seismic events.

As stated above, sudden depressurization of a vessel from impact without external heating may not result in a BLEVE, but may result in other situations that warrant evaluation. For example, it could lead to a pool fire if the breach is below the vapor-liquid interface and the liquid is combustible or flammable. Or it could lead to a jet fire if the content release is pressurized and contacts a sufficient energy source. The jet fire would need to come from a breach in the vapor space and be turbulent enough to entrain and mix air. However, if the jet flame could impinge on another vessel, a BLEVE of the adjacent vessel could occur.

Unmitigated assessment of BLEVE is performed similarly to pressure vessel burst, for (a) blast effects, (b) fragmentation effects, and (c) thermal effects.

4.3.2.2.1 BLAST EFFECT FROM BLEVE

Blast effect assessment is performed in similar fashion as with pressure vessel burst described above. See subsection 4.3.2.1.1 of this Handbook. (CCPS, 1994, Section 9.2)

4.3.2.2.2 FRAGMENTATION FROM BLEVE

Fragment effect assessment is performed in similar fashion as with pressure vessel burst described above. See subsection 4.3.2.1.2 of this Handbook.

4.3.2.2.3 THERMAL EFFECTS FROM BLEVE

The thermal effects from a BLEVE can be evaluated similar to the thermal effects from a pressure vessel burst with combustion, as discussed in Section 4.3.2.1.3, based on the fire analysis methodologies.

Fireball Diameter and Duration

In order to simplify calculations of BLEVE effects, it is often assumed that the fireball touches the ground, the fireball is spherical and its center is at height $D_c/2$. This should give a somewhat conservative estimate of radiant heat flux. Note that in practice, the fireball rises as a function of time and that greater accuracy requires the use of numerical models.

The fireball diameter and its duration can be calculated by the following equations (CCPS, 1994; ALOHA, 2013 page 68; EPA-550-B-99-005, page D-22):

$$D_c = 5.8 \cdot m_f^{1/3}$$ **Equation 4-29**

$$t\_c = 0.45 \cdot m\_f\text{\^{}}(1 / 3) \qquad for\ mf\ <\ 30{,}000\ kg$$ **Equation 4-30**

$$t\_c = 2.6 \cdot m\_f\text{\^{}}(1 / 6)tc \qquad for\ mf\ >\ 30{,}000\ kg$$ **Equation 4-31**

Where:

D_c [m] – final fireball diameter

m_f [kg] – mass of fuel in fireball

t_c [s] – duration of fireball

Damage Distance

From the equations to determine q (heat flux) and F (view factor) the hazard distance, L (i.e., the maximum distance at which that level of damage will occur) can be calculated as (from as cited in CCPS, 1994, pages 178-179):

$$L = \left(\frac{D_c}{2}\right)\sqrt{\left(\frac{E \cdot cos\,\Theta \cdot \tau_a}{q}\right)}$$ **Equation 4-32**

For propane BLEVEs, the following empirical, simplified formula for the hazard range that could inflict severe burns to people was developed (original source from Lihou and Maund, 1982, "Thermal Radiation Hazard from Fireballs," *I. Chem. E. Symp. Ser., No. 71* as cited in CCPS, 1994 page 183):

$$L \sim 3.6 \cdot m_f^{0.4}$$ **Equation 4-35**

Heat Flux

Finally, the incident radiation per unit area at which a receptor receives thermal radiation or the heat flux that causes a specific level of damage over a minimum duration is given by (CCPS, 1994 page 178 and ALOHA, 2013 page 65, which are similar to the fire analysis discussion in Section 4.2.2 of this Handbook):

$$q = E_s \cdot F \cdot \tau_a$$ **Equation 4-34**

Where:

q [kW/m^2] – rate at which thermal radiation is received by the receptor/incident radiant heat flux

E_s [kW/m^2] – surface emissive power. A value of 350 kW/m^2 for E_s is consistent with experiments on BLEVEs for most hydrocarbons involving a vapor mass of 1,000 kg or more.

$F = D_c^2 \cos\Theta / 4L^2$ [dimensionless] – View factor. For a point on a plane surface at a distance L from the center of a spherical fireball (with no obstructions between)

Θ is the angle between the normal to the surface and the line connecting the point to the center of the fireball.

τ_a [dimensionless] – atmospheric transmissivity (CCPS, 1994 Equation 9.1.6)

RH is the relative humidity

$$\boldsymbol{\tau_a = log[14.1 \cdot RH^{-0.108}\left(L - \frac{D_c}{2}\right)^{-0.13}}$$ **Equation 4-35**

Fuel Contribution to Fireball

A simple rule of thumb based on a "Study of Fireball Following Steam Explosion n-Pentane" (Hasegawa and Soto, 1977) is that the amount of gas in a BLEVE can be taken to be three times the flash fraction, up to a limit of 100 percent.

4.3.2.3 VAPOR CLOUD EXPLOSION

In the DOE Complex, examples of vapor cloud ignition involve the release of different gaseous mixtures into the environment and depending on the time factor, could envelope the MAR in the proximity of the vapor cloud.

Depending of the substance content and its flammability, a vapor cloud ignition can be developed into a deflagration or detonation. The initiation energy plays a fundamental role after a flammable gas has ignited. Detonations and deflagrations are often distinguished by the speed or rate of propagation of the combustion wave through the material.

In a deflagration, the flame or combustion wave is below the speed of sound in air at 20 °C (68 °F), which is approximately 330 m/sec (1,082 ft/sec).

In a detonation, the flame or combustion wave propagates through the reactants at supersonic speeds on the order of 2,000 m/sec (6,562 ft/sec).

4.3.2.3.1 VAPOR CLOUD DEFLAGRATION

A vapor cloud deflagration is characterized by the sudden energy release when the gas ignition results in a pressure increase starting at the ignition location (center of initial cloud). For an unconfined vapor cloud deflagration, the pressure wave, sometimes referred to as a constant-volume combustion pressure, expands from the initial location at a subsonic propagation rate and reduces rapidly as a function of distance. The combustion propagates through the gas medium from mass diffusion and heat transfer. This phenomenon can exert excessive force on confinement features (e.g., cause a glovebox breach or overturn a vessel) or can cause collateral damage due to debris impacts to the MAR from failed equipment and interior furnishings, examples being collapse of lighting, piping, ventilation ductwork. For a confined vapor cloud deflagration in a process room or enclosure, for other than minor deflagrations, the damage is not caused by a pressure wave as a function of distance and instead it is due to a uniform pressure rise in the room which can fail structural boundaries causing debris-impacts to the MAR.

4.3.2.3.2 VAPOR CLOUD DETONATION

A Vapor Cloud Detonation is considered when the gas ignites in a detonation with a sudden release of energy and a pressure increase at the ignition location. However, even if the flammable gas concentration levels are high, detonation may not occur if the geometry is not favorable for a shock wave to occur. (It is generally known that the pressure wave for a detonation, resulting in an overpressure, is referred to as a shock wave or Chapman-Jouguet (CJ) pressure). Long pipes are a more favorable geometry for a detonation to occur than a vessel with a length to diameter ratio of one and no interior obstructions.

4.3.2.3.3 VAPOR CLOUD DEFLAGRATION AND DETONATION PRACTICAL DIFFERENCES

When comparing a deflagration to a detonation, the pressure wave progresses outward from the detonation source at a much higher rate. The pressure wave for a detonation travels at supersonic velocities. At the wave front, the unburnt gases are compressed. The combustion occurs at the wave front from the compressive heating of the gases.

The practical distinction between deflagrations and detonations relates to the amount of damage caused by the overpressures and depend on the material involved in the detonation or deflagration.

For example, the overpressure in a typical unconfined deflagration wave without obstructions is on the order of 1 atmosphere (14.70 psi) for C_2H_2 in air (NUREG-1805). By contrast the pressure attained during a detonation can be up to 20 atmospheres (294 psi), which would cause significant debris impacts from failed equipment and structural features.

In closed vessels, deflagration overpressures from stoichiometric fuel-air concentrations at initial conditions (25 C and 1.013 bar) when the burning rate is low (Bjerketvedt et al., 2012), are summarized in Table 4-4, for various explosive substances. In addition, according to the *Loss Prevention in the Process Industries* (as reported in the 1980 first edition of Lees, 1996), the CJ pressure is approximately twice of the constant-volume combustion pressure. Doubling the pressures increases in Table 4-4 result in pressures during a detonation of up to 20 atmospheres (294 psi).

Table 4-4. Deflagration Overpressures in Closed Vessels
(Source: Extracted from Bjerketvedt et al., 2012 Table 4.5).

	Hydrogen	Ethylene	Propane	Methane
P (bar)	8.15	9.51	9.44	8.94

Original source as cited in Bjerketvedt et al., 2012: Baker, W.E., et al., 1983. *Explosion Hazards and Evaluation*, Elservier Science Publishing Company, Amsterdam.

According to the *Loss Prevention in the Process Industries* (as reported in the 1980 first edition of Lees, 1996), the CJ pressure is approximately twice of the constant-volume combustion pressure. Doubling the pressures increases in Table 4-4 results in pressures during a detonation of up to 20 atmospheres (294 psi).

4.3.2.3.4 BLAST EFFECT FROM VAPOR CLOUD EXPLOSION

Different techniques are used for determining the blast effect from vapor cloud explosions. The two techniques discussed in this section can roughly be characterized as being applicable to near- and far-field impacts.

The TNT-equivalency method is recommended for determining far-field potential damage. It takes the fuel (flammable gas) energy and determines an equivalent energy of TNT.

As long as the far-field potential damage is the concern, the TNT-equivalent method is a poor model for a gas explosion. This method is known to give non-conservative results for peak overpressure in the far field, because the positive phase duration and shape of the blast waves are not well reproduced. For this reason, determining peak overpressure for the purpose of accident analysis can lead to erroneous results. In order to apply the model, conservative TNT-Equivalency values, α_e, are introduced as seen in the content of this section.

The Multi-energy method is better suited to determining near-field potential damage than the TNT model, although can also be used for determining far-field evaluations. Through the use of this method’s scaling equations, side-on and overpressures and duration of pressures can be determined. The Multi-energy method provides a better prediction of the positive phase duration of the pressure and shape of the blast waves.

TNT-Equivalency Method

A “TNT-equivalency” concept has been used in the literature for evaluation of potential damage from an explosion overpressure, and in particular, has been applied to the evaluation of vapor cloud explosions. Baker et al., 1977 summarized it as follows:

> A common method of assessment of possible energy release or correlation of the results of experiments has been to assess the energy release on the basis of equivalent pounds of TNT. This method is used because a large body of experimental data and theoretical analyses exist for blast waves generated by TNT or other solid explosives. Although the comparison with TNT is convenient, the correlation is far from exact. Specific energies, which can be released, i.e., energy per unit volume or mass of material, differ quite widely between TNT, various liquid propellants or mixtures of liquid propellants and oxidizers, and gases stored in pressure vessels.

The concept of TNT-equivalency was introduced for blast prediction purposes when the mechanisms of blast generation in vapor clouds were not fully understood. The method simply converts the available combustion energy into an equivalent charge weight of TNT. This TNT method is for gas explosions outside of facilities that are unconfined explosions, i.e., this method is not valid for inside building explosions). The "TNT-equivalency factors" come from assessing the damage to the exterior of buildings from the gas explosion vs. the quantity of TNT to cause the same damage.

A simplified method for assessing the blast wave effects from a vapor cloud explosion is based on blast wave energy, i.e., TNT-equivalent. NUREG-1805 Equation 15-1, NRC Regulatory Guide 1.91, *Evaluation of Explosions Postulated to Occur at Nearby Facilities and on Transportation Routes Near Nuclear Power Plants*, and SFPE, 2008, estimate the energy released as follows:

$$\boldsymbol{E_{TNT} = \alpha_e H_f W_f} \qquad \textbf{Equation 4-36}$$

Where:

E_{TNT} [J] = explosive energy released or blast wave energy

W_f [kg] – the mass of fuel involved. The weight of the fuel W_f in the cloud is equal to the flash fraction (F) times the quantity (mass) of fuel released.

H_f [kJ/kg] – theoretical net heat of combustion of the fuel in question. This information is available in NUREG-1805 Table 15-2, Heat of Combustion, Ignition Temperature, and Adiabatic Flame Temperature* of Flammable Gases; and in Factory Mutual Loss Prevention Data Sheet 7-42, "Guidelines for the Estimation of Property Damage from Outdoor vapor cloud explosions in Chemical Processing Facilities," March, 1990 (as cited in NRC Regulatory Guide 1.91).

α_e [dimensionless] – TNT-equivalency based on energy; the fraction of available combustion energy participating in blast wave generation

Note that the literature on this subject does not use consistent terminology, hence it is common that TNT-equivalency (α_e) is also called equivalency factor, yield factor, efficiency, or efficiency factor.

For a catastrophic failure of a vessel containing a gas liquefied under pressure (such as liquid propane), some fraction (F) of the liquid flashes into vapor and the rest cools to the boiling point of the liquid (or lower). The flash fraction can be determined on the basis of actual thermodynamic data using the following equation:

$$\boldsymbol{F = 1 - exp\left(-\frac{C_p \Delta T}{L}\right)} \qquad \textbf{Equation 4-37}$$

Where:

- F [dimensionless] – Flash Fraction
- C_p [kJ/(kgK)] – mean specific heat of the flashing material at constant pressure
- ΔT [K] – difference in temperature between the temperature of the vessel and the atmospheric boiling point
- L [kJ/kg] – latent heat of vaporization

Some of the unvaporized liquid from the ruptured vessel forms aerosols, and thus adds to the fuel in the vapor cloud. The UK Health and Safety Executive recommends calculating the cloud inventory by using the flash fraction and then multiplying by 2 to allow for spray and aerosol contributions to the cloud.

The corresponding TNT equivalent mass in (kg), W_{TNT}, is:

$$\boldsymbol{W_{TNT} = \frac{E_{TNT}}{H_{TNT}}}$$ **Equation 4-38**

Where:

W_{TNT} [kg] – equivalent mass of TNT or yield

H_{TNT} [J/kg] – heat of combustion of TNT

The heat of combustion of TNT is 4,680 kJ/kg per EPA-550-B-99-009 Section C.1, Equation for Estimation of Distance to 1 psi Overpressure for vapor cloud explosions. However, other values have also been selected, e.g., 4500 kJ/kg was used in NUREG-1805, Section 15.8.2, TNT Mass Equivalent Calculations, and 4,420 kJ/kg was used in the 1995 second edition of the *SFPE Handbook of Fire Protection Engineering* (as cited in NRC Regulatory Guide 1.91).

If the explosive energy is not calculated, the TNT equivalent mass can be determined from:

$$\boldsymbol{W_{TNT} = \alpha_e \frac{(H_f W_f)}{H_{TNT}} = \alpha_m W_f}$$ **Equation 4-39**

Where:

$\alpha_m = \alpha_e (H_f / H_{TNT})$ [dimensionless] – TNT-equivalency based on mass

In order to apply the TNT-equivalency model, a conservative value of α_e (TNT-Equivalency value based on energy) is selected. A brief discussion of practices for choosing these values is provided below.

For stoichiometric, hydrocarbon-air detonation, the theoretical maximum efficiency of conversion of heat of combustion into blast is approximately 40% (CCPS, 1994, Section 4.3.1). In practice, because vapor cloud explosions are usually deflagrations and not full detonations and gas mixtures in air are rarely fully stoichiometric, the efficiency is usually less than 40%.

Table 4-5 provides a range of values of α_e that have been estimated based on past accidents or recommended (see CCPS, 1994 or the original references for further discussion and understanding of their bases to select a conservative value for purpose of the DSA accident analysis).

Table 4-5. Sources for TNT Equivalency Factor Estimations.

References	α_e
Dow Chemical (CCPS, 1994, Section 4.3.1; Brasie and Simpson, 1968)	$0.02 \le \alpha_e \le 0.05$
United Kingdom Health and Safety Executive (CCPS, 1994, Section 4.3.1; HSE, 1979)	$\alpha_e = 0.03$
Exxon (CCPS, 1994, Section 4.3.1; unpublished)	$0.03 \le \alpha_e \le 0.10$
Industrial Risk Insurers (CCPS, 1994, Section 4.3.1)	0.02
Factory Mutual Research Corp (CCPS, 1994, Section 4.3.1) {Note: These values are also recommended in NRC Regulatory Guide 1.91.)	0.05-0.15
The U.S. Environmental Protection Agency (EPA-550-B-99-005) in its guidance for explosion modeling in the context of its Risk Management Program regulations, recommends: • For worst-case explosion analysis • For "alternative" or "more likely" scenarios	 0.1 0.03

Original sources (as cited in CCPS, 1994):

Brasie and Simpson, 1968. Brasie, W.C. and D.W. Simpson, "Guidelines for Estimating Explosion Damage," Proc. 63rd Nat. AIChE Meeting, American Institute of Chemical Engineers, New York, NY.

HSE, 1979. "Second Report of the Advisory Committee on Major Hazards," Health and Safety Executive, United Kingdom, London, UK.

Industrial Risk Insurers, 1990. "Oil and Chemical Properties Loss Potential Estimation Guide*," IRI-Information February 1, 1990*.

Factory Mutual Research Corporation, 1990. "Guidelines for the Estimation of Property Damage from Outdoor Vapor Cloud Explosions in Chemical Processing Facilities," Technical Report, March.

For other than catastrophic releases (such as a jet release from a vessel containing a gas under pressure or a gas liquefied under pressure, where the release approximates a steady state), it is in principle possible to use an atmospheric dispersion model to determine the amount of fuel at any one time that lies between the upper and lower flammable limits.

EPA-550-B-99-009, Section C.1 assumes that the entire contents of the cloud is within the flammability limits for a worst-case release scenario. As shown in Table 4-5, EPA-550-B-99-009 also assumes that 10% of the flammable vapor in the cloud participates in the explosion blast wave. This Handbook considers the EPA worst-case guidance conservative for the purposes of the DSA accident analysis; however, the TNO Multi-Energy method discussed in the next subsection may be more defensible.

Once W_{TNT} has been determined, the "scale distance" can be calculated by the following simple expression:

$$Scaled\ Distance = \frac{Actual\ Distance}{\sqrt[3]{W_{TNT}}} \Rightarrow \bar{R} = \frac{R}{\sqrt[3]{W_{TNT}}}\left[\frac{m}{\sqrt[3]{kg}}\right] \qquad \textbf{Equation 4-40}$$

This equation has been plotted in Figure 4-17 where the side-on overpressure can be estimated on the vertical axis. The figure is from 1976 a paper by V.C. Marshall, "The Siting and Construction of Control Buildings – a Strategic Approach," *I. Chem. E. Symp. Series, No. 47* (as cited in CCPS, 1994 page 117).

Alternate correlations to determine the overpressure distance from an explosion have been used in other methods (EPA-550-B-99-005; NRC Regulatory Guide 1.91; ARCHIE, 1989).

There are, however, certain caveats. The TNT-equivalent methodology explosion is a poor model for a gas explosion. In particular, the positive phase duration and shape of the blast waves are not well reproduced. However, TNT-equivalency methods are satisfactory, so long as far-field potential damage is the concern.

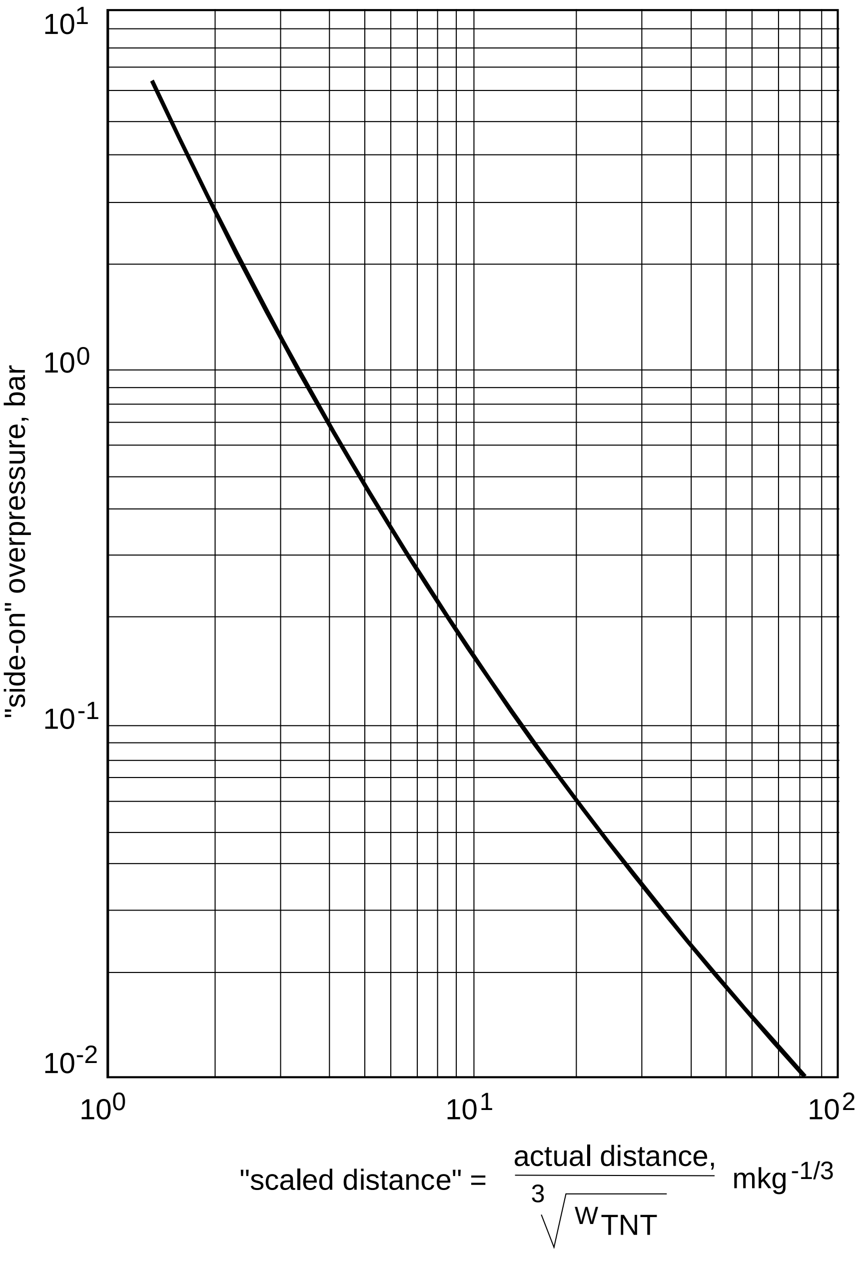
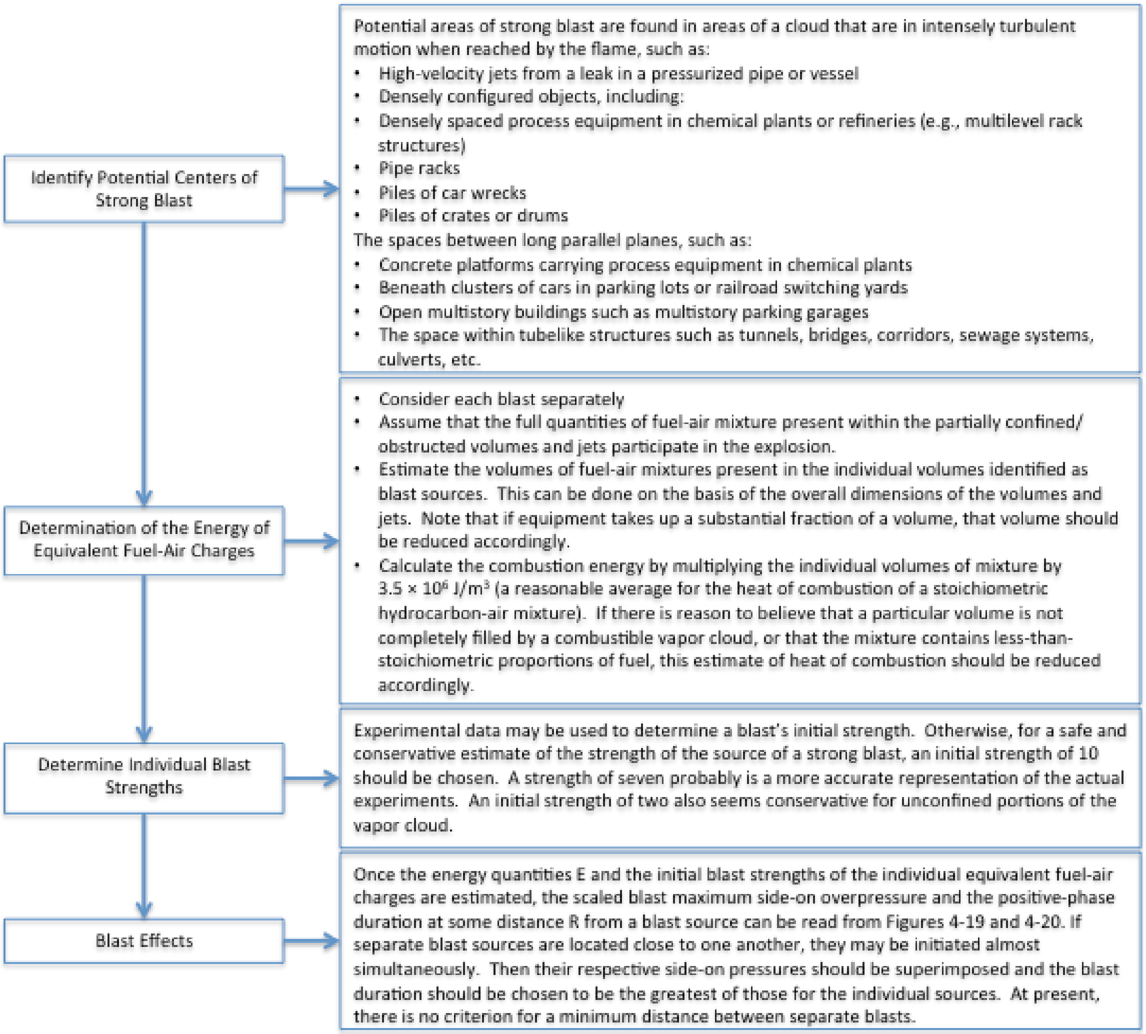


Figure 4-17. Hopkinson-Scaled TNT Charge Blast
(Source: 1976 Marshall paper as cited in CCPS, 1994 Figure 4.18)

TNO Multi-Energy Method

A summary of the necessary steps to apply the TNO Multi-Energy method with the needed calculations is provided in Figure 4-18.



Potential areas of strong blast are found in areas of a cloud that are in intensely turbulent motion when reached by the flame, such as:

- High-velocity jets from a leak in a pressurized pipe or vessel
- Densely configured objects, including:
- Densely spaced process equipment in chemical plants or refineries (e.g., multilevel rack structures)
- Pipe racks
- Piles of car wrecks
- Piles of crates or drums

The spaces between long parallel planes, such as:

- Concrete platforms carrying process equipment in chemical plants
- Beneath clusters of cars in parking lots or railroad switching yards
- Open multistory buildings such as multistory parking garages
- The space within tubelike structures such as tunnels, bridges, corridors, sewage systems, culverts, etc.

- Consider each blast separately
- Assume that the full quantities of fuel-air mixture present within the partially confined/obstructed volumes and jets participate in the explosion.
- Estimate the volumes of fuel-air mixtures present in the individual volumes identified as blast sources. This can be done on the basis of the overall dimensions of the volumes and jets. Note that if equipment takes up a substantial fraction of a volume, that volume should be reduced accordingly.
- Calculate the combustion energy by multiplying the individual volumes of mixture by 3.5×10^6 J/m^3 (a reasonable average for the heat of combustion of a stoichiometric hydrocarbon-air mixture). If there is reason to believe that a particular volume is not completely filled by a combustible vapor cloud, or that the mixture contains less-than-stoichiometric proportions of fuel, this estimate of heat of combustion should be reduced accordingly.

Experimental data may be used to determine a blast's initial strength. Otherwise, for a safe and conservative estimate of the strength of the source of a strong blast, an initial strength of 10 should be chosen. A strength of seven probably is a more accurate representation of the actual experiments. An initial strength of two also seems conservative for unconfined portions of the vapor cloud.

Once the energy quantities E and the initial blast strengths of the individual equivalent fuel-air charges are estimated, the scaled blast maximum side-on overpressure and the positive-phase duration at some distance R from a blast source can be read from Figures 4-19 and 4-20. If separate blast sources are located close to one another, they may be initiated almost simultaneously. Then their respective side-on pressures should be superimposed and the blast duration should be chosen to be the greatest of those for the individual sources. At present, there is no criterion for a minimum distance between separate blasts.

Figure 4-18. Multi-Energy Calculation Method Steps
(Source: Adapted from CCPS, 1994)

The basic tool for the application of the TNO Multi-Energy model is based on a set of scaling equations also known as Sach's scaling equations. Additional information on the Multi-Energy Method to establish a conservative evaluation for the DSA accident analysis can be found in CCPS, 1994, Section 4.3.2, Methods Based on Fuel-Air Charge Blast (other methods are also provided that reference), or in the original development of that method in "The Multi-Energy Method—A Framework for Vapor Cloud Explosion Blast Prediction" (van den Berg, 1985).

The scaling equations are:

$$\overline{R_s} = \frac{R}{\sqrt[3]{\frac{E}{P_0}}}$$ **Equation 4-41**

$$\overline{t_{+s}} = \frac{t_+ c_0}{\sqrt[3]{\frac{E}{P_0}}}$$ **Equation 4-42**

$$P_s = \overline{\Delta P_s} P_0$$ **Equation 4-43**

Where:

R_s [dimensionless] – energy scaled distance

Once calculated, a number ranging from 1 (very low strength) up to 10 (detonative strength) represents the initial blast strength in Figure 4-19 and Figure 4-20.

In addition, Figure 4-19 and Figure 4-20 show a rough indication of the blast-wave shape, which corresponds to the characteristic behavior of a gas-explosion blast.

R [m] – actual distance from source of explosion

E [J] – charge combustion energy

P_0 [Pa] – ambient pressure

t_{+s} [dimensionless] – positive-phase duration as a function of the combustion

t_+ [s] – the positive-phase duration

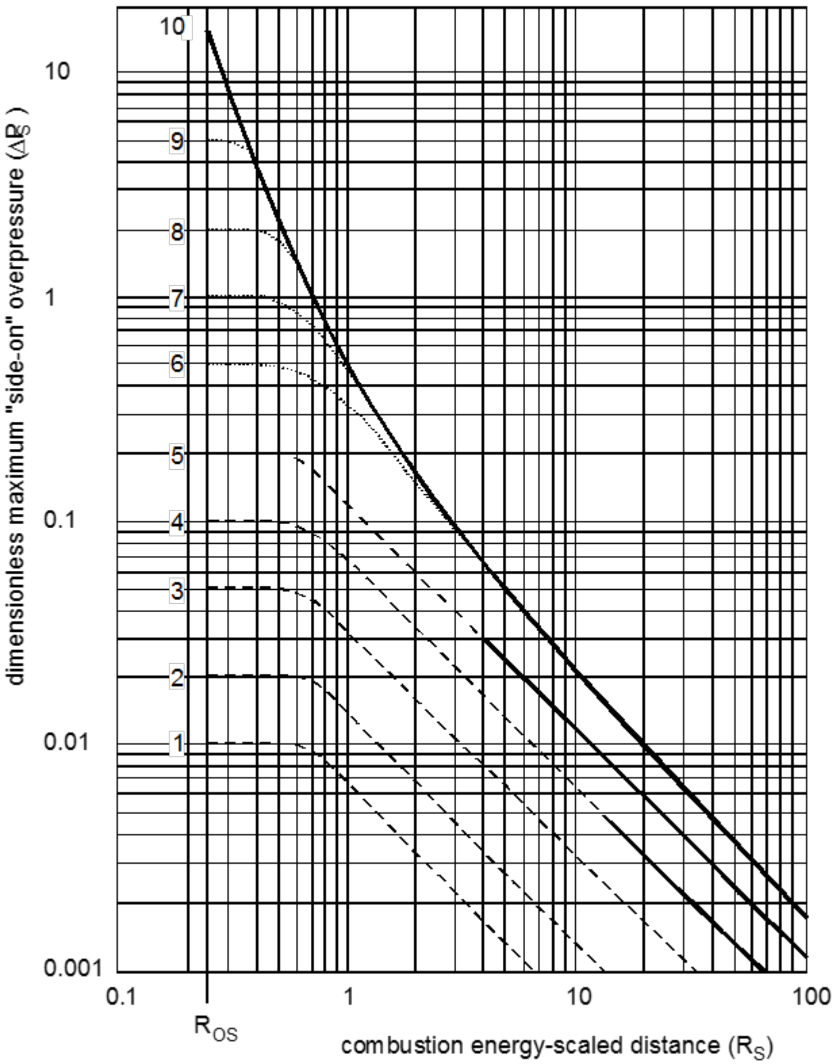
c_0 [m/s] – ambient speed of sound

P_s [Pa] – side-on blast overpressure

ΔP_s [-] – Scaled side-on blast overpressure

R_o [m] – charge radius

Once P_s has been estimated form the graphic, use Equation 4-42 to calculate the positive phase duration and Equation 4-43 to calculate the overpressure.



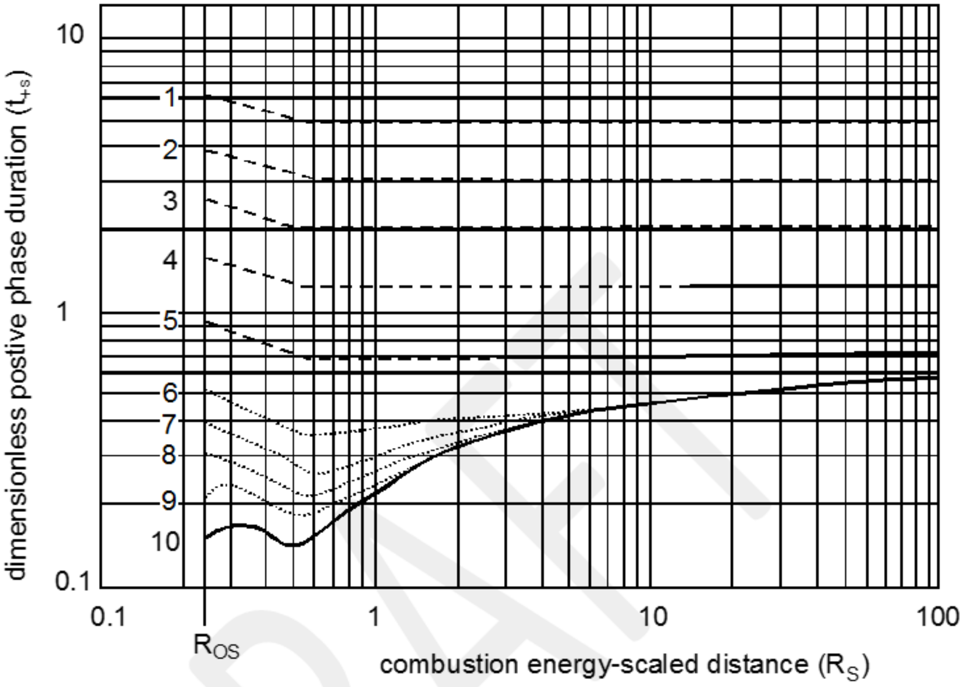


Figure 4-19. Sachs-Scaled Side-on Peak Overpressure of Blast from a Hemispherical Fuel-Air Charge
(Source: Adapted from CCPS, 1994 Figure 4.24)

Figure 4-20. Sachs-Scaled Positive-Phase Duration of Blast from a Hemispherical Fuel-Air Charge
(Source: CCPS, 1994 Figure 4.24**)**

4.3.2.3.5 FRAGMENTATION FROM VAPOR CLOUD EXPLOSION

Fragment effect assessment is not performed for vapor cloud explosion since the vapor cloud is the result of a flammable gas release over time t and it does not involve catastrophic functional failures of receptacles (vessels, containers, jugs) containing the gas, vapor, or mixture. If a vapor cloud explosion is credible, then fragmentation and other failures of SSCs should be considered.

4.3.2.3.6 THERMAL EFFECT FROM VAPOR CLOUD EXPLOSION

The thermal effects from a vapor cloud explosion can be evaluated similar to the thermal effects from a pressure vessel burst with combustion, as discussed in Section 4.3.2.1.3, based on the fire analysis methodologies.

4.3.2.4 FLASH FIRE

A flash fire is the non-explosive combustion of a vapor cloud—it does not produces a blast. (See Section 4.2; see also the scenario description summary in Table 4-1.)

4.3.3 CONSEQUENCES OF EXPLOSIONS BEYOND RELEASES OF HAZARDOUS MATERIALS

Consequences of explosions are characterized for the purpose of the DSA hazard and accident analysis to assess the potential unmitigated damages that explosions can inflict to the public, the co-located workers the facility worker, and to the environment.

Unmitigated consequences of the explosions are grouped in:

- Damages caused by overpressures of vessel burst, BLEVEs and vapor cloud explosions;
- Damages caused by fragmentation of vessel burst and BLEVEs; and
- Damages caused by thermal radiation from the fireball generated after a vessel burst, BLEVEs and vapor cloud explosions.

Section 9.5.5 of this handbook presents a brief summary of consequences of energetic events which includes detonations, deflagrations, BLEVEs, and impacts from radiant heat exposure to fires. This section also discusses ALOHA V 5.4.6 which is a Central Registry toolbox code that is capable of providing quantitative results from each of these energetic events.

4.3.3.1 DAMAGE CAUSED BY OVERPRESSURE (DETONATIONS AND DEFLAGRATIONS)

NUREG-1805 Section 15.8 describes the potential damage from overpressure as follows:

> The damage caused by a shock or blast wave striking an object or a person is a complex function of many factors, and it is well beyond the scope of this chapter to describe all of the complex interactions involved. Instead, we will simply refer to the wave as a rapidly expanding shell of compressed gases. We can then measure the strength of the wave in terms of units of pressure (psi), and we can relate the effects of peak overpressure within the wave (i.e., the maximum pressure in the wave in excess of normal atmospheric pressure) to the level of property or personal injury that is likely to result.

Table 15-1[30] lists damage effects on people and property, which might be expected to result from explosions characterized by various peak overpressures (Clancey, 1972). Peak overpressures in a shock or blast wave are highest near the source of the explosion and decrease rapidly with distance from the explosion site. The extent of damage incurred is heavily influenced by the location of the blast relative to nearby reflecting surfaces.

Table 4-6. Estimated Damage Attributable to Explosive Overpressure.
(Source: Adapted primarily from NUREG-1805, Table 15-1,
with additions as noted from other references)

Overpressure * (psig)	Expected Damage
0.03	Occasional breaking of large windows that are already under strain.
0.04	Glass failure caused by loud noises (143 dB) or sonic booms.
0.1	Breaking of small windows under strain.
0.15	Typical glass failure.
0.4	Some damage to house ceilings; 10% window glass breakage.
0.4	Limited minor structural damage.
0.50–1.0	Windows usually shattered; some damage to window frames.
0.7	Minor damage to house structures.
1.0	Houses made uninhabitable by partial demolition.
1.0	ALOHA V. 5.4.6 PAC: Shatters glass. EPA-550-B-99-009 applies this threshold for vapor cloud explosions to define the endpoint distance for worst-case evaluation. NRC Regulatory Guide 1.91 conservatively selected this value below which no significant damage would be expected, which establishes the safe distance from a source of potential explosions to critical plant structures for a nuclear power plant.
1.0–2.0	Failure and buckling of corrugated metal panels; housing wood panels are blown in.
1.0–8.0	Slight to serious injuries (e.g., skin lacerations from flying glass).
1.3	Slight distortion of the steel frames of clad buildings.
2	Partial collapse of walls and roofs of houses.
2.0–3.0	Shattering of non-reinforced concrete or cinder block walls.
2.3	Lower limit of serious structural damage.
2.4–12.2	Up to 90% eardrum rupture among exposed populations.
2.5	50% destruction of home brickwork.
3	Distortion of steel frame buildings; may pull away from their foundations.
3.0–4.0	Ruin of frameless steel panel buildings.
3.5	ALOHA V. 5.4.6 PAC: Serious injury.
4	Rupture of cladding of light industrial buildings.
5	Snapping of wood utility poles.
5.0–7.0	Nearly complete destruction of houses.

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[30] Table 4-6 in this document.

Overpressure * (psig)	**Expected Damage**
7	Overturning of loaded train cars.
7.0-8.0	Shearing of flexure causes failure of 8–12-inch thick non-reinforced brick.
8.0	ALOHA V. 5.4.6 PAC: Destruction of buildings.
9	Demolition of loaded train cars.
10	Probable total destruction of building.
15.5 - 29	Up to 99% fatalities among exposed populations as a result of direct blast effects. (ARCHIE, 1989 Table B.1)

* These are the peak pressures formed (in excess of normal atmospheric pressure) by blast and shock waves.

For SI units, 1 psi = 6.894757 kPa.

Sources:

Clancey, V.J., “Diagnostic Features of Explosion Damage,” *Sixth International Meeting of Forensic Science*, Edinburgh, England, 1972 (as cited in NUREG-1805 Table 15-1, Estimated Damage Attributable to Explosive Overpressure (Clancey, 1972)).

Lees, F.P., *Loss Prevention in the Process Industries*, Vol. 1, Butterworth, London and Boston, 1980 (as cited in ARCHIE, 1989 Table B.1, Explosion Overpressure Damage Estimates).

Additional sources added, as identified above:

EPA-550-B-99-009.

NRC Regulatory Guide 1.91, page 3.

ALOHA V. 5.4.6 PAC values.

4.3.3.2 DAMAGE CAUSED BY FRAGMENTATION

Damages caused by fragments originating from an explosion may have a significant impact on surrounding SSCs. Section 4.3.2.1.2 discusses the techniques that determine the characteristics (shape, velocity, angle of elevation) of fragments on SSCs or the MAR. By knowing the characteristics of fragments, it is possible to judge whether a SSC will continue to operate after an explosion.

In the qualitative analysis of consequences to the facility worker, fragmentation injuries to the facility worker should be considered.

4.3.3.3 DAMAGE CAUSED BY THERMAL EFFECTS TO FACILITY WORKERS

The information collected in Table 4-7 summarizes the type of injury that may result from various thermal dose levels. A thermal analysis may be performed to show the thermal dose as a function of distance, and the impact of the thermal dose to the worker. The analysis can be the basis for establishing a barrier around a flammable area to prevent workers from entering the area and becoming potential casualties, unless the workers have appropriate personal protective equipment, or for emergency planning and responses.

However, DOE-STD-3009-2014, Section 2.6.1.3, excludes the minor consequences in the previous paragraph for qualitatively assessing consequence levels for facility worker hazard analysis. If the event is classified as a SIH, then Chapter 4 of DOE-STD-3009-2014 is not applicable. For an explosion that is not a SIH, then the thermal effects as well as physical injury from flying shrapnel need to be considered in the qualitative consequence assessment for the facility worker in the DSA.

Table 4-7. Approximate Rate of Radiant Flux

(Source: NFPA 921 Table 5.5.4.2.8, CCPS 1994 Table 6.6, ALOHA V. 5.4.6 PAC)

Approximate Radiant Heat Flux [kW/m^2]	**Comment or Observed Effect**
170	Maximum heat flux as currently measured in a post-flashover fire compartment. (1)
80	Heat flux for protective clothing Thermal Protective Performance (TPP) Test. [a]
52	Fiberboard ignites spontaneously after 5 seconds. [b]
37.5	Sufficient to cause damage to process equipment. Minimum energy required to ignite wood at indefinitely long exposures. (2)
29	Wood ignites spontaneously after prolonged exposure. [b]
20	Heat flux on a residential family room floor at the beginning of flashover. [c]
16	Human skin experiences sudden pain and blisters after 5-second exposure with second-degree burn injury. [a]
12.5	Wood volatiles ignite with intended exposure [d] and piloted ignition.
10.4	Human skin experiences pain with 3-second exposure and blisters in 9 seconds with second-degree burn injury. [a,b]
10.0	ALOHA V. 5.4.6 PAC: Potentially lethal within 60 seconds.
9.5	Pain threshold reached after 8 s. Second degree burns after 20 s. (2)
6.4	Human skin experiences pain with a second exposure and blisters in 18 seconds with second-degree burn injury. [a,e]
5.0	ALOHA V. 5.4.6 PAC: Second degree burns within 60 seconds.
4.5	Human skin becomes blistered with a 30-second exposure, causing a second-degree burn injury. [a]
4.0	Sufficient to cause pain to personnel if unable to reach cover within 20 s; however, blistering of the skin (second degree burns) is likely; 0 percent lethality. (2)
2.5	Common thermal radiation exposure while firefighting. [f] This energy level may cause burn injuries with prolonged exposure.
2.0	ALOHA V. 5.4.6 PAC: Pain within 60 seconds.
1.4	Thermal radiation from the sun. Potential sunburn in 30 minutes or less.[g]
1.0	Approximate solar radiation intensity on a clear, hot summer day. (2)

(1) NFPA 921 Table 5.5.4.2.8

Original sources as cited in NFPA 921, Table 5.5.4.2.8

[a] From NFPA1971, *Standard on Protective Ensemble for Structural Fire Fighting*.

[b] From Lawson, "Fire and the Atomic Bomb."

[c] From Fang and Breese, "Fire Development in Residential Basement Rooms."

[d] From Lawson and Simms, "The Ignition of Wood by Radiation," pp. 288-292.

[e] From Tan, "Flare System Design Simplified," pp. 172-176.

[f] From U.S. Fire Administration, "Minimum Standards on Structural Fire Fighting Protective Clothing and Equipment."

[g] From Bennett and Myers, *Momentum, Heat, and Mass Transfer*.

(2) CCPS 1994, Table 6.6

(3) ALOHA V. 5.4.6 PAC values added above, as identified.

Table 4-8 shows the time restrictions on workers with respect to potential thermal radiation from a fire to avoid reaching the pain threshold.

Table 4-8. Exposure Time t_c to Reach the Pain Threshold.

Radiation Intensity		t_c
[$Btu/hr/ft^2$]	**[kW/m^2]**	**[s]**
500	1.74	60
740	2.33	40
920	2.90	30
1,500	4.73	16
2,200	6.94	9
3,000	9.46	6
3,700	11.67	4
6,300	19.87	2

Source: API 521, 1982, *Recommended Practice 521*, American Petroleum Institute (as cited in CCPS, 1994, Table 6.5, Exposure Time to Reach the Pain Threshold (API 521, 1982).

Figure 4-21 shows the combination of heat flux and time that result in various injury levels to a worker (CCPS, 1994, Figure 6.10).

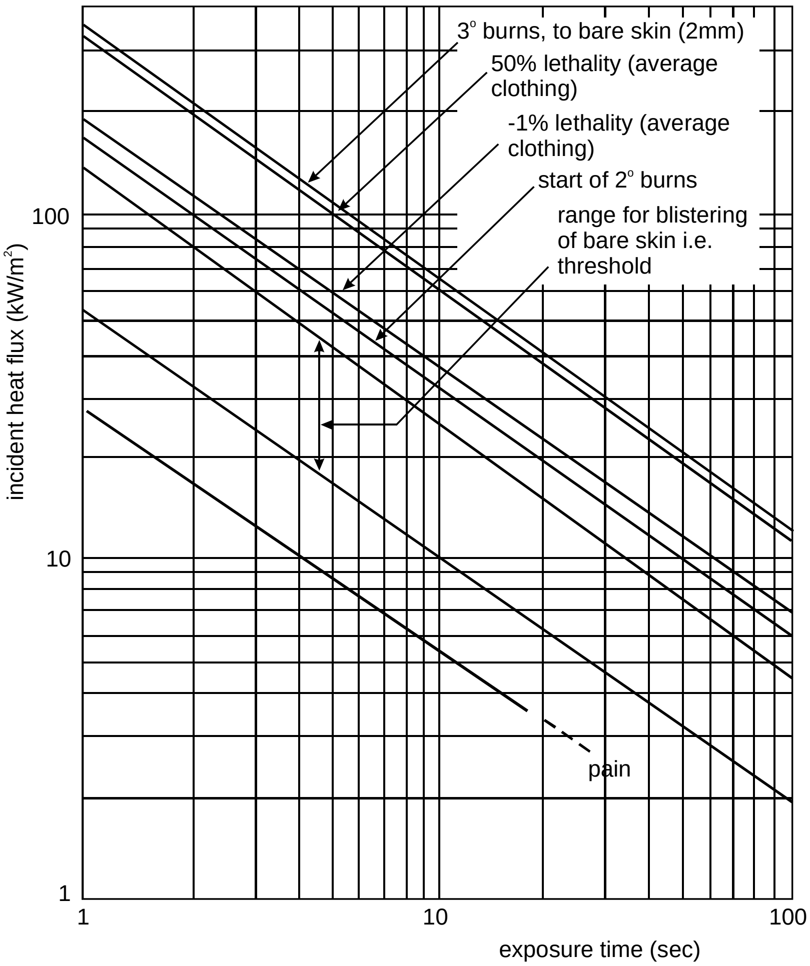

Figure 4-21. Injury and Fatality Levels for Thermal Radiation
(Source**:** CCPS, 1994 Figure 6.10)

ALOHA, 2013, Section 6.2, Levels of Concern for Thermal Radiation, reviewed the literature to present the technical basis for thresholds that are used in the ALOHA code: 10 kW/m^2 for a fatality; 5 kW/m^2 for second degree burns on unprotected skin; and 2 kW/m^2 for pain. A value of 1.7 kW/m^2 was reported to not even cause pain regardless of exposure time, and the 5 kW/m^2 was based on the U.S. Department of Transportation regulations for liquid natural gas facilities.

4.3.3.4 DAMAGE CAUSED BY THERMAL EFFECTS TO SSCS

In addition to potential adverse personnel impacts, thermal flux can adversely impact SSCs. Thermal flux data can be used to determine appropriate locations for SSCs to prevent adverse effects of a potential fire. A fire analysis as discussed in Section 4.2.2 is completed to determine the potential heat flux over the fire duration. With the transient heat flux profile, it is possible to use Table 4-7 and Table 4-8, to determine potential injury to workers and damage to SSCs.

From Table 4-7 it can be observed that process equipment and buildings suffer severe damage for incident heat fluxes of 37.5 kW/m^2 and 12.5 kW/m^2 respectively. As a rule of thumb, flammable materials in buildings and process installations would be damaged after having been exposed to the above-quoted heat fluxes for longer than 1,000 s (CCPS, 1994).

4.3.4 SOURCE TERM CALCULATION FOR EXPLOSION SCENARIOS

The following discusses the effect of an explosion on radiological and hazardous material in terms of parameters important to the source term calculations, as further discussed in Chapter 5, *Source Term Analysis*. This section provides basic guidance in the determination of MAR, DR, and ARF/RF to estimate the release from an explosion event, and considerations related to release durations. No additional considerations are presented for the selection of a mitigated LPF for explosions since the analysis would be unique for the type of explosion and facility features (refer to Section 5.2.5 for further discussion of LPFs for a mitigated analysis).

4.3.4.1 EXPLOSION MAR

For vessel bursts or BLEVEs, the MAR, quantity, form, and location is subject to assessment of following:

a. For events where the MAR is outside of the exploding vessel, the effects of the blast are assessed as a function of distance.
b. The impacts from fragments over a specific distance. The material could be in the nearby proximity or directly within the reach of fragments projected by the burst vessel.
c. The thermal effects, as the result of thermal radiation produced during BLEVEs. If flammable substances are released out of a pressurized vessel and form a cloud, the impact on the MAR will depend on the distance the MAR is from the edge of the flammable cloud/fireball.

For vapor cloud explosions, the MAR, quantity, form and, location is subject to assessment depending on the conditions where the explosion scenario event develops, for example:

a. A confined vapor cloud explosion causes a uniform pressure rise in the room until the walls/ceiling fails, resulting in potential debris impacts to the MAR throughout the room.
b. For large enough enclosures or unconfined vapor clouds, where no significant over-pressure is predicted; depending upon the size of the vapor cloud; the MAR may be determined by a physical area subject to accelerated airflow that could suspend powders and liquids. If the vapor cloud produces detonation-like overpressures (e.g., as predicted with the TNO Multi-Energy Method), detonation and over-pressurization to rupture (if applicable) explosive forces on the MAR are assessed.
c. No fragmentation is considered since the vapor cloud is the result of a gas release over time. If a vapor cloud explosion is credible, then fragmentation and other failures of SSCs should be considered.
d. Thermal effect is assessed on MAR if the material exposed to the thermal radiation is in the area or in the proximity of the ignited cloud.

Explosions have a primary and secondary effect. The primary effects are discussed above. A secondary effect is the possibility of secondary fires of other combustibles/flammables in the room or facility. These fires could impact MAR that was not directly affected by the original explosion, or serve as a mechanism for damaging the same MAR in a second way.

4.3.4.2 EXPLOSION DAMAGE RATIO (DR)

Generally, a DR of 1.0 is appropriate for the unmitigated case, unless it is feasible to justify a technical basis for a different value. For all explosion cases, the type of explosion, distance, and mitigative and/or design control features are taken into account to justify the calculated results that various types of material and/or quantity either would not or would be subjected to certain physical stresses.

For vapor cloud explosions, additional considerations include height of the cloud, radius, impulse, and energy content. Fragmentation effects also consider energy deposited at impact, and the size of the fragments.

Section 5.2.2 provides a discussion of DRs. Additional guidance regarding explosions DRs are provided in Section 5.2.2.2, Examples.

4.3.4.3 EXPLOSION ARF/RF

In the development of DOE-HDBK-3010-94, available experiments and other data were correlated with the major types of material forms present at DOE nuclear processing and material handling facilities. The MAR is not necessarily the explosive material, but rather the material exposed to the explosion stresses of shock (detonation) and blast (deflagration) waves from an explosive source. In some cases the material is the explosion source.

The Material at Risk (MAR) pertinent to the major types of radioactive materials that were addressed include:

1. Gases, most specifically tritium;
2. Liquids
   a. Aqueous solutions
   b. Organics, combustible liquids
3. Solids
   a. Metals
   b. Nonmetallic or composite solids
   c. Powders
4. Surface contamination
   a. Contaminated, combustible solids
   b. Solid, noncombustible unyielding surface
   c. HEPA filters – venting of pressurized gases through filters

An important distinction to mention is that the TNT equivalent method, as discussed in section 4.3.2.3.4, is used to calculate shock effects (detonations) on MARs located in the near field (or practically adjacent) where the explosion occurs, but this equivalency should not be associated with the MAR itself, unless any of the listed above materials in question is the explosive source.

4.3.4.4 EXPLOSION RELEASE DURATION

For unmitigated explosions indoors and all explosions outdoors, the release duration for atmospheric dispersion should be the same as the sampling time base for the dispersion parameters (viz., 3 or 10 minutes), as discussed in Chapter 6, *Atmospheric Dispersion*.

For mitigated explosions inside facilities, the analyst may consider the use of a leakpath factor from the facility geometry to effect a longer release time than 3 or 10 minutes. The analyst is cautioned that Section 5.2.4 of this states that the total airborne quantity is assumed to exit the facility at one moment in time because simple physical principles showing holdup may not be available. If crediting the facility with holdup, the analyst should use acceptable physical principles to show that facility holdup is possible, and more importantly, obtain approval from the regulatory authorities that facility holdup is an acceptable mitigation. In many cases, building holdup does not limit the total release but only serves to spread the total release over a longer time period. Section 5.2.4 provides a discussion of events that are not amenable to potential facility holdup calculations.

For explosions releasing hazardous chemicals located outdoors, the release duration should be considered to be 1 minute when calculating the 15-min time weighted average (TWA) as discussed in Chapter 9, *Chemical Dispersion and Consequence Analysis*.

4.3.5 CASE: SOURCE TERM CALCULATION FOR HYDROGEN EXPLOSION

The source term is dependent on whether a detonation or deflagration occurs. The explosion is modeled in the source term calculation using either the detonation model or deflagration model, depending on the flammable gas concentration.

- If the hydrogen concentration is below the LFL, no event will occur. A concentration of 12% volume at 25 °C and 1 atmosphere is conservatively selected for detonation of hydrogen and air system in vessels.
- If the hydrogen concentration is between 4% and the 12% volume at 25 °C and 1 atmosphere in the hydrogen-air system, a deflagration is assumed to occur.
- If the hydrogen concentration is at 12% or above, a detonation is assumed to occur. There is some uncertainty in the 12% value due to equipment geometry [unfavorable to Deflagration to Detonation Transition (DDT)] and lack of a credible ignition source. However because of the uncertainty in the 12% value, the analyst should use the 12% for hydrogen LEL. The consequences of a detonation are large and it is conservative to assume that the 12% value is appropriate for hydrogen's LEL.

The above values were taken from (Klotz, 2005: Section 2 for the 4% value, Section 5 for the 12% value). Different values apply for other flammable gases. The conditions for achieving DDT deal in particular with the geometry and path of the flame front. Since some process areas have a geometry that is favorable for DDTs (e.g., a tank with numerous obstructions), a concentration of 12% at 25 °C and 1 atmosphere in air has been conservatively used for the DSA accident analysis. Other factors, such as presence of water vapor and energy of the ignition source, affect this parameter and would make a detonation less likely, but are conservatively ignored.

The following subsections are structured to address the important parameters and considerations for selecting MAR, DR, ARF/RF, and release duration, rather than as a narrative scenario of a case study that would be documented for the DSA or its supporting calculation.

The LFL value of 4% for hydrogen should be corrected if used for other than the 25 °C and 1 atmospheric conditions. The following correction is used for air temperature greater than 25 °C (Klotz, 2005, p. 7):

$$LFL_{H2} = LFL_{H2@4\%} - 0.0011 \times (T - 25)$$ **Equation 4-44**

Where:

LFL_{H2} = hydrogen LFL at temperature T, volume %
$LFL_{H2@4\%}$ = hydrogen LFL at 25 °C and 1 atmosphere, volume %
0.0011 = Attenuation Factor
T = temperature, °C

There are different values for the Attenuation Factor in the literature. If a different factor can be justified by the user for their unique situation, then the justification should be provided in the document that the user produces. Different flammable gases have different Attenuation Factors. There are also different correction formulas for LFL in the literature. If a different correction formula is applicable for the event scenario under evaluation, the analyst should consider the different correction formula and provide justification for using the different correction formula.

It is conservative to use no correction for temperature less than 25 °C.

The LFL and LEL values for hydrogen are given at one atmosphere pressure. The data base for LFL and LEL values at other than atmospheric pressure is near zero. Typically, most LFL and LEL calculations are completed for near atmospheric pressure and any potential correction for pressure is negligible. If experimental data become available for pressures different than atmospheric, then the new data should be examined for applicability to the analyst's event scenario. If a pressure correction is needed and no experimental data are available, a suggested correction from the ideal gas relationship is:

$$LFL_{H2} = LFL_{H2@1atm} \cdot \left(\frac{P_{1atm}}{P_{act}}\right)$$

Equation 4-45

Where:

LFL_{H2} = hydrogen LFL at pressure P_{act}, volume %
$LFL_{H2@1atm}$ = hydrogen LFL at 25 °C and 1 atmosphere, volume %
P_{1atm} = standard atmospheric pressure, atm
P_{act} = actual atmospheric pressure, atm

LEL values can be corrected using the same formulas as above. However in practice, LEL corrections are seldom performed as the correction is generally very small. Also, hydrogen LEL values in the literature shows some variation from the 12%. A potential small correction to the 12% value is generally not worth the effort.

The hydrogen LFL and LEL values in this section are based on an oxidizing environment of air. A different oxidizing environment could lead to different results.

The preceding paragraphs have discussed the LFL and LEL for hydrogen in air. In many cases across the DOE complex, hydrogen is not the only flammable gas in a vapor space. For a combination of flammable hydrocarbons, Le Chatelier's Law [Joseph M. Kutcha, "Investigation of Fire and Explosion Accidents in the Chemical, Mining, and Fuel-Related Industries – A Manual", Bureau of Mines Bulletin 680, 1985, Equation 35; Michael G. Zabetakis, "Flammability Characteristics of Combustible Gases and Vapors", Bureau of Mines Bulletin 627, 1965, Equation 46] is used to develop a composite LFL or CLFL. Two similar expressions for Le Chatelier's Law are:

$$CLFL = \frac{1}{\sum_i \frac{M_i^{mole}}{M_{tot}^{mole} \cdot LFL_i}} = \frac{1}{\sum_i \frac{f_i}{LFL_i}}$$

Equation 4-46

Where:

CLFL = composite LFL, volume %
LFL_i = the lower flammability limit of gas i, volume %
M_i^{mole} = the mole fraction of flammable gas i
M_{tot}^{mole} = the total mole fraction of all flammable gases
f_i = fraction of combustible gas represented by the ith combustible

An example calculation for a vapor space containing two flammable gases follows. Let the fraction of gas1 with a LFL of 2% in the vapor space equal 0.011 while gas 2 with a LFL of 5% has a fraction in the vapor space equal to 0.035. The flammable fraction for gas 1 is 0.011 / (0.011 + 0.035) = 0.239 and for gas 2 is 0.035 / (0.011 + 0.035) = 0.761. The resulting CLFL is:

$$CLFL = \frac{1}{\frac{f_1}{LFL_1}+\frac{f_2}{LFL_2}} = \frac{1}{\frac{0.239}{2\%}+\frac{0.761}{5\%}} = 3.68\%$$ **Equation 4-47**

The preceding paragraphs have discussed the LFL of gases and potential corrections to the nominal LFL value of a gas. For control of flammable gases, the industry standard for allowable LFL or CLFL conditions is NFPA 69. This standard states that the concentration of a flammable gas is controlled to 25% of the LFL (or CLFL) unless there is real-time monitoring of the gas concentration, in which case the gas concentration is allowed to reach 60% of the LFL or CLFL. In DOE facilities, the control points for flammable gas concentrations are typically the 25% or 60% levels, depending on the control is use. There are cases where LFL (CLFL) levels different than 25% or 60% are allowed, depending on the process and what is allowed by the local regulatory agencies. Also, allowable gas concentrations during accident conditions may be allowed to differ from the 25% or 60% guideline values in NFPA 69.

Controlling LFL or CLFL conditions is typically accomplished with purge flows through the vapor space containing the flammable gas. The purge flow is based on the maximum LFL or CLFL level that is permitted by the facility in question.

4.3.5.1 GAS EXPLOSION SOURCE TERM (ST)

The source term from a gas explosion is based on the TNT-Equivalency model. As discussed in Section 5.2, the source term is determined from the five-factor formula:

$$ST = MAR \times DR \times ARF \times RF \times LPF$$ **Equation 4-48**

Where:

MAR = material at risk
DR = damage ratio
ARF = airborne release fraction
RF = respirable fraction
LPF = leakpath factor

In fitting this formula to a gas explosion over a liquid containing radionuclides, the TNT equivalent mass from Equation 4-38 provides the equivalent of the MARxDR. If one prefers to define DR = 1, then Equation 4-38 defines the MAR. For an explosion, the ARF/RF is one. The LPF equals one for unmitigated analyses and is usually one for mitigated events as acceptable methodologies for determining LPF values less than one are not available. The end result is that the source term (ST) is simply the result from Equation 4-38. In this example, the TNT equivalent mass model simply converts energy into a quantity of liquid that is vaporized to become a ST for radiological dose calculations.

An additional item should be considered in using the ST from the previous paragraph in determining a receptor dose consequence. This item is whether the radionuclides in the liquid MAR are uniformly distributed throughout the liquid. The ST from the simple TNT model is the surface of the MAR. If settling of solids in the original liquid mass has occurred, then the radionuclide content of the evaporated liquid would be less than the original uniform distribution of radionuclides in the liquid. Another scenario is that the waste material has trapped flammable gas that is suddenly released. As part of the release, there is the possibility that the rising gas bubbles in the waste will bring more hazardous materials to the top layer of liquid that is susceptible to evaporation from the gas detonation.

In the previous paragraphs, the MAR is defined as the quantity of liquid that is evaporated. The original quantity of material in the tank is more accurately termed the MAR.

This treatment for an explosion assumes that the explosion is the only stress imposed on the original mass of liquid involved in the explosion.

4.3.5.2 GAS DEFLAGRATION SOURCE TERM (ST)

Calculations for determining a ST for a flammable gas deflagration are more involved than the calculations for a detonation event. There is no single set of equations available for a deflagration event. Depending on the defined accident scenario from the HA process, there are different paths that a release can take. For example, a deflagration may or may not rupture the vessel or pipe containing the flammable gas that caused the deflagration.

With deflagrations, it is possible to have multiples stresses on the MAR in a vessel, depending on the accident scenario progression. For the deflagration discussion in the following paragraphs, the accident scenario is assumed to occur inside a vessel.

The initial step in a deflagration is to determine the mass quantity that is evaporated from the liquid surface due to the deflagration. The fraction of energy available for evaporation is determined:

$$F = \frac{A_F}{A_W + A_C + A_F}$$ **Equation 4-49**

Where:

E_T - total energy from the combustion of flammable gas
A_F - footprint area (the liquid surface area)
A_W - area of exposed walls
A_C - ceiling area

In this equation, the fraction of the energy (F) that is deposited into the liquid surface is taken to be equal to the fraction of the total surface area represented by the liquid; this assumes that no energy is lost by venting and that the heat flux from the product gas volume is uniform. One difficulty in using the equation is that the liquid level in the vessel experiencing the deflagration can vary, resulting in different values for A_w. To eliminate this potential question on side wall area, A_w can be set to zero and the area ratio reduces to the simple value of 0.5 because for a simple vessel model, $A_F = A_C$.

Equation 4-49 assumes that the flammable gas is uniformly distributed throughout the vapor space. Also, the heat flux from the hot gas after the deflagration is uniform on the vessel walls, vessel top surface, and waste surface that surround the vapor space of the vessel. If a localized deflagration is possible near the waste surface, the analyst will need to justify the use of Equation 4-49 or a possible modification to Equation 4-49.

Once the fraction of energy is calculated from Equation 4-49, the mass quantity that is evaporated from the deflagration is determined:

$$MAR = \frac{E_H * F}{(C_p * \Delta T + H)}$$ **Equation 4-50**

Where:

E_H – Total heat from combustion of flammable gas

C_p - Specific heat of liquid
ΔT - Temperature differential to raise the liquid temperature to boiling
H - Latent heat of vaporization of liquid

As in Section 4.3.5.1, the MAR from the above equation is defined as the actual quantity that is evaporated from the deflagration and not the original mass of the liquid exposed to the deflagration. Typically, the original mass would be defined as the MAR but the value from Equation 4-50 is used as the MAR variable in the five-factor formula.

With a deflagration for a stoichiometric gas/air mixture in an enclosed space, there is a pressure increase and this increase is specific for different gases. This pressure is referred to as the adiabatic, constant-volume combustion constant (AICC) pressure, and the table below provides examples of AICC pressures.

Table 4-9. Constant Volume Combustion Pressures for Various Gases.

Gas	P (bar)
Hydrogen	8.15
Ethylene	9.51
Propane	9.44
Methane	8.94

Source: D. Bjerketvedt, et al., "Gas Explosion Handbook," GexCon, (internet version).

At this point in the analysis, specific information is needed regarding the accident scenario sequence for a deflagration. Possible accident sequences are discussed in the following paragraphs.

One possible accident sequence for the deflagration is that the deflagration has pressurized the vessel, and that the relief is through a simple vent pipe through which the gas flow is not choked. The analyst for a simple unmitigated analysis can use the MAR from Equation 4-50. The unmitigated ST for this MAR is determined from Equation 4-48 with DR = 1, LPF = 1, and ARF/RF = 0.1 × 1.0. This ST is due to the original stress on the MAR. In this scenario, no entrainment of liquid in the vessel occurs and the dose consequence is totally dependent on the ST from Equation 4-50.

A second accident scenario for the deflagration assumes that the vessel containing the deflagration bursts. In this scenario, venting of the pressurized liquid from the vessel occurs as well as the release of the ST from the evaporation of the waste from the first accident scenario in the previous paragraph. Depending on the pressure magnitude (AICC value) and on the location of the venting process, different ARF/RF values are used for the venting calculation. Section 3.1, subsection "Explosive Stress" of DOE-STD-3010 presents information on the selection of ARF/RF values.

A third accident scenario for the deflagration assumes that the vessel breach is well above the liquid level in the vessel. In this scenario, the analyst is referred to the technique described in (Paddleford, D. F. and J. K. Thomas, 1995.) The total ST for this third scenario would be sum of the STs from the volume of vaporized waste and from the mass quantity that is entrained and exits through the breach in the vessel wall.

The above accident scenarios for a gas deflagration do not include all possible STs. The analyst should carefully review the accident scenario as defined by the HA process and determine the appropriate analytical technique to determine the STs.

4.4 SPILLS

A spill is of concern in accident analysis, as it results in an airborne release of radiological and toxic chemical materials from the puddle that is formed through evaporation. DOE-HDBK-3010-94 describes a spill event as follows:

> Material experiences instability/shear stress at the surface of the mass resulting in sub-division of the overall mass. Airflow patterns around and through the material mass, including induced turbulence, accelerate overall sub-division. Mass breakup is further enhanced by impact with ground surface. The material sub-division can generate particles sufficiently small that they remain airborne for a significant period of time.

4.4.1 TYPES OF LOSS OF CONFINEMENT/SPILLS AND SCENARIOS

Spills can be defined as the accidental falling or flowing of material out of a confinement boundary. Spills can result from either a closed confinement system (e.g., sealed drum or tank) or an open confinement system (e.g., open container being handled in a glovebox [GB]). The GB, room, and exterior building walls can also be considered confinement barriers, but these barriers are used to determine the leak path of the spill.

DOE-HDBK-3010-94 provides estimates of ARF/RFs for the following spill/loss of confinement events:

- Free-fall spill of aqueous solutions, 3-m fall distance.
- Free-fall spills of slurries, 3-m fall distance, <40% solids.
- Free-fall spills of viscous solutions, viscosity >8 centipoise.
- Free-fall spills of aqueous solutions, slurries and viscous solutions, fall distances >3 m.
- Free-fall spill of cohesionless powders <3m.
- Free-fall spill of cohesionless powders >3m.
- Suspended solid dispersed into flowing air.
- Aqueous solution, slurries, and viscous liquids (non-Newtonian fluids) spilled onto a hard, unyielding surface.

Spills of powders, liquids, or gases can be initiated via human error or by an external energy source. Examples of such events include puncture of a container by a forklift or missile, crushing of a container, drop of container, or other impact, shock, vibration, and abrasion forces.

For nonvolatile and volatile liquids, evaporation is generally the dominant mechanism for release of hazardous materials. For spills of these types, the surface area of the spill and temperature of the pool formed by the spill dominate the release. DOE- Central Registry Toolbox codes such as EPICode and ALOHA, have pool evaporation models that can be used to evaluate spills of liquids and volatile organic compounds. See Section 9.7 for a further discussion of these codes.

For spills of gases and cryogenic compounds, the impact on surrounding equipment needs to be considered. Concurrent spills of dissimilar compounds from a common-cause event (e.g., seismic) may result in adverse chemical reactions. Analysis of adverse chemical reactions is discussed in Section 4.5 of this Handbook.

4.4.2 ANALYSIS OF SPILLS

The analysis of spills requires the analyst to be able to identify the amount of material that is spilled and the mechanical mechanism involved, that is, the accident phenomenology, so that the MAR, DR, ARF, and RF can be determined utilizing information in DOE-HDBK-3010-94. Spill source terms is further discussed in Chapter 5. NUREG/CR-6410, Section 3.2.3.3, provides the following descriptions of insults to containers or enclosures that may result in a spill:

A. Puncture-Perforation of a container or confinement can release materials in a number of ways. For the release of a volatile material, evaporation is the dominant mechanism (Brereton et al., 1997). Some solids (e.g., phenol) may vaporize/sublime on release from perforated containers. Materials that are flammable gases or have combustible vapors can be vented and, in the presence of an ignition source, result in secondary fires. Solutions with non-volatile solvents and powder may vent if the volume is pressurized and can vent either above the level of the material in the vessel (fragmentation of the liquid by bubble formation and rupture at the surface, or separation of particles at rest by the expansion of the gas in the inter-particle void space) or below it (spray formation of liquids either at temperatures above or below the boiling point of the solvent, or by venting of pressurized volume containing powders). Free-fall spill/release of a solid may be followed by a period of evaporation or even sublimation for volatile solids.

B. Free-Fall Spill (Result of Perforation) - The release and free-fall of liquids and powders can result in suspension from shear stress at the air-material interface. A falling slug can thus shed particles/droplets during the fall. Air resistance can result in the disruption of the face of the falling slug of powder, and particles can be shed into the area of lower pressure resulting from the restoration of the streamlines on the back face of the slug. Impact can induce breakup of solids, powder slugs, and liquids. Volatile materials may evaporate on release (Brereton et al., 1997).

C. Crush-Impact - This phenomenon imposes force on the surface of the material impacted and can fragment both solids (brittle fracture, displacement of powders) and liquids (splashing and droplet formation by displacement and shear). If the force is applied to less than the total surface of the material, fragmentation of the material is limited to the volume that experiences shock wave transmission and reflectance in solids, or the surface area affected for liquids.

D. Shock-Vibration - If the surface is not fragmented, particles lying on the surface (surface contamination, corrosion products) can be jarred from the surface and suspended by vibratory/shock effects.

E. Abrasion - This phenomenon consists of forces applied to the surface layer that induce fragmentation of the surface by mechanical action. Particles generated may be suspended by the mechanical action more efficiently than by aerodynamic forces.

The following three subsections provide a brief treatment of glovebox spills, spills from material handling and waste container accidents, and spills due to over-pressurizations. Aerodynamic entrainment is also briefly treated. Pressurized gas releases are addressed in Section 9.5.2.

4.4.2.1 GLOVEBOX SPILLS

Loss of confinement inside a GB could be caused by an operator inadvertently dropping an open can of material during an operation such as a bagout operation, by equipment failure, or by an airflow reversal. A spill from a can or bottle may occur as the result of a human error while performing some particular action in the GB. A chemical reaction could also occur either inside or outside a container, resulting in a container breach. The MAR is the amount of material that could be spilled from the GB. The DR represents the amount damaged from the accident, while the ARF/RF can be determined by the energy of the released material if any is imparted on it from the release event, height of the release, and environmental conditions (i.e., temperature, pressure, humidity) into which the spill occurs. The release from the glovebox into the process room is of interest for evaluation of consequences to the FW, while the release to the environment is of interest for evaluation of consequences to the CW and MOI.

4.4.2.2 MATERIAL HANDLING AND WASTE CONTAINER ACCIDENTS

A number of energy sources can cause a spill or loss of confinement during material handling. The movement of waste containers or primary containers with dispersible forms of Pu or U used in processes can be subjected to such energy sources. The most common include: (1) kinetic energy sources such as maintenance equipment (e.g., drills, grinders), handling equipment (e.g., forklifts), and internally generated missiles (e.g., shrapnel from failed rotating plant equipment); (2) potential energy sources (e.g., high storage shelves); (3) NPHs (e.g., earthquakes); and (4) man-made external events (e.g., airplane crashes). In addition, chemical reactions such as from nitric acid or chlorinated solvent corrosion of the container and exothermic pyrophoric Pu reactions can also fail the primary confinement boundary. Loss of confinement events involving a single drum, crate, or container can result from all energy sources during handling operations. Events involving multiple drums, crates, or containers require a large energy source from mechanical equipment such as a forklift truck.

Table 4-10 provides an example of an approach for defining spill sizes for handling accidents for containers without interior packaging and for tanks/piping. Evaluating different spills sizes may be important if the preventive or mitigative controls that need to be credited are different, otherwise, the bounding spill size important to establishing the safety basis within a likelihood category is generally evaluated.

Spill sizes, however, depend heavily on spill type, interior packaging, size of packaging, internal pressure, orifice size, and form and type of hazardous material. For example, the amount of material released from a drum punctured by a fork lift may be different from the amount released from an identical drum that fell from the top of a stack of drums from the effects of an earthquake. Also, if the material within a container is packaged in additional containers, such as plastic bags, not all of these interior containers would be breached in an accident. A drum puncture, for example, would probably breach only one interior container, so that the amount of spilled material (i.e., MAR) would be reduced by a factor equal to the number of bags in the drum, assuming each bag contains the same amount.

Table 4-10. Spill Sizes for Handling Accidents.

Spill Size	Drums	Tanks/Piping
Small	one drum	≤10% content of tanks/piping
Medium	Two to three drums	>10% but <50% content of tanks/piping
Large	≥ four drums	100% content of tanks/piping

4.4.2.3 OVER-PRESSURIZATIONS

Over-pressures can result from a build-up of pressure in a container through increasing temperature or through radiolysis, or from the force of a pressure wave of an explosion. For a pressurized container, a small hole in the vessel can result in a spray release of liquid or rapid depressurization and release of powder whereas a rupture of the container of powder would release a cloud of powder. Explosions that cause over-pressurizations are discussed in Section 4.3.

4.4.2.3.1 PRESSURIZED POWDER RELEASES

If the gases in and around a powder are compressed, the gases will expand rapidly during a sudden release of pressure, resulting in airborne dispersal of the powder. Experiments involving the venting of pressurized powders is discussed in Chapter 4, Solids, of DOE-HDBK-3010-94, in which different amounts of powders are subjected to sudden venting under a variety of over-pressures. In general, the larger the over-pressure the larger the amount of powder that becomes airborne, but does not change the original host material particle size distribution.

4.4.2.3.2 PRESSURIZED LIQUID RELEASES

There are three main regimes of pressurized venting of liquids: (1) venting below liquid level, (2) venting above liquid level, and (3) venting of superheated liquid (i.e., flashing spray). This phenomenon covers general pressurized venting, including deflagration induced pressurized venting effects. Experiments involving the venting of pressurized liquids is discussed in Chapter 3 of DOE-HDBK-3010-94. Further discussion is provided in Section 9.5.2 of this handbook.

4.4.2.4 AERODYNAMIC ENTRAINMENT

Aerodynamic entrainment needs to be considered in two situations: (1) air flow past material spilled on the floor or ground, and (2) backdraft of a confinement ventilation system.

Air and other gases passing over a surface or directed onto a surface can induce flow and turbulence that can suspend particles on or from the surface impacted. The presence of obstructions around or over the surface can affect the air flow and, therefore, the suspension of materials from the surface. Sources for gases at accelerated velocities are the passage of or impact by the pressure impulse generated by explosions, ambient or extreme wind conditions, or other conditions such as indoor ventilation airflows.

In DOE-HDBK-3010-94, the approach has been to consider aerodynamic entrainment or resuspension[31] conditions as best evaluated for quantification of hazardous release scenarios using empirical relationships based on field and laboratory data. While the transport phenomena described in Chapters 6 and 9 are applicable to these situations and improve the understanding of the effects of these phenomena, the analyst is directed to Chapter 5 for quantitative inputs applicable to the accident conditions being addressed so that the physical release potential from aerodynamic entrainment/resuspension is conservatively estimated as defined for the DOE-STD-3009 unmitigated analysis. Two scenarios below are discussed in more detail.

- **Air flow past spilled material:** An airborne release rate (ARR), and the length of time that air is flowing past the material, are required to estimate the potential airborne release from postulated accident conditions. In some situations, the release rate may not be uniform with time.

- **HVAC backdraft (or flow reversal):** For the airflow reversal scenario resulting from a loss of HVAC Zone I functionality, a GB breach could occur and result in the release of holdup material in the GB and exposed material in open containers within the GB. Since the Zone II Ventilation System is still functional, the rest of the building ventilation system is operating under partial system flow or even near normal ambient conditions depending upon the ventilation system design. Other factors that affect the airflow reversal scenario are the DR for the holdup material and the release duration.

4.5 ANALYSIS OF CHEMICAL REACTIONS

Several specific chemical reactions rise from the hazards analyses and may require accident analysis due to their ability to contribute to the airborne release of radioactive materials or toxic chemicals in nuclear materials processing and waste management as they can lead to loss of confinement, fire and/or explosions. This section briefly discusses a selection of reactions relevant to DOE accident analysis, including:

- Organic-Based Ion Exchange Resin Reaction;
- “Red Oil” Reaction;
- Organic Reaction Event; and
- Hydroxylamine Nitrate Reaction.

This information may be useful in identifying and analyzing chemical reaction events. It may also be useful to determine whether a fire, explosion, or loss of confinement may occur (which can be further evaluated per information provided in Sections 4.2, 4.3, and 4.4 of this handbook).

4.5.1 ORGANIC-BASED ION EXCHANGE RESIN REACTION

Synthetic ion exchange resins are used in nuclear processing operations such as with plutonium nitrate solutions. Because the separation and purification processes involve contacting nitric acid solutions with

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[31] Resuspension as used when referring to the stress caused by an accident or to calculate the airborne source term, refers to the initial suspension of materials from the surface of the particulate mass being affected by the accident stress or air turbulence. This should not be confused with a more limited definition of resuspension used in the Chapter 6 and 7 atmospheric dispersion analyses that refers to the amount of contaminated materials initially deposited as the plume travels downwind that becomes airborne again due to wind effects overcoming saltation.

organic materials, conditions for safe operation should be clearly defined and resolutely maintained.

Under conditions of rapid reaction between nitric acid and organic materials, the nitrogen oxides produced by the reaction are also reactive, and this further tends to accelerate the reaction. The result in a confined system can be rapid and accelerating pressurization, with the resulting hazard of bursting the ion exchange column or vessel.

The presence of a large number of active sites designated to exchange ions accompanied by extensive polymer cross-linking in the overall resin matrix creates an inherent potential for instability in the type of resin used. Under the right circumstances, this instability can be expressed in a wide variety of exothermic reactions. A variety of reactions is possible, but once the thermal excursion reaches an autocatalytic state, an over-pressurization incident of some type is the inevitable result.

Various types of theoretical models for assessing the airborne release have been postulated. Precedents within DOE for source term estimation have used the model of a thermal explosion since this model seems to predict damage that best matches what has been historically observed. The model is based on exothermic resin degradation reactions, including the recombination of plutonium with nitrate. In thermal explosion events, the initial source of the resin exotherm is highly localized. The localized area may dry out the resin and heat it above the resin autocatalytic ignition temperature, at which point the column condition can no longer be stabilized. Accelerated heat and gas generation results in rapid pressure build up to the onset of structural failure of the ion exchange vessel.

A pressurized spray of superheated liquid occurs when the vessel fails either catastrophically or leaks. For a catastrophic failure, the amount of release depends on the failure pressure of the ion exchange column since this will determine the degree of superheating. The ARF increases with higher degrees of superheat. Assuming the properties of water as expressed in the steam tables, a superheat of 50 °C corresponds to 0.76 MPa (110 psia), and a superheat of 100 °C corresponds to 3.1 MPa (450 psia). If the accident occurs with process solutions present, the ARF should be obtained from DOE-HDBK-3010-94, Section 3.2.2.2 for blast effects over the surface of the liquid and Section 3.2.2.3 for venting below or above the liquid surface, and Sections 4.4.2.2 and 4.4.2.3 for blast effects and venting of solids/powders, respectively. Ignition of the dried-out organic resin, such as polystyrene resin, whether still in the ion exchange column or packaged as waste, may occur before, during, or after the explosion and represents another potential source term mechanism (1E-2 ARF / 1.0 RF per Table 5-1 of Chapter 5).

4.5.1.1 REACTIONS OF NITRIC ACID WITH ORGANIC MATERIALS

Nitric acid, in addition to being a strong acid, is a powerful oxidant when concentrated. It “reacts violently with many organic compounds, for example turpentine, charcoal, and charred sawdust. The concentrated acid may react explosively with ethanol. Nitric acid is used with certain organics, such as furfuryl alcohol and aniline, as rocket propellant” (Clarke and Mazzafro, 1996). The explosive properties of such reactions are aggravated by the production of gaseous reaction products, including steam, carbon dioxide, and nitrogen oxides. The concentrated acid can induce nitration in many organic compounds, including both aromatic and aliphatic hydrocarbons, and the products may be unstable to shock or heat.

The nitrating reaction of concentrated HNO_3 with organic materials proceeds by one of several mechanisms. With aromatic compounds and alcohols, the reaction is believed to involve the ion NO_2^+. Consider a reaction of nitric acid (HNO_3+) with benzene (C_6H_6) and ethanol (C_2H_5OH).

Reaction of nitric acid with aromatic compound and ethanol

$$HNO_3 + C_6H_6 + C_2H_5OH ==> NO_2^+ + H_2NO_3- + H_2O + 8CO_2 \quad \textbf{Equation 4-51}$$

From the principles of mass action, it is evident that in strong acid this equilibrium is shifted to the right. In dilute nitric acid, this equilibrium is shifted to the left and the rate of nitration is negligible. The addition of sulfuric acid favors the nitrating reaction, and sulfuric acid is used for this purpose in the chemical industry.

Another mechanism that leads to the nitration of aliphatic hydrocarbons involves reaction of the NO_2 radical. This normally occurs only with concentrated acid at very high temperatures. However, ionizing radiation produces this radical in nitrate solutions (Miner, 1969), making such reactions possible at ordinary temperatures. Nitric oxide also reacts with metal to create hydrogen gas. Other hazards involving nitrates and organics are mentioned in Section 4.5.3.

4.5.1.2 COMPOSITION AND REACTIONS OF ION EXCHANGE RESINS

Synthetic ion exchange resins are made in many types, and used for a wide variety of industrial purposes. Those used in nuclear separations processes are primarily of two types: cation exchange resins, and strong base anion exchange resins. Both cation and anion exchange resins are composed of polystyrene with active sites chemically bound to the aromatic rings. Cation resins contain sulfonic acid groups, which carry a negative charge and bind the positively charged cations through electrostatic forces. The active sites in anion resins are quaternary amine groups, which take on a positive charge that need to be neutralized by a negative ion.

Other active groups, such as chelating agents, are sometimes present in resins used for specialized purposes, such as concentrating samples for chemical or radiochemical analysis. Full characterization of ion exchange resins requires specifying resin bead sizes and the extent of cross-linking. Small resin particles permit more rapid exchange, but offer greater resistance to flow. Development of macroreticular resins, which contain large channels that facilitate diffusion, has enabled improved sorption and desorption kinetics. The extent of cross-linking determines the rigidity of resins, and their tendency to shrink and swell as the solution composition varies.

4.5.1.3 CHEMICAL DEGRADATION OF ION EXCHANGE RESINS

Both strongly basic anion and cation resins are quite stable in neutral and moderately acid aqueous solution at ordinary ambient temperatures. Strong-base anion resins are used for plutonium and neptunium separations at nitric acid concentrations in the range of 6 to 8 molar (M). Chemical degradation of the resin is unimportant under these conditions. However, at higher acidities there is an increasing likelihood of reaction between the nitric acid and the amine groups that give the resin its character. The rate of nitric acid reaction with the resin also increases with temperature. Acidity control and low temperatures are therefore important safety factors. For example, at the Savannah River Site, column temperatures during anion exchange processing of plutonium are limited to a maximum of 60 °C, and the nitric acid concentration is held below 9 M. Temperature control becomes especially important when processing highly radioactive alpha-emitting isotopes, such as Plutonium-238 or Americium-241. In these, nearly all the decay heat is released within the ion exchange bed on which they are sorbed.

A number of incidents have occurred in the chemical process industry when weak-base anion resins were exposed to nitric acid. A review has recommended that nitric acid not be used with these resins, as they are apparently more sensitive to attack by nitric acid than the strong-base resins (Calmon, 1980). Calmon also recommends that the presence of ions such as copper, which may catalyze resin decomposition, should be excluded from processes involving nitric acid and resins.

4.5.1.4 RADIATION EFFECTS ON ION EXCHANGE RESINS

Like all organic material, synthetic ion exchange resins are degraded by ionizing radiation. Although aromatic compounds are less vulnerable to radiation degradation than aliphatic compounds, ionizing radiation can still break chemical bonds within the ring and elsewhere in the resin. Additionally, free radicals formed by radiolysis of water in the resin bed can remove bound hydrogen or attach to the resin. Substituent groups may be removed, and the resin backbone may cross-link. The extensive literature on radiolysis of ion exchange resins has been reviewed by Pillay (1986). Again, the highest radiation dose rates are associated with short-lived alpha-emitting isotopes, which release nearly all their radiation into the bed on which they are sorbed.

Empirical relationships have been developed to establish the maximum radiation dose that a resin can tolerate. For very radioactive material, such as Curium-244, only a single use of a given resin batch may be allowed. For less radioactive material, such as Plutonium-239 or Neptunium-237, repeated use over a long period is allowable. The U.S. Nuclear Regulatory Commission (NRC) adopted a maximum allowable dose to anion resin of 1E+08 rad (1E+06 gray) based on a survey of practices in the nuclear power plant industry and considering uncertainties (NUREG/CR-2830, *Permissible Radionuclide Loadings for Organic Ion-Exchange Resins from Nuclear Power Plants*), a value that also has been adopted at some DOE sites such as Savannah River (Smith, F.G., et al., 2007). Generally, the effectiveness of the resin as a separations medium begins to degrade before nitration makes the resin itself a reaction hazard. However, the handling of spent resins should take into account the possibility of radiation-induced nitration, which makes the resin more flammable and more easily subject to chemical degradation.

4.5.1.5 INCIDENTS INVOLVING CHEMICAL REACTIONS OF RESINS

A number of events, including vessel rupture, fire, and explosion, have occurred in ion exchange equipment exposed to nitric acid. Calmon (1980) has reviewed 14 events occurring prior to 1980, including 8 in nuclear processing operations. Pillay (1986) cites 13 articles dealing with incidents in the nuclear industry, including those cited by Calmon. Several of these incidents were reviewed by Miles (1969). There has also been at least one serious incident in Russia that has not been described in western literature. It was informally reported during bilateral meetings on safety at Hanford in 1993.

Cation resin is considered less vulnerable to degradation than anion resin. However, a major incident in 1976 (BNWI--107) involved the explosion of a cation column at Hanford that had been loaded with more than 100 g americium, and allowed to stand for more than five months as the result of a plant shutdown. The resin was Dowex 50, 8 percent cross-linked, and the liquid phase was 7 M nitric acid. The column was 6-in. schedule 10 stainless steel pipe. On resumption of work, the column pressurized and burst violently, causing considerable damage and one serious injury. The resin had been exposed to a high radiation dose from absorbed americium during the outage. It is unclear whether the pressure relief vent was open at the time of the accident.

The Russian incident of 1993 involved an anion column loaded with the highly radioactive isotope Plutonium-238. As the result of a valve leak, the column dried out, and the cooling jacket was unable to maintain the central part of the column at a safe temperature. (Heat transfer through dry resin is poor.) The resin was heated by the radioisotope and reacted with enough violence to burst the column. This operation was in a remote facility, and there was no personal injury. However, cleanup and repair were very difficult.

4.5.1.6 DISCUSSION OF ACCIDENT CONDITIONS

Precautions against resin reactions are of two types: (1) those that prevent the reaction from occurring, and (2) those that mitigate the results.

Precautions to prevent a runaway reaction include temperature control, acid concentration control, and providing adequate cooling. Because most of the heat transfer within a column of resin involves the aqueous phase the column should not be allowed to dry out. At the Savannah River Site, a maximum flow interruption of 48 h is allowed for processing Pu-239, and a maximum interruption of 15 min is allowed when processing Pu-238. Maintaining flow carries away heat, and helps prevent the formation of bubbles in the resin bed. As previously indicated, maximum values for radiation doses (10^8 rad), nitric acid concentration (9 M) and temperature (60 °C) are also imposed. The values chosen were based on experience and on the results of laboratory studies of the materials and reactions.

Another method of prevention is to use resins less susceptible to these phenomena. For new resins or processes, the reactivity of the system should be determined using techniques such as thermogravimetric analysis, differential thermal analysis, and differential scanning calorimetry.

Mitigation primarily takes the form of venting. The design of vents should take into account measured reaction rates and the corresponding gas generation. Design is important; vents should be of the “ever open” type wherever possible. Where this is not possible, as in high-pressure separations systems, careful analysis of the system and control of operating parameters is important to ensure safe operation.

4.5.2 “RED OIL” REACTION

4.5.2.1 BACKGROUND AND PRIOR RED OIL INCIDENTS

The Plutonium Uranium Extraction (PUREX) solvent extraction process (and its variants) uses tri-n-butyl phosphate (TBP) and concentrated nitric acid as two principal components (>70 wt% HNO_3). These components, under certain extreme conditions of heating (temperatures greater than 135 degrees C) and strong nitric acid concentration, can react in an uncontrolled manner that could result in very serious consequences such as over-pressurization and rupture of a vessel, and fire or deflagration of flammable gases generated. The stronger the concentration of the nitric acid, the more violent the reaction. In the absence of high temperatures, or the presence of dilute nitric acid (e.g., 30 wt% HNO_3), this reaction does not occur.

Incidents with TBP and concentrated nitric acid are often referred to as “red oil” incidents because of the red oily intermediates that form in the TBP phase in the course of the reaction. The red oily intermediates are nitrated compounds that are flammable and produce significant amounts of NO_x gases. Red oil looks similar to the red fumes present with red fuming nitric acid (> 90 wt% HNO_3).

The consequences from a TBP/nitric acid runaway reaction (i.e., “red oil explosion”) can vary significantly depending upon assumed initial conditions and vessel design and other factors, which influence the accident progression. Common to all scenarios is the oxidation of TBP by nitric acid or nitrates dissolved in it. Possible scenarios range from benign reactions to intense uncontrolled reactions followed by primary vessel failure and/or flammable gas deflagration. Small-scale reactions between

TBP and nitric acid can result in slow reactions similar to boiling and a more reactive scenario. In the slow reaction, the release of radioactivity from the vessel would be very small due to a small airborne and respirable release fraction product of 3E-5 ARF / 1.0 RF (see Chapter 5, Table 5-1 for simmering liquid). In the more reactive scenario in which the solution boils, the fraction of radioactivity released could be as high as 2E-3 ARF / 1.0 RF (see Chapter 5, Table 5-1). (See also the DOE-HDBK-3010-94, Section 3.2.2.2 for blast effects over the surface of the liquid; Section 3.2.2.3 for venting below or above the liquid surface). For worst-case uncontrolled reactions of large quantities of TBP and nitric acid in vessels without adequate venting, an ARF/RF as high as 1E-1 has been postulated based on insights from the Tomsk-7 accident considering source term contributions from the initial explosion that ruptured the vessel, subsequent deflagration of combustible gases released into the room that blew out the building walls, and the ensuing fire (Howard, 1994).

While proper vent area will ensure process vessel integrity, a pressurized radiological release or free-fall spill of liquids would be expected. Also, the consequences of potential flash fire or deflagration of the vented gases on containment structures should be evaluated as well as radiological source terms based on the type of accident stress.

Several reported incidents of damage have occurred in the nuclear industry as the result of high-temperature reactions between TBP and nitric acid or nitrates. The most recent was the damaging explosion at the Tomsk-7 nuclear fuel reprocessing plant in Russia during April 1993 (Hyder, 1996; IAEA, 1998). At least four incidents in North American plants have been attributed to such reactions. Two of these were at the Savannah River Site. One other incident in the Soviet Union has been informally reported.

Damaging incidents occurred at Hanford and the Savannah River Site in 1953 (Colven et al., 1953; Campbell and Mailen 1998). In each case, TBP solution was inadvertently allowed to enter an evaporator in which a nitrate solution was being concentrated at a relatively high temperature. The damage at Hanford was minor; however, the unit at the Savannah River Site was destroyed by the explosion. Temperature controls were established by the two sites following investigations of these incidents, and these have successfully prevented any recurrence within the DOE complex. However, an incident that damaged a Canadian evaporator in 1980 appears to have been caused by a nitrate-TBP reaction (Hyder, 1994a).

A damaging incident at the Savannah River Site in 1975 resulted from the accidental introduction of TBP into a vessel in which uranyl nitrate was being calcined (Gray, 1978). In this case, the calciner was adequately vented, but flammable fumes were released to the process room and ignited, producing a fireball deflagration and a pressure wave loading in that blew out the lightly constructed walls.

The explosion in the Tomsk-7 plant involved reaction of strong nitric acid with organic material originating from the PUREX solvent extraction process. The organic material was not well characterized but presumably contained TBP and its degradation products. The materials were contacted in a tank that also contained evaporator bottoms (probably still thermally hot). There was no venting or pressure relief until a substantial pressure had been generated in the vessel. During a period of about 100 min, an accelerating reaction occurred that overwhelmed the pressure relief and finally burst the vessel. Substantial damage to the building was done by the resulting pressure wave and/or ignition of flammable gases released from the vessel.

Investigations of the above incidents have produced much of the available information on TBP-nitrate reactions. Hyder (1996) summarized investigations regarding TBP-nitrate reactions and provided an interpretation of the experimental results and their pertinence to past incidents. Experimental studies were conducted at the Savannah River Site by Nichols in the 1950s (Colven et al., 1953) and by a team under Harmon in the middle 1970s (Harmon et al., 1976). Other investigations have been made at Hanford (Wagner, 1953; Watkins and Gordon, 1993), by the Du Pont Engineering Department at the Savannah River Site (Hyder, 1996), and in Russia (Vladimirova et al., 1991). Additional studies have been conducted at the Savannah River Site and Los Alamos (Hyder, 1994b; Davis et al., 1966; Smith and Cavin, 1994; Fauske, 1994).

The Defense Nuclear Facilities Safety Board issued a technical report on red oil hazards and explosions, DNFSB/TECH-33**,** *Control of Red Oil Explosions in Defense Nuclear Facilities* (2003). It is an assessment of the potential for a red oil explosion in the DOE defense nuclear facilities complex. This reference describes the connection between the process of solvent extraction and red oil production, identifies the types of process equipment and the necessary materials capable of producing red oil, defines what red oil is and what conditions cause it to decompose in a runaway reaction, summarizes four of the previous red oil events described above, and provides discussions of controls for prevention or mitigation of a red oil explosion (generally categorized as controls for temperature, pressure, mass, and concentration).

Reactions of concern involve oxidation of TBP by nitric acid or nitrates dissolved in it. The oxidant content is a small fraction of the amount required for complete oxidation, and most of the TBP is unaffected by this reaction. In sealed tubes the products include principally carbon monoxide, carbon dioxide, water, nitrogen gas, nitrogen oxides (NO and N_2O), and phosphoric acid. Other non-volatile organic materials are also produced, but have not been well characterized. In open vessels, intermediate products such as NO, NO_2, and CO can escape, and the amount of oxidation is less. The heat produced is also much less, as reactions giving these products are less energetic. Heat produced ranges from a measured value of about 100 cal/g in DTA experiments (Watkins and Gordon, 1993), to a calculated value of about 340 cal/g for sealed-tube experiments (Hyder,1994b).

At high temperatures (above 130 C), TBP is thermally decomposed to 1-butene and phosphoric acid. This appears to be the principal source of flammable gas produced in this reaction. This decomposition is endothermic and requires the oxidation reaction (or some other heat source) to produce the necessary heat (Harmon et al. 1976; Watkins and Gordon, 1993).

TBP that has been contacted with aqueous solutions will contain some water (Davis et al., 1966). Savannah River Site experiments (Smith and Cavin, 1994) have shown that heat removal by evaporation is very effective if the water content can be maintained and water vapor removed by proper venting of the atmosphere above the TBP. Hanford experiments have also confirmed this phenomenon (Watkins and Gordon, 1993). Further, the experiments indicate that if the vessel were adequately vented, the transport of water from the underlying aqueous phase to the TBP phase would be sufficient to maintain continuous evaporation and a net cooling.

Formation and thermal decomposition of red oil during unit operations of nuclear fuel cycle process flowsheets is a severe risk. Solvent extraction is a cost effective industrial process to recover, purify, or separate metals. Although several solvents can effectively extract uranium, plutonium, or thorium from acid solutions, the commercially chosen solvent is only TBP. Results of unique experiments on adiabatic thermal decomposition of red oil, red oil equilibrated with excess of 4N nitric acid and 100% TBP equilibrated with excess of 4N nitric acid are discussed (Kumar et al., 2011). The provision of sufficient vent area in the equipment to avoid closed-vent conditions during worst case scenario needs to be considered (Kumar et al., 2011).

If sufficient venting of process vessels is available for the quantity of TBP present, failure of the process vessel can be precluded. The basis for determining the proper vent area is the work by Fauske & Associates for the Savannah River Site (1994). In this experimental work a number of tests were performed with the Reactive System Screening Tool (Creed and Fauske, 1990) and Vent Sizing Package (Fauske and Leung, 1985) calorimeters. These small (10 ml and 110 ml, respectively) calorimeters have been specifically developed for the purpose of studying runaway reactions and determining vent sizes to support safe design and operation in the commercial chemical industry.

In open (well-vented) systems, a runaway is much less likely to occur because of release of reactive intermediate gases and evaporative cooling mechanisms. The Fauske experiments show, that even when runaway is induced in the TBP and nitric acid system, dangerous pressure buildup is prevented with practical vent sizes. In particular, scale up of a test in which TBP was saturated with concentrated (> 70 weight percent) nitric acid indicated pressures should remain low (less than 22 psig) provided the effective vent area was greater than 0.0022 in^2/kg of TBP and nitric acid solution. By contrast, identical tests with a closed system, i.e., no vent, was destructive, and an identical test with the vent but with a back pressure of 2 atm. (to simulate the Tomsk control valve opening pressure) resulted in a large pressure with severe bulging of the test vessel

4.5.2.2 DISCUSSION OF RED OIL ACCIDENT CONDITIONS

A discussion of the operating or faulted conditions that resulted in each of five historical accidents follows:

- Savannah River Site, TNX Facility, 1953. TBP was inadvertently introduced into an evaporator concentrating uranyl nitrate solution. The evaporation was poorly controlled, and the uranyl nitrate was heated to incipient solidification. Gases from the reacting TBP pressurized and/or ignited and the burst the evaporator.
- Hanford, 1953. This event was very similar to the 1953 event at the Savannah River Site. Pressurization occurred, but it was not sufficient to burst the vessel.
- Savannah River Site. A-Line, 1975. TBP was inadvertently introduced into a heated calciner. Venting allowed gases to escape the primary vessel; however, they were flammable and a deflagration occurred in the process room.
- Port Hope, Ontario, 1980. TBP was inadvertently introduced into a uranyl nitrate evaporator. It appears that the evaporator was operated at a temperature much higher than the normal conservative value. A pressure pulse damaged the upper part of the unit.
- Tomsk-7, Russia, 1993. Concentrated nitric acid was contacted with an undetermined but large amount of PUREX organic residues (possibly containing aromatic and cyclic contaminants) in a feed tank. The tank also contained hot, freshly evaporated uranyl nitrate solutions, and was initially unvented. The reaction of nitric acid and the organic material pressurized and destroyed the vessel. The pressure surge, and possibly an external ignition of the released gases, seriously damaged the building.

In four of the five events, TBP was externally heated in the presence of nitrate to a relatively high (though in no case well determined) temperature. In the cases of the evaporator incidents, two errors were involved: introduction of TBP and heating to a high temperature. In the case of the Savannah River Site A-Line calciner, the high temperature was essential to the process, and safety was dependent on keeping TBP out of the unit.

Temperature controls placed on the Savannah River Site, and at other locations, since the 1953 incident have succeeded in preventing further evaporator incidents. It is noteworthy that the TBP in the calciner incident had passed through an evaporator without incident because of these temperature controls. Replacement of batch calciners by continuous calciners has reduced the potential for inadvertent reaction in the Savannah River Site A-Line. This, along with material control measures, has prevented a recurrence of the 1975 incident.

The Tomsk-7 incident involved the following conditions: contact of strong nitric acid with a large volume of TBP (possibly containing aromatic and cyclic contaminants); a quiescent system with no mixing, hence the organic material need not be in thermal equilibrium with the underlying solution; no venting, and hence no evaporative cooling. In contrast, all similar tanks at the Savannah River Site are vented and mixed. Nitric acid concentrations are limited, as are the volumes of TBP allowed to pass into such tanks.

4.5.2.3 APPROACH TO PREVENTING RED OIL ACCIDENTS

The information in the previous sections indicates the set of reactions that take place in an organic-nitric system are exothermic with the reaction rate being a very strong increasing function of temperature. They also indicate the overall reaction rate and energy released is significantly higher in a closed system, as opposed to an open system, because of more energetic intermediate reactions and higher boiling points that results from the increase in constituent partial pressures.

The basic approaches to prevent an uncontrolled reaction include the following administrative controls:

- **Prevent high temperature TBP and nitric acid by ensuring that the cooling mechanisms are capable of removing the heat being generated.** The reaction will only run away if the temperature exceeds some critical value (dependent on TBP mass and vessel heat removal mechanisms) above which the rate of heat generation exceeds the rate of heat loss. Vessel cooling systems can remove sufficient heat. Vessel agitation systems can ensure sufficient aqueous phase mixing with an organic phase to ensure evaporative cooling. In unagitated vented vessels (e.g., evaporators), the transport of water from the underlying aqueous phase to the TBP phase can be sufficient to maintain continuous evaporation and net cooling. This approach is valid for temperatures up to at least 121 C and organic depths to at least 6.2 ft (Smith and Cavin, 1994).
- **Maintain the vessel vent areas to reduce constituent partial pressures in the vessel that could feed back to increase energy release rates and limit evaporative cooling.** If the mixture is open to the atmosphere, evaporation of water, diluent, and nitric acid is an efficient heat loss mechanism, which will limit the temperature of the mixture to the atmospheric pressure boiling point. Also, adequate venting allows the escape of reactants and intermediates from the reaction mixture, and limits the extent of the reaction. In contrast, a closed, inadequately vented system allows the pressure to increase as gaseous reaction products accumulate, which raises the boiling point, suppresses the heat loss due to evaporation, and retains partially reacted intermediates, which can continue to react and generate heat. Process vessels can readily have vents of sufficient area.
- **Limit the mass of TBP present.** The total amount of heat generated and total amount of gases generated will be proportional to the amount of TBP that is reacted. With limited amounts of TBP, uncontrolled reactions can be accommodated with minimal consequences.
- **Limit the acid concentration.** The reaction rate is proportional to the acid concentration.

4.5.2.4 PREVENTIVE CONTROLS

The preventive controls that can be employed to prevent runaway TBP reactions in a processing facility are given below:

- Ventilation system for the process vessel
- Ventilation system for the process room
- Agitation system for the process vessel;
- Evaporator maximum temperature interlock with steam heating system
- Liquid level instrumentation and low level interlocks
- Vessel vent areas
- Sampling of vessels for TBP content
- Time between vessel transfers
- Controls to prevent transfer of solvent wash solutions to acidic evaporators
- Procedural requirements to compare specific gravities of feed tank solutions
- Control of TPB mass of various process locations

With potentially large quantities of TBP, sufficient preventive measures should be selected from the above list to ensure the likelihood of uncontrolled reactions in beyond the extremely unlikely likelihood bin. For small to intermediate quantities of TBP, the approach in the previous section can be used to predict consequences that may be acceptable.

4.5.3 ORGANIC REACTION EVENT

4.5.3.1 BACKGROUND AND DISCUSSION

Nitrated organic compounds are in widespread use as propellants and explosives. The generation or accumulation of such materials in nuclear facilities may present a risk of runaway reaction, loss of confinement, fire, or explosion. The materials of primary potential concern include organic compounds containing nitrate or nitrite, but also may concern mixtures of organic material and nitric acid. These materials may be solids, liquids, gels, or slurries.

Waste materials are a particular concern. Once a material is set aside as waste, it is easy to ignore, especially if it is kept in a remote tank or waste drum because of its radioactivity. Such materials may include spent resins, degraded solvents, analytical reagents, lubricants that have been exposed to acid, and the like. In this environment, over a long time, further reactions may occur. For example, the explosion at Tomsk-7 appears to have involved degraded, impure solvent that had been stored for a long time in contact with nitric acid solution in a radioactive environment. The resulting material appears to have been highly reactive toward strong nitric acid.

Another concern is the accumulation of materials in unexpected locations. Decomposition of sulfamic acid during processing has led to the accumulation of ammonium nitrate, a potentially explosive material, in the offgas system. The “red oil” incident in the SRS A-Line involved a situation in which, unexpectedly, the organic phase was denser than the aqueous material in the tank with it, and so settled to the bottom. It was then unknowingly drawn off and sent to a drying kettle, where it decomposed into flammable gases.

Ammonium nitrate (NH_4NO_3) is a colorless crystal that is a powerful oxidizer used in commercial explosives. It has a heat of formation of–340 kJ/mol at 25 °C. Ammonium nitrate can undergo a decomposition reaction when heated to 250 °C, and can react with other constituents at a variety of temperatures. Ammonium nitrate fuel oil is a type of reaction with a maximum energy release at a concentration of 94 percent ammonium nitrate with 6 percent absorbed fuel oil. Ammonium nitrate may react with other organics less vigorously at other concentrations.

An uncontrolled reaction can occur in waste tanks or drums when organic salts are in contact with nitrate/nitrite salts, if high concentrations of both exist and temperatures are above the reaction onset temperature. Decay heat and chemical reactions can lead to waste heating over relatively long periods. Increasing temperatures result when heat is dissipated to the environment at a rate slower than it is generated within the waste. The increase in reaction rate with temperature provides a positive feedback mechanism and can lead to an energetic event. Reactions produce high-temperature gases that pressurize the tank. A tank breach results in a pressurized release of reaction product gases that entrains aqueous tank material.

In the chemical and radiological conditions found in the Hanford Site tanks, the organic materials in the solution decompose to low energy compounds such as formate, oxalate, and carbonate. These low energy compounds do not support deflagration propagation. This aging process greatly reduces hazards associated with organic materials in these tanks (Meacham et al., 1998).

The radiological source term from an organic reaction is evaluated based on whether the consequences are from a chemical detonation or thermal runaway reaction with rapid generation of gases that could over-pressurize and rupture the vessel or container leading to a high pressure release of the radioactive material. In addition to or instead of a pressurized release of radioactive material, if the vented gases are flammable, the physical consequences of potential flash fire or deflagration on containment structures is evaluated to estimate the radiological source terms based on the type of accident stress.

An organic fuel-oxidizer reaction causing a release of radioactive material occurred on February 14, 2014 at WIPP. The DOE Accident Investigation Board determined that the release was a result of an exothermic reaction involving the mixture of the organic materials (Swheat Scoop® absorbent and/or neutralizer) and nitrate salts present inside a single TRU drum. Chemical reactions heated the drum's contents, leading to a thermal runaway reaction with an exponential temperature rise in the core and rapid generation of gases. Gas generation exceeded the drum's relief venting capacity. The drum lid extruded beyond the lid retention ring, deflected the lid, and resulted in a rapid release of the materials from the drum. The combustible gases and solids ignited, spreading the fire to other combustible materials (fiberboard and polyethylene slip sheets, reinforcement plates, stretch wrap, cardboard stiffeners and polypropylene super sack fabric) within the waste array. The energetic release propelled TRU waste from the drum up into the polypropylene magnesium oxide (MgO) super sacks on top of the container stack, onto adjacent stacked waste containers, and throughout the underground exhaust path from the drum's location. The results of the Phase 2 investigation were issued on April 16, 2015, and are available at: http://energy.gov/em/downloads/radiological-release-event-waste-isolation-pilot-plant-february-14-2014.[32]

Dealing with waste materials therefore involves locating them, sampling them, and developing safe-handling methods. Each case is likely to be unique. The methods for evaluating the problems are general, however, and have been based on long experience in the chemical industry.

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[32] For a detailed discussion of the reaction mechanism, see SRNL-RP-2014-01198 and Clark and Funk, 2015.

4.5.3.2 ANALYTICAL AND TEST METHODS

A variety of methods have been developed for characterizing the hazards associated with potentially reactive chemicals. In general, reaction of unstable chemical systems will be initiated or accelerated by heating. The tests therefore generally involve heating of small samples under controlled conditions. Differential thermal analysis (DTA) is important in identifying exothermic processes as a function of temperature. The combination of DTA, thermogravimetry, and analysis of the offgases can provide an adequate description of reactivity in many cases. These techniques are adaptable to contained and shielded facilities. For systems in which venting is provided to control the pressure, the method of Fauske has been widely used in the chemical industry to determine vent sizes. This method was used in evaluating the red oil problem. However, it does not appear to have been applied to contained radioactive facilities. Instrumented bomb calorimetry was also applied in studies of the red oil reaction, but again in nonradioactive facilities.

Where the explosive potential is of concern, tests using small explosive initiators have been developed within the explosive industry. These methods are difficult to adapt to radioactive systems, and have mainly been applied to nonradioactive materials. The potential initiator of an explosion is usually fire or heating, so the methods given above will give an indication of the explosive potential.

4.5.3.3 PREVENTION AND MITIGATION

Prevention of these reactions first involves locating and characterizing the materials, identification of possible reactive chemicals from references, such as *Brethericks' Handbook of Reactive Chemical Hazards* (Urben, 2006), and developing an appropriate handling and storage plan. In some cases it may be possible to destroy the material safely. For handling and storage, temperature control is important. Contact with potentially reactive materials should be prevented. When safety analysis determines that the most likely concern for initiating reaction is an external fire, as is often the case, then measures to prevent such fires can be imposed.

Venting will also be important. Nitrogen oxides from slow reactions should not be allowed to accumulate. These can accelerate nitrate oxidation.

4.5.4 HYDROXYLAMINE NITRATE REACTION

Hydroxylamine, NH_2OH, has been used in the nuclear industry as a reducing agent and in decontaminating solutions. It is used as the nitrate (HAN) or sulfate (HAS) salt in solution. It has the advantage of reducing plutonium smoothly to the trivalent state without creating solid waste.

Hydroxylamine is unstable against decomposition in the presence of nitric acid, and this reaction is catalyzed by dissolved iron. This reaction occurs more readily at higher nitric acid concentrations. It appears that the formation of nitrous acid (HNO_2) is an important element in the mechanism. The net reaction is:

$$\text{Reaction of nitric acid and Hydroxylamine} \Longrightarrow 3\ HNO_2 + 7\ H_2O + 2\ HNO_3$$ **Equation 4-52**

This reaction, once begun, can accelerate to a dangerous rate, producing great quantities of gas and pressurizing containers. At least seven damaging incidents involving the decomposition of HAN have occurred in DOE facilities. The last of these occurred in May 1997 at the Plutonium Reclamation Facility in Hanford.

Since the vented gases are not flammable, the radiological source term from decomposition of HAN that results rapid generation of gases that could over-pressurize the vessel or container is based on a pressurized release of the solution. For over-pressurization of process solutions present, the ARF should be obtained from DOE-HDBK-3010-94, Section 3.2.2.2 for blast effects over the surface of the liquid and Section 3.2.2.3 for venting below or above the liquid surface.

4.5.4.1 PREVENTION AND MITIGATION

The recommendations in DOE/EH-0555, *Technical Report On Hydroxylamine Nitrate,* include the following:

- HAN concentrations should not be allowed to exceed 2 M, and the nitric acid concentration should be less than twice the HAN concentration.
- The long term storage of in-process HAN-nitric acid solutions should be avoided.
- Tankage containing HAN solutions should be evaluated to ensure adequate venting in the event of rapid HAN decomposition.
- In preparing HAN solutions the sequence of mixing is important in avoiding autocatalytic systems.
- Care should be taken to avoid the accumulation of HAN solutions as heels or in process lines.
- Strict procedures should be used to avoid contaminating HAN or its solutions with metal ions.
- HAN solutions should be maintained below 40° C.

The detailed recommendations consider five scenarios and discuss the precautions necessary in each case.

4.5.5 CHEMICAL REACTIONS ACCIDENT ANALYSIS

Estimating the consequences from plausible scenarios that have radioactive materials involved in a chemical process to accident analysis in a DSA may be challenging. Evaluate a loss of confinement and/or a fire or explosion event as separate events. For example, if a process with plutonium dissolved in nitric acid has a loss of confinement event and the vessel loses enough liquid such that the plutonium in solution dries and is exposed to ambient oxygen, then the risk of a pyrophoric fire exists after the loss of confinement event. Consider the radiological and chemical consequences with any event involving radioactive material involved in a chemical reaction accident.

For a thorough evaluation, use the source term parameters that provide a conservative conclusion that drive a control set. Changing the parameters by an order of magnitude may not change the conclusion or the resulting control set.

For example, use DR of one for resin columns, waste drums or process vessels. Evaluate the total MAR in the vessel for the loss of confinement and fire or for an explosion of a vessel. Evaluate accident progression from loss of confinement to fire or explosion and with a range of ARF/RF in the range of 1E-2 to 1E-4, which approximates the information from the DOE-HDBK-3010-94 for these type accidents, as summarized in Chapter 5 of this Handbook.

By using a bounding MAR of the entire vessel contents, a DR of one, an ARF/RF in the range of 1E-2 to 1E-4, and a LPF of one, a conservative accident analysis can be described in a DSA. Simple and conservative analysis can be used as a starting point. In some cases, no further insight or changes to the control set would result from expending analytical effort on a more refined analysis. In other cases, refinements could provide insight, but in all cases, the analysis should be bounding, technically justified, and consistent with DOE Standard 3009. If the resulting consequence driven control set can enable safe operations without being too difficult to implement, then the source term parameters used are sufficient. Only if further refinement in a particular parameter is needed to reduce consequences to receptors do the accident analyses warrant such refinements. If the postulated event in the DSA closely resembles an event that has either happened in the past or has been analyzed in a technical journal or report, then this information can be used to support a technical justification of the DR, ARF, and RF. A technical justification that cites actual or previously analyzed events should discuss whether these events bound the severity of the accident conditions postulated in the DSA and describe how any non-bounding aspects of the cited events were addressed in the derivation of DR, ARF, and RF.

4.6 NATURAL PHENOMENA HAZARD EVENTS

Natural phenomena hazard (NPH) events are quantitatively evaluated in accident analysis due to their ability to contribute to the airborne and/or waterborne release of radioactive and toxic chemical materials that may result when SSCs fail to perform their safety function during and after the NPH events. Furthermore, the NPH events may cause fires or explosions that could provide energy for transporting the radioactive and toxic chemical material and at the same time degrade the functions of the SSCs.

4.6.1 NPH EVENT TYPES

NPH events that affect DOE sites are:

- Seismic events (earthquakes);
- Extreme winds (straight-line winds, tornadoes, and hurricanes);
- Floods (seiches, tsunamis, storm surges);
- Extreme precipitation;
- Lightning;
- Volcanic eruptions (ashfall); and
- Wildland fires.

DOE-STD-1020-2016 provides criteria and guidance for evaluation and design for all of these NPHs, except wildland fires, which is addressed in DOE-STD-1066-2016, *Fire Protection*. Additional guidance on implementing DOE-STD-1020-2016 is available in DOD-HDBK-1220-2017, *Natural Phenomena Hazards Analysis and Design Handbook for DOE Facilities*.

4.6.2 NPH EVENT ANALYSIS OVERVIEW

Unmitigated accident analysis of NPH events is performed differently for safety basis documents for new nonreactor nuclear facilities and major modifications to existing nuclear facilities, than for existing facilities where the DSA is to be updated as a result of revised NPH criteria based on periodic reassessments. These approaches are addressed in the following subsections, followed by a summary of the general methodology for these evaluations.

4.6.2.1 ACCIDENT ANALYSIS FOR A NEW NUCLEAR FACILITY OR MAJOR MODIFICATION OF AN EXISTING NUCLEAR FACILITY

In preparing a safety design basis document for the purpose of designing a new nuclear facility or major modification of an existing nuclear facility, the evaluation of NPH events is different from the evaluation of operational accidents. The magnitude of a design basis NPH event (e.g., the peak ground acceleration from an earthquake) is determined based upon: (a) the unmitigated dose consequences of the SSC failure that determines the NPH design category (NDC) of that SSC as described in Section 2.3 of DOE-STD-1020-2016 and the associated performance goal (expressed as annual probability of failure), and, (b) a factor that is a measure of the degree of inherent conservatism in the design criteria and analysis methods specified for the NDC of the SSC in DOE-STD-1020-2016 and the categorization scheme described in supporting national consensus standard ANSI/ANS-2.26-2004. DOE-STD-1020-2016 also provides direction on how to determine the site-specific NPH hazard values corresponding to each NDC level. Some of these values can be directly obtained from national consensus standards[33] while a site-specific probabilistic NPH hazard analysis (e.g., Probabilistic Seismic Hazard Assessment) may need to be performed if consensus standards are silent on them or do not provide the requisite level of specificity.

For new facilities, the NDC of an SSC establishes a risk-based target performance goal for the SSC, and the return period[34] of the specific hazard, as established in DOE-STD-1020-2016, to which the SSC will need to be designed. The NDCs were formerly called Performance Categories (PCs) in previous versions of the DOE NPH design-related orders, guides, and standards, which are roughly equivalent from a performance goal perspective to the numerical assignments for NDC. For example, a PC-3 SSC may be viewed as equivalent to an SDC-3 SSC.

Subsections 4.6.3 through 4.6.8 provide additional guidance on unmitigated analyses of specific NPH types to estimate radiological and toxic chemical source terms based on conservative estimates of MARs and DRs. Atmospheric dispersion, aquatic dispersion and radiological dose calculations are performed in accordance with Chapters 6, 7, and 8 of this Handbook. To determine MARs and DRs for safety classification and NDC categorizations of the SSCs during a new facility design, the unmitigated consequence analysis should assume that the building structure inside which the SSCs are located would not maintain confinement and may collapse during the design basis NPH event.

The NDC for SSCs that provide protection from toxic chemical hazards are determined based on the unmitigated consequences of SSC failure from an NPH event, similar to the unmitigated consequence methodology for radiological releases. The methodology for this unmitigated analysis should be consistent with DOE-STD-3009-2014 and Chapter 9 of this Handbook, to determine the need for SS SSCs, which influences the NDC determinations. The higher of the NDCs determined from the application of radiation dose criteria and the criteria for toxic chemical consequences should be used; therefore, it is possible that an SSC categorized as NDC-2 based on radiation hazards may be assigned to the NDC-3 category based on toxic chemical hazards.

4.6.2.2 ACCIDENT ANALYSIS FOR EXISTING NUCLEAR FACILITY DSA

For existing facilities, the NDC or PC establishes the return period of the specific NPHs to which the SSC design will need to be evaluated. For the DSA evaluation of NPH impacts on existing facilities, the initial step is to establish, for each SSC, which NDC from the requirements in DOE-STD-1020-2016 should apply, or which PCs from the previous DOE NPH standards apply as discussed below. Evaluations of SSC capacities should have previously been performed as required by an implementation plan when required by the DOE Program Secretarial Office per DOE O 420.1B or DOE O 420.1C, and its facility conditions assessment should be used for the development of the existing DSA.

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[33] ASCE 7-10, ANSI/ANS-2.3-2011 (R2016), *Estimating Tornado, Hurricane, and Extreme Straight Line Wind Characteristics at Nuclear Facility Sites*.

[34] The return period is the reciprocal of the frequency of exceedance of the NPH event: a 100-yr flood has a 1E-2/yr frequency of exceedance.

DOE O 420.1C and DOE-STD-1020-2016 require that sites with any facilities rated NDC-3 or higher, review existing NPH assessments every 10 years. The results of the updated evaluations should be used in the unmitigated radiological and toxic chemical consequence evaluations to support any required updates of the accident analyses.

If a new NPH assessment yields increased NPH loads and they exceed the capacity of existing SSCs, the DOE Site Office would evaluate and determine whether to upgrade SSCs and whether such evaluation results need to be integrated with the DSA annual update. DOE-STD-1020-2016, Section 9.3, *Facility Condition Assessments,* allows for a factor of two reduction in the return period and lesser design loads, with caveats, when evaluating existing SSCs. If an engineering evaluation concludes that the existing structure will not withstand the higher NPH loads, with allowances, a collapse event should be further evaluated in DSA Chapter 3 accident analysis as an EBA.

Situations where increased NPH loads exceed the capacity of existing SSCs should also be evaluated to determine whether this new information requires entry into the Potential Inadequacy of the Safety Analysis (PISA) process. This evaluation can be performed using DOE Guide 424.1-1B, *Implementation Guide for Use in Addressing Unreviewed Safety Question Requirements*. For SSCs that are found deficient, a fragility analysis or seismic margin study may be performed to assist in the PISA and Unreviewed Safety Question Determination, and to justify continued operation of the facility.

Another outcome of a new NPH assessment is that higher NPH loads might be within the DBA and EBAs already evaluated in the DSA. Thus, no changes would be necessary for the DSA upgrade.

In performing an NPH engineering evaluation for the existing facility, an unmitigated dose consequence analysis is required that would assume that the structure will suffer major damage, exceed Limit States, and/or collapse. This evaluation is used to determine the safety significance of the SSCs, i.e., whether the SSCs provide a SC or SS safety function. If the engineering evaluation concludes that the SSCs can withstand the NPH loads, then the unmitigated analysis can also credit the SSC as an initial condition that provides the SC or SS safety function and would be protected by a TSR Design Feature. This analysis applies only to passive features. Chemical consequences can be evaluated in the same manner as discussed for new facilities or major modifications, as described in Section 4.6.2.1.

For an unmitigated analysis in Section 3.2.2 of DOE-STD-3009-2014, if a building structure, or any of its components, is credited to maintain confinement, the NPH engineering evaluation using the revised or updated NPH loads is required to demonstrate that the building structure and its components that have confinement function will not be deformed more than the Limit State commensurate with the permissible leak rate (see Section 5 and Appendix B of ANSI/ANS-2.26-2004; R2010). To ensure required confinement function, such an evaluation considers not only the relationship between the predicted deformation level/Limit State and leak rate, but also the existence of various openings and penetrations in the building components. The analyst should carefully consider and account for any leak paths that could be caused by expected event-driven actions such opening exterior doors to facilitate personnel evacuation. However, if other SSCs fail at the revised NPH loads, the unmitigated dose consequence analysis should recognize that some damage to other SSCs, such as fire sprinklers, may occur and could cause collateral damage resulting in potential radiological or hazardous chemicals releases.

The unmitigated radiological and toxic chemical consequences of the SSC failure that determines the NDC of an SSC is based on the same criteria and methods described above for evaluation of new facilities and major modifications, and guidance from other chapters of this Handbook. Subsections 4.6.3 through 4.6.8 address additional guidance for unmitigated analyses of specific NPH types to estimate source terms based on conservative estimates of MAR and DRs.

With respect to evaluation of existing structures, systems and components (SSCs) following an updated NPH assessment (required periodically by DOE-STD-1020-2016, *Natural Phenomena Hazards Design and Evaluation Criteria for Department of Energy Facilities*, and its 2012 predecessor), a question arises regarding selection of the appropriate bounding DBA or EBA. Two outcomes are possible: (1) the original DBAs or EBAs developed for the design or evaluation of the facility are bounding; or (2) new EBAs with higher NPH loads are defined by the NPH assessment are bounding. New bounding EBAs would require further DSA evaluation using the results of the facility condition assessments required by DOE-STD-1020. If the existing DBAs or EBAs are bounding, then a DSA revision should:

- Document that the updated NPH evaluations did not change the existing accident analyses in the safety basis document. If the safety class and safety significant SSCs have been concluded to provide their safety functions for the applicable NPH EBA criteria for existing facilities, their failure during a higher level NPH event is considered to be a Beyond DBA and therefore the consequence of their failure is not evaluated in the DSA Chapter 3 accident analysis, except in regards to potential cliff edge effects associated with evaluation of Beyond DBAs (addressed in the next bullet).

- Evaluate SSCs for Beyond DBAs using NPH event return periods applicable for an NPH Design Category (NDC) one level higher than the design or evaluation basis NDCs. For example, if the design or evaluation basis NDC of an SSC is NDC-3, its Beyond DBA can be defined using a return period applicable to NDC-4. See Section 3.4, Beyond Design/Evaluation Basis Accidents, of this Handbook for further discussions.

- For existing facilities, all SSCs, including confinement barriers, that have been evaluated to meet the requirements of DOE-STD-1020-2016 or its predecessor used for the existing DSA accident analysis, can be credited when considering potential interaction effects of these SSCs on SSCs of the same or lower NDC level.

4.6.2.3 GENERAL METHODOLOGY

For preparing the DSA of a nuclear facility, the list of DBA/EBAs would include those resulting from NPH events. The selection of the size of these NPH events and their evaluation and mitigation are required to be performed in accordance with DOE-STD-1020-2016 and the accompanying NPH Handbook.

In general, for all nuclear and hazardous facilities in the DOE complex, DBA/EBAs related to NPH events selected per the criteria in DOE-STD-1020-2016 are evaluated using requirements and guidelines given in DOE-STD-3009-2014. For TRU waste facilities, additional NPH event evaluation guidance is provided in DOE-STD-5506-2007. Since the NPH evaluation provisions in DOE-STD-5506-2007 were developed independent of those in DOE-STD-1020-2016; therefore, during the DSA development process, some inconsistencies between the provisions in these two documents may be identified. Any such identified inconsistency should be reported to the DOE with proposed resolution.

SSC failures from NPH events may also cause toxic chemical releases from nonreactor nuclear facilities with chemical hazards requiring further DSA evaluation as described in Section 2.3.2, Chemical Hazard Evaluation, of this Handbook. NPH-induced toxic chemical releases are evaluated in a similar manner to other operational accident types as described in Chapters 3 and 4 of this Handbook. For example, an NPH event can cause spills of process solutions or powders and result in impacts of debris on process equipment or impact of process equipment with the floor, or potential fires or explosions. The DR, ARF and RF are similar to those from operational accidents. Moreover, care should be taken to determine if the effect of the NPH will cause abnormal process conditions. These types of events should be identified and analyzed in the DSA. For example, it might be more conservative to assume that a process tank remains intact, but suffers an overpressure event due to lack of power or cooling. Failure of tanks or vessels could result in energetic chemical reactions, which may cause a release as discussed in Sections 4.3 through 4.5. A rupture of a line could result in a spray release.

NPH events can initiate several separate accident progressions (e.g., fires, explosions, spills, collapses) simultaneously. Therefore, the overall consequence analysis should sum up the contributions from all the individual accident progressions.

4.6.3 SEISMIC EVENTS

Seismic events result in ground motions that can affect all the SSCs in a facility, so the unmitigated consequences, assuming the failure of all SSCs—including the facility structure itself—should be considered. The seismic ground motions result in accelerations and displacements that are transmitted into the facility structure and to all the systems and components in the facility structure. Seismic events can also result in soil-structure interactions, ground displacements that can impact the behavior of the facility structure foundations and result in failures. The facility's foundations should be evaluated to address any potential structural concerns. Seismic events can cause secondary events, such as failure of ground slopes near the facility structure, tsunamis, and seiches, which can result in additional flooding concerns, facility fires, explosions, deflagrations, and unwanted interaction between SSCs in the facility.

NPH requirements for seismic events are provided in Chapter 3 of DOE-STD-1020-2016. The unmitigated accident analyses performed for the facility determines the SDC of the SSCs, which, in conjunction with a proper seismic hazard analysis, defines the size of the seismic event to be used to design/evaluate the facility SSCs. According to DOE-STD-3009, accident analysis for a seismic event is intended to determine the unmitigated consequences of release of the radioactive and/or toxic chemical inventory of the facility. As stated above, the results of the accident analysis determine the SDC for the facility SSCs.

The simplest evaluation of the unmitigated consequence assessment is to consider all hazardous material to be released in a seismic event, that is, all the facility MAR is included with DR=1. While this assumption may not be true in all situations, the analyst should justify taking an approach that does not not make this bounding assumption.

The initial conditions and assumptions for the analysis are documented and evaluated to determine if controls are needed to maintain the validity of the evaluation. If the presence of an assumed passive SSC prevents significant consequences, it is evaluated for classification as either SS or SC (see section A.3 in Appendix A of DOE-STD-3009-2014). Earthquake experience information or previous seismic evaluations of similar SSCs may be used to estimate the extent of MAR and DR for each SSC. These judgments of damage, MAR, and DRs should be determined working with the discipline engineers responsible for the seismic design and evaluation. Accordingly, to analyze the seismic event, the analyst should:

1. Define the scenarios;
2. Identify the type of material involved and appropriate MAR, DR, and LPF (for mitigated scenarios only);
3. Determine the unmitigated consequences;

4. Determine the SSCs which will be used to mitigate or prevent the consequences; and
5. Define the SDC for the SSCs that mitigate or prevent the consequences.

4.6.4 EXTREME WIND EVENTS

Extreme wind events can be straight-line winds, tornado, or hurricane. A tornado can also insult a SSC from a rapid atmospheric pressure change. NPH requirements for extreme wind events and evaluation of SSC capabilities or damages is provided in Chapter 4 of the DOE-STD-1020-2016. The unmitigated accident analyses performed for the facility determines the Wind Design Category (WDC) of the SSCs, which, in conjunction with a proper extreme wind hazard analysis, defines the size and return period of the extreme wind event to be used to design and evaluate the facility SSCs.

According to DOE-STD-3009, accident analysis for a wind event is intended to determine the unmitigated consequences of release of the radioactive and/or toxic chemical inventory of the facility. As stated for seismic events, the results of the accident analysis determines the WDC for the facility SSCs. For extreme wind events, if properly designed in accordance with the requirements of DOE-STD-1020-2016, the facility structure can usually be considered to protect the systems and components inside of it. This is dependent on the number of openings in the facility structure, which could result in internal wind-induced pressures on the systems and components inside of it. The facility structure's failure should be considered in determining the unmitigated consequences of the release of the hazardous material to the environment.

The initial conditions and assumptions for the analysis are documented and evaluated to determine if controls are needed to maintain the validity of the evaluation. If the presence of an assumed passive SSC prevents significant consequences, it is evaluated for the need to classify as either SS or SC (see section A.3 in Appendix A of DOE-STD-3009-2014). Wind experience information or previous wind evaluations of similar SSCs may be used to estimate the extent of MAR and DRs for such SSCs. These judgments of damage, MAR and DRs should be determined working with the discipline engineers responsible for the wind design and evaluation.

SSCs located outside of the facility structure are also susceptible to the extreme winds and associated missiles. The failure of these SSCs should also be considered in the accident and consequence analyses. To analyze the extreme wind event, the analyst should:

1. Define the scenarios;
2. Identify the type of material involved and appropriate MAR, DR, and LPF (for mitigated scenarios only);
3. Determine the unmitigated consequences;
4. Determine the SSCs which will be used to mitigate or prevent the consequences; and
5. Define the WDC for the SSCs that mitigate or prevent the consequences.

4.6.5 FLOOD AND PRECIPITATION EVENTS

Flood events for a facility can result from several sources, such as river flooding, dam, levee, or dike failure, storm surge, tsunami, seiche, landslide, extreme precipitation (both rainfall and snow/ice) run-off, and extreme precipitation loading on roofs, parapets, or outside utilities. Floods can also cause water-borne debris impacts which should also be considered.

NPH requirements for floods and extreme precipitation events are provided in Chapters 5 and 7 of DOE-STD-1020-2016. The unmitigated accident analyses performed for the facility determines the Flood

Design Category (FDC) of the SSCs which, in conjunction with a proper flood hazard analysis, defines the size of the flood event to be used to design/evaluate the facility SSCs. For dry sites, which are defined as sites that have no external flood threat outside of extreme precipitation, the unmitigated accident analyses performed for the facility determines the Precipitation Design Category (PDC) of the SSCs which, in conjunction with a proper extreme precipitation hazard analysis, defines the size of the extreme precipitation event to be used to design/evaluate the facility SSCs.

According to DOE-STD-3009, accident analysis for a flood or extreme precipitation events is intended to determine the unmitigated consequences of release of the radioactive and/or toxic chemical inventory of the facility. As stated for seismic and extreme wind insults, the results of the unmitigated accident analyses determine the FDC and PDC for the facility SSCs.

For flood and extreme precipitation events, if properly designed in accordance with the requirements of DOE-STD-1020-2016, the facility structure can usually be considered to protect the systems and components inside the facility structure. This is dependent on the number of openings in the facility structure, which could result in inflow of flood water. The facility structure's failure should be considered in determining the unmitigated consequences of the release of the hazardous material in the facility. The initial conditions and assumptions for the analysis are documented and evaluated to determine if controls are needed to maintain the validity of the evaluation. If the presence of an assumed passive SSC prevents significant consequences, it is evaluated for the need to classify as either SS or SC (see section A.3 in Appendix A of DOE-STD-3009-2014). Flood and precipitation experience information or previous flood and precipitation evaluations of similar SSCs may be used to estimate extent of MAR and DRs for such SSCs. These judgments of damage, MAR, and DRs should be determined working with the discipline engineers responsible for the flood and extreme precipitation design and evaluation. Some SSCs, even though capable of withstanding mechanical loads from flood water, may fail to perform their safety function when subjected to water intrusion or inundation. These modes of failure should also be considered in performing flood and extreme precipitation hazard evaluations.

SSCs located outside of the facility structure would be susceptible to the flood, extreme precipitation, and associated water debris. The failure of these SSCs should also be considered in the accident and consequence analyses.

To analyze the flood and precipitation events, the analyst should:

1. Define the scenarios;
2. Identify the type of material involved and appropriate MAR, DR, and LPF (for mitigated scenarios only);
3. Determine the unmitigated consequences;
4. Determine the SSCs which will be used to mitigate or prevent the consequences; and
5. Define the FDC and PDC for the SSCs that mitigate or prevent the consequences.

4.6.6 LIGHTNING EVENTS

Chapter 6 of DOE-STD-1020-2016 is focused on NPH design criteria and does not provide a detailed discussion about the effects of lightning events or guidance regarding the safety analysis. Accordingly, the following additional guidance is provided with respect to the DSA evaluation.

Lightning is a high-current electrical discharge in the atmosphere with a path length measured in kilometers. Natural lightning is almost always associated with clouds, normally those of severe weather (e.g., thunderstorms), but can also be present in volcanic clouds and clouds from dust storms.

Assessing the severity and frequency of lightning strikes at, or nearby, a site is essential because lightning can:

- Start a fire inside a building, outside of a building but within the industrial area, or on the area surrounding the industrial area of a site; fire can also arise from contact of combustibles with a lightning-heated non-combustible;
- Can start a wildland fire at sites surrounded by forests intense enough to breach site barriers;
- Breach a building, providing an open pathway for radioactive or other hazardous substances to be released into the atmosphere;[35] and
- Cause failure of sensors, communications and electronic components, and power supply systems.

The analyst can consult a map of the United States given in the *Standard for Installation of Lightning Protection Systems*, NFPA 780 (NFPA, 2017).[36] NFPA 780 provides an Annex L, Lightning Risk Assessment, which may be applied in the facility FHA when determining the requirement to install a lightning protection system. Per NFPA 780 Section L.1.4, "Lightning risk for a structure is the product of the lightning frequency, exposure vulnerability, and the consequence of the strike to the structure or object." The results of the lightning frequency calculation can be directly used to estimate the DSA likelihood of a strike to the facility. This frequency calculation relies on local ground flash density data as referenced in NFPA 780 and other factors such as the footprint of the facility ("equivalent collection area") to estimate the" annual threat of occurrence (lightning strike frequency)." The NFPA risk assessment methodology also estimates a "tolerable lightning frequency" and "acceptable frequency of property loss" based on other considerations, and these frequency estimates should not be used for the DSA determination of the likelihood. The DSA likelihood determination may further modify the annual threat of occurrence lightning strike frequency to estimate the likelihood of a lightning-induced fire or fire from a lightning-induced wildland fire based on facility-specific justifications.

The severity of a lightning flash is usually defined by the peak amplitude of its return stroke current, which range from one to hundreds of kA. The upper one-percentile current (i.e., 99 percent of all lightning flashes have a lower current) has been determined to be about 200 kA. Lightning scientists identify this level of current as the severe threat level. The 50th percentile value lies in the 20-30 kA range.

For flat terrain without buildings or other structures, the probability of a lightning strike is the same throughout the area. However, structures, especially tall ones such as stacks, water towers, and power poles, are more likely to attract lightning and thus increase the probability of a strike at those locations, while concomitantly decreasing the probability at other nearby locations. These taller structures provide some protection for nearby shorter structures. The extent of this protection, however, is not readily quantifiable except for properly grounded conductive structures (or buildings protected by a code-compliant Lightning Protection System). Elevated conducting wires that are horizontal and grounded can also protect facilities below them. Power lines could therefore be considered to provide some protection for certain buildings. In general, the stacks, water towers, and power lines may offer protection for only a

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[35] Because filter plenums are electrically conductive, they can attract lightning and can therefore be breached by lightning even within a building. This phenomenon would provide another leak path to the environment as well as a hazard to personnel within the building.

[36] This standard was originally issued as NFPA 78, *Lightning Protection Code*.

small portion of an industrial area.

If a particular facility is not protected, the expected number of lightning strikes per year can be determined by multiplying the footprint area of the facility by the lightning strike density applicable for the site. This quantitative estimate of the annual frequency of lightning strikes to the facility can then be used to qualitatively assign a hazard scenario likelihood as suggested on Table 2-9.

Not every lightning strike is damaging to structures. The amount of structural damage depends on the amount of current in the return stroke, the magnitude of any continuing current, and the susceptibility of the target to lightning damage. Electronic equipment, for example, is more susceptible to failure from a lightning strike than a concrete pad is to fire damage. The main danger from lightning for the site is from fire, as fire can potentially lead to a release of radioactive or toxic chemic material. Lightning-induced fire can be caused in several ways:

1. Fire can be started in dry combustible material, such as a wooden structure or dry grass, by the weak "continuing current" between lightning strokes.[37] About 20 percent of the lightning strikes have a continuing current large enough to start such a fire (Hasbrouck, 1989). The magnitude of the peak current is not relevant for this circumstance, as the return stroke is too brief to start a fire. This type of fire will be mainly confined to wildland fires and wooden power poles, unless there are wooden structures on the site and a lack of a requirement that any wood brought onto the site be treated with fire retardant. Range fires can occur only when the wildland grass is dry during drought conditions. Lightning-induced wildland fires should be anticipated. In addition, power poles have been set on fire by lightning, showing that this type of fire also needs to be anticipated.

2. If a facility is constructed of non-combustible building materials, a so-called Highly Protected Risk (HPR) facility, or if it is constructed as a Faraday cage, the frequency of a lightning-induced in-facility fire is qualitatively assessed as *extremely unlikely*, whether or not the facility has a properly functioning lightning protection system, unless the NFPA 780 lightning risk assessment determines that the probability of a lightning strike is so small that a lightning protection system is not required by the code.

3. For a facility that has a code-compliant lightning protection system that can perform its designed function as determined by the FHA or Fire Protection Engineering, a qualitative reduction of one likelihood bin for the mitigated analysis may be taken for lightning-induced in-facility fires. This is based on the general rule of thumb discussed in Section 2.5.2, Qualitative Likelihood, for failure of a SSC.

4. A lightning strike on a building can induce large currents in the electrical wiring in the building. It is possible that the high current will cause a breakdown in both the insulation on the wiring and the insulation provided by the air, causing an electrical arc to form between the wire and a nearby grounded object. (This is called a "side-flash.") A follow-on current from the electrical circuit would then sustain the arc and could continue for many seconds or even minutes, long after the lightning strike is gone. Combustible material in the immediate vicinity could then be ignited. Although arcing is more likely with the larger-current strikes, any magnitude of strike should be considered. This type of fire for facilities without functional lightning protection systems should

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[37] The continuing current will probably not start a fire within a concrete structure or Butler-type building.

be considered as the same likelihood as determined above from the NFPA 780 method.

5. A lightning-induced spark in the building could ignite volatile gases, such as from rags damp with cleaning fluids. This could occur with a lightning strike of any magnitude current. This type of fire may thus be considered *less likely* for facilities with functional lightning protection systems depending on process-specific and facility-specific considerations.

For DOE facilities performing explosive operations, and/or handling nuclear weapons, lightning represents an additional hazard. For a more complete discussion, refer to Chapter X of DOE-STD-1212-2012, *Explosives Safety*. Lightning presents a hazard to explosives in at least five ways:

1. The electrical current produced by a voltage gradient resulting from a lightning strike could initiate the explosives directly.

2. The surface flashover or arcing of the generated electrical current between conductive surfaces that are not at equilibrium could initiate the explosives directly by the heat, sparks, and molten metal generated by the arc.

3. This same arcing could cause damage or fires in electrical fixtures and equipment.

4. Lightning could initiate a fire involving combustible materials in the facility, including the containers around explosives.

5. The spalling generated by the heat of the current flowing through the structural components of the facility could initiate, by impact, unprotected explosives. In addition, lightning could affect support systems such as fire protection and security. Lightning can reach a structure not only by direct strike, but also indirectly by coupling to a conductor that penetrates the structure.

From this information the analyst can determine the potential impact of lightning strikes on hazardous materials. The methodology to analyze lightning-initiated accidents is to:

1. Define the scenario;
2. Estimate the damage to facility SSCs and support systems from lightning strikes;
3. Identify materials and appropriate MAR, DR, and LPF (for mitigated scenarios only); and,
4. Calculate the radiological or toxic chemical consequences for this type of event.

4.6.7 VOLCANIC ERUPTION AND ASHFALL EVENTS

Volcanic eruption events can pose a number of hazards to facilities such as ashfall (“tephra”), lava flows, ballistic projections, pyroclastic flows, mudflows, low-level seismic activity, ground deformation, tsunami, atmospheric effects, and emission of gasses that can result in acid rains. For existing DOE sites, the primary volcanic hazards are from ashfall. Designing facilities to withstand any other volcanic hazard is not feasible, and such hazards should be mitigated by siting facilities far enough from active volcanoes to preclude being affected by these hazards. The primary issues with ashfall are the potential clogging of ventilation systems and equipment exhaust, structural roof loading, and other concerns include disruption or shorting of electrical equipment and interference with emergency response.

Volcanic eruptions may pose hazards to select DOE sites in the western United States. For practical application, volcanic hazards are assessed at DOE sites and facilities lying within 400 kilometers of a volcanic center that erupted within the geologic Quaternary Period (i.e., 2.6 million years before present).

Chapter 8 of DOE-STD-1020-2016 provides NPH requirements for volcanic eruption events. The unmitigated accident analyses performed for the facility determines the Volcanic Design Category (VDC) of the SSCs, which, in conjunction with a proper volcanic hazard analysis, defines the size of the volcanic-induced event to be used to design/evaluate the facility SSCs.

According to DOE-STD-3009, accident analysis for a volcanic eruption event is intended to determine the unmitigated consequences of release of the radioactive and/or toxic chemical inventory of the facility. As stated above, the results of the accident analyses determine the VDC for the facility SSCs. For volcanic eruptions, the facility structure can usually be considered to protect the systems and components inside the facility structure with the exception of the potential clogging of ventilation systems from ashfall which have openings to the outside of the facility structure. The facility structure's failure should be considered in determining the unmitigated consequences of the release of the hazardous material in the facility.

SSCs located outside of the facility structure could be susceptible to the volcanic ashfall and potential extreme rainfall induced by the volcanic eruption. The failure of these SSCs should also be considered in the accident and consequence analyses.

To analyze the volcanic ashfall events, the analyst should:

1. Define the scenarios;
2. Identity the type of material involved and appropriate MAR and DR (for mitigated scenarios only);
3. Determine the unmitigated consequences;
4. Determine the SSCs which will be used to mitigate or prevent the consequences; and
5. Define the VDC for the SSCs that mitigate or prevent the consequences.

4.6.8 WILDLAND FIRES

Wildland or range fires (also called wildfires) present an external exposure to site facilities, and as such, their potential severity needs to be evaluated. The potential severity of a wildland fire may be assessed through an analysis of the chief factors that contribute to its growth and spread. These factors include the characterization of the fuel available, the terrain, and environmental conditions. The damage potential from a wildland fire is dependent on factors such as including the construction of potential target structures, spatial separation distances, existing automatic fire suppression, and the effectiveness of the responding fire fighters.

A wildland fire in the site buffer zone or exclusion area of the DOE site may threaten the structural integrity (i.e., MAR confinement capabilities) of site facilities located in this region, as well as facilities located in the site's industrial area that normally have minimal or extremely limited vegetation. The fire may spread by flame or radiative heat from building-to-building, or it may be spread to various building roofs by flying brands. Wildland and other fire hazard potentials are addressed in a facility FHA. (See Appendix B of DOE-STD-1066-2016, *Fire Protection*, for details.) An FHA analysis of wildland fire potential should be incorporated into the DSA. The following section details the methods available to subject matter experts in determining wildland fire potential.

4.6.8.1 WILDLAND FIRE EVENT DESCRIPTION AND ANALYSIS

Wildland fires may be caused by various natural and human initiators. These initiators include lightning, human action, mechanical incidents, and an explosion and/or fire at an off-site facility. Lightning can occur any time of the year; however, it is primarily a spring and summertime phenomenon. Human action-caused incidents include improper disposal of smoking materials, poor control of a campfire, hot work, prescribed burns, ignition by tracer fire during training, ignition by explosives during training, carelessness, and arson. Mechanical incidents include sparks generated from railways and passing automobiles.

The methodology to analyze a wildland fire is to:

1. Define the bounding scenario.
2. Identify the type of material involved and appropriate damage ratios.
3. Determine the consequences.
4. Determine appropriate design/operational criteria for the SSCs needed to prevent or mitigate the event.

Expected wildland fire intensity may be determined by characterizing the material available for combustion, such as trees, grasses, forbs (weeds), and low shrubs. Vegetation types are to be identified within the outlying areas, such as marshland, woodland, shrubland, and grassland. Other vegetation types may be located in small isolated pockets. The average plant production in terms of kilograms per hectare or tons/acre is estimated.

In the bounding scenario, a wildland fire would burn the entire area surrounding a site. Some facilities within this area (for example, those of wood construction) would be damaged or potentially destroyed. Smoke might necessitate site evacuation, road closures, and reconfiguration of building ventilation systems. In general, wildland fires are of such an extent and unpredictable nature that multiple buildings/facilities will likely be threatened, requiring fire department and other firefighting resources to be deployed accordingly.

NFPA 1144, *Standard for Reducing Structure Ignition Hazards from Wildland Fire* (2013), provides guidance for the analysis of the susceptibleness of a structure to wildland fires. The NFPA standard identifies the elements of the structure and the surrounding environment that require evaluation. These elements contribute to the safety analyst's understanding and selection of controls for the mitigated analysis.

NFPA 1144 provides an example hazard assessment in its Table A.4.1.2, "Example of Structure Assessment Rating Form." The five areas of evaluation are:

- Overview of the surrounding environment – topography, weather, and surrounding structures;
- Chimney to eaves – roof construction, skylights, and roof attachments;
- Top of exterior wall to foundation – wall construction, openings and penetrations;
- Foundation to Immediate Landscaped Area (ILA)[38] – vegetative fuels and other combustibles around the structure, heat and flame sources, other structures and vehicle parking within 30 ft;

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[38] ILA definition: "The area of the structure ignition zone extending at least 30 ft (9 m) from the foundation of the structure, including the footprint on decks and all extensions, and the area in which vegetation has been modified for reduced flammability or aesthetic purposes, such as lawns and gardens." This area is often referred to as "defensible space."

- ILA to the extent of the Structure Ignition Zone (SIZ) [39] – vegetation, heat and flame sources, and vehicle parking between the outer edge of the ILA and the extent of the SIZ.

The FHA application of this hazard assessment methodology will result in four hazard ratings that can be used to aid in assessing the likelihood of a wildland fire causing a release of radiological or hazardous chemical MAR. The evaluation areas also aid in identifying existing passive design features that may be credited in the DSA unmitigated hazard evaluation or accident analysis or may need to be improved to provide the necessary protection of MAR. This NFPA methodology may be used to perform iterative analysis as well since it identifies controls (e.g. vegetation control/treatment within the SIZ).

This Handbook provides some amplifying information on the NFPA 1144 table (highlighted in yellow in the example that follows) for use by fire protection subject matter experts in the DSA development/ revision process. Annex A of NFPA 1144 provides additional detailed explanatory information that may provide insights into assigning a value where a range of values is provided. If not obvious, assigned values should be documented with a basis either within the cell or use of footnotes, as illustrated in the example provided in the next subsection.

Building design, location and construction standards that reduce structural susceptibility to wildland fires are provided in Chapter 5 of NFPA 1144, in NFPA 1141 (2017), *Standard for Fire Protection Infrastructure for Land Development in Wildland, Rural, and Suburban Areas*, and in local building codes. Section 4.2.5.8 of NFPA 1144 states, "Any structure that fails to comply with the requirements of Chapter 5 shall be deemed to increase the risk of the spread of wildland fire to improved property and the risk of fires on improved property spreading to wildland fuels."

Some additional sources of guidance for fire hazards analysis, building design and construction, exterior exposure protection, and wildland fire management are:

- DOE-STD-1066-2016, *Fire Protection*, was developed to address the special or unique fire protection issues at DOE facilities and includes guidance (and additional references) for wildland fire management and facility design against wildland fire exposures. Specifically, Chapter 8 addresses wildland fires.

- NFPA 801 (2014), *Fire Protection for Facilities Handling Radioactive Materials*, addresses fire protection requirements intended to reduce the risk of fires and explosions at facilities handling radioactive materials. NFPA 801, Section 5.5 specifically states, "Buildings in which radioactive materials are to be used, handled, or stored shall be fire-resistant or noncombustible construction in accordance with NFPA 220, *Standard on Types of Building Construction*, Type I or Type II construction."

- NFPA 80A (2012), *Recommended Practice for Protection of Buildings from Exterior Fire Exposures*, provides guidance on fire exposure hazards. NFPA 80A, Chapter 4 provides guidance for determining minimum building separation distances, and Chapter 5 identifies various means by which facilities may be protected from fire damage due to exterior exposure.

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[39] SIZ definition: "The "ignition zone" includes the area around a specific structure and associated accessory structures, including all vegetation that contains potential ignition sources and fuels that can affect ignition potential during an intense wildland fire." The zone extends 0–200 ft (0–60 m) out from a structure's foundation.

- NFPA 1143 (2014), *Standard for Wildland Fire Management,* provides guidance that aids in the development of wildland fire management programs, which include the full range of activities and functions necessary to plan, prepare, and respond to potential fires.

4.6.8.2 EXAMPLE: WILDLAND FIRE FACILITY/STRUCTURE HAZARD ASSESSMENT

A simple example of the application of the Wildland Fire Facility/Structure Hazard Assessment is presented in Table 4-11. For this example, the most significant characteristics of the facility are listed below. However, for specific facilities, additional detailed information should also be available. The values for the hazard risk ratings and the Hazard Rating Scale are established in NFPA 1144. For each of the example characteristics listed below, cross-references are provided as a brief basis for the selected values in Table 4-11. Note that the evaluated characteristics include existing facility controls.

Topographical Features (TF):

- The facility location is in a semi-arid region {evaluated as identified by TF1}
- The region has a history of wildland fires (about 1 every 10 years) {justifying a relatively high rating of 4 as shown for TF2};
- The surrounding environment is timberland (mostly ponderosa pine) and grassland with minimal slash or undergrowth due to regular forest management, thus there is moderate wildland combustible material present {evaluated as identified by TF3}.
- The location may be subjected to significant straight, dry winds, as well as thunder/lightning storms {supporting values identified by TF4}.
- The nearest sloping grade of greater than 15% is more than 400 ft from facility, except for the northerly direction where a slope of 15% to 20% begins at 30 ft from the facility and continues out several hundred feet {thus resulting in relatively low values for the evaluations of topography slope (rating range from 0 to 15) and the Building Setback (rating range of 0 to ~5) for which slopes greater than 30% are several hundred feet away; evaluations are identified as TF5}.
- A neighboring structure is a single story transportable building of combustible materials with an attached wood deck with no underpinning or screening. This structure is 60 to 70 feet away {evaluated as a moderate risk of 3 (for a risk factor range of 0 to 5) for separation of structures as shown by TF6}.

Fuel Modifications and Vegetation (FM):

- Large trees have been removed and the brush is thinned out to a distance of at least 210 ft. Trees and brush are removed out to 100 ft, leaving primarily grasses and forbs. {This fuel modification treatment significantly reduces the flame and radiative heat threat to the structure from the SIZ, justifying very low values from 30 to 100 feet; when properly performed it may be judged to support the low values identified by FM1}.
- A controlled defensible space, concrete slab, is provided for a minimum of 30 ft from the foundation of the structure in all directions {essentially eliminating combustibles and justifying a value of 0 for FM2; without this defensible space the hazard risk would significantly increase}.

Building Construction (BC):

- Although the concrete structure of the walls are 1 to 2 hour fire resistance capable, multiple penetration seals in several concrete walls are not fire-rated, resulting in fire resistance vulnerabilities in the exterior walls {judged for this example to pose a significant fire propagation risk into the building and thus elevated value of 9 for the siding identified by BC1};

- There are no skylights in the roof and the facility roof has been evaluated by fire protection engineering and is considered to meet UL Class A/FM Class 1 requirements (i.e., provides adequate fire resistance, supporting a very low risk evaluation shown by BC2);
- Large external ventilation fan suction and discharge duct openings are not covered by metal screening, making it possible for sparks or fire brands to reach combustible ventilation filters (hence a high hazard value of 20 is assigned as shown by BC3);
- Existing gutters are constructed of metal (supporting a very low risk evaluation shown by BC4);

Additional Fuel Modifications Relevant to Fire Hazards (FM):

- Vehicles are parked within the SIZ on paved parking lots clear of vegetation. (FM3)
- The facility is equipped with a concrete dock (deck) for equipment and material shipping and receiving. (FM4)
- No vehicles are parked or left unattended within 30 ft of the facility. (FM5)
- No other significant combustibles are permanently located or stored within 30 ft of the facility. (FM6)

Additional Fire Risk Factors (FF):

- An above ground, dry transformer (1750 kVA) is located approximately 50 feet away from the building exterior, stepping down 13.8 kV commercial power to 600 V electrical service for the facility (evaluated as a moderate utility fire hazard shown as FF1). There is no gas service to this facility.

Fire Protection System (FP):

- Facility is equipped throughout with an NFPA-compliant wet-pipe sprinkler fire suppression system (therefore the building can be considered fully protected, resulting in a 0 hazard rating under the Fixed Fire Protection category identified as FP1).

Table 4-11. Example Application of Wildland Fire Facility/Structure Hazard Assessment

Analyzed Parameters	**Environment ‡**	**Building Structure ‡**		**Landscape/Combustibles ‡**	
Rating Values by Areas Assessed	Overview of Surrounding Environment (4.2.1*)	From Chimney to Eaves (4.2.2*)	From Top of Exterior Wall to Foundation (4.2.3*)	From Foundation to ILA (0 to 30 ft) (4.2.4*)	From ILA to Extent of SIZ (30 to 200 ft) (4.2.5*)
Topographical Features					
Topographical features that adversely affect wildland fire behavior (4.2.1*)	3 {TF1, TF3, TF5, general judgement}				
Areas with history of high fire occurrence (4.3.4*)	4 {TF2}				

Analyzed Parameters	**Environment ‡**	**Building Structure ‡**		**Landscape/Combustibles ‡**	
Rating Values by Areas Assessed	Overview of Surrounding Environment (4.2.1*)	From Chimney to Eaves (4.2.2*)	From Top of Exterior Wall to Foundation (4.2.3*)	From Foundation to ILA (0 to 30 ft) (4.2.4*)	From ILA to Extent of SIZ (30 to 200 ft) (4.2.5*)
Areas exposed to unusually severe fire weather and strong, dry winds (4.2.1.3*)	5 {TF4}				
Local weather conditions and prevailing winds (4.2.1.2*)	4 {TF4}				
Separation of structures on adjacent property that can contribute to fire spread/behavior (4.2.1.3*)	3 {TF6}			0 {TF6}	3 {TF6}
Vegetation—Characteristics of predominant vegetation					
Light (e.g. grasses, forbs, sawgrasses, and tundra) NFDRS Fuel Models** A, C, I, N, S, and T	5 {TF3, FM1}			0 {FM2}	0 {TF3, FM1}
Medium (e.g. light brush and small trees) NFDRS Fuel Models** D, E, F, H, P, Q, and U	0 {TF3, FM1}			0 {FM2}	5 {TF3, FM1}
Heavy (e.g. dense brush, timber, and hardwoods) NFDRS Fuel Models** B, G, and O	0 {TF3, FM1}			0 {FM2}	0 {TF3, FM1}
Slash (e.g. timber harvesting residue) NFRDS Fuel Models** J, K, and L	0 {TF3, FM1}			0 {FM2}	0 {TF3, FM1}
Topography					
Slope 5-9%				0 {TF5}	0 {TF5}
Slope 10-20%				4 {TF5}	2 {TF5}
Slope 21-30%				0 {TF5}	0 {TF5}
Slope 31-40%				0 {TF5}	0 {TF5}
Slope >41%				0 {TF5}	0 {TF5}
Building Setback, relative to slopes of ≥ 30%					
≥30 ft (9.14 m) to slope	NA {TF5}				
<30 ft (9.14 m) to slope	NA {TF5}				
Roofing Materials and Assembly, nonrated***		0 {BC2}			
Ventilation Soffits, without metal mesh or screening		20 {BC3}			

Analyzed Parameters	**Environment ‡**	**Building Structure ‡**		**Landscape/Combustibles ‡**	
Rating Values by Areas Assessed	Overview of Surrounding Environment (4.2.1*)	From Chimney to Eaves (4.2.2*)	From Top of Exterior Wall to Foundation (4.2.3*)	From Foundation to ILA (0 to 30 ft) (4.2.4*)	From ILA to Extent of SIZ (30 to 200 ft) (4.2.5*)
Gutters, combustible		0 {BC4}			
Building Construction (predominant)					
Siding and Deck—noncombustible/fire-resistive/ignition-resistant ††			9 {BC1, FM4}		
Siding—noncombustible/fire-resistive/ignition-resistant siding, but Deck—combustible ††			NA {BC1, FM4}		
Siding and Deck—combustible ††			NA {BC1, FM4}		
Fire resistance of wall components (e.g. doors, windows, and penetrations) are also considered in the building construction evaluation. Value (0 to 9) of item 1 above may increase up to 9 based on extent of vulnerabilities created in the walls. Likewise the value (10 to 14) of item 2 may increase up to 14 due to vulnerabilities.					
Fences and Attachments					
Combustible					
Non-combustible			1.	NA {None}	
Placement of Gas and Electric Utilities					
2. One underground, one aboveground	3 {FF1}				
Both aboveground					
Both underground					
Fuel Modifications within structure ignition zone					
71-100 ft (21-30 m) of vegetation treatment from the structures	3.				0 {FM1, FM3}
30-70 ft (9-21 m) of vegetation treatment from the structures					0 {FM1, FM3}
<30 ft (9 m) of vegetation treatment from the structures				0 {FM2, FM5, FM6}	
Note: Evaluate the presence and location of heat sources, flame sources and vehicle parking from the foundation to the ILA (4.2.4.2 and 4.2.4.5*) and throughout the SIZ (4.2.5.3 and 4.2.5.5*). For example, even with no vegetation in the Defensible Space (<30 ft), the presence of fuel, heat and flame sources (e.g. propane tanks, parked vehicles, combustible waste containers) could be sufficient cause to result in a high evaluation value of 15.					

Analyzed Parameters	**Environment ‡**	**Building Structure ‡**		**Landscape/Combustibles ‡**	
Rating Values by Areas Assessed	Overview of Surrounding Environment (4.2.1*)	From Chimney to Eaves (4.2.2*)	From Top of Exterior Wall to Foundation (4.2.3*)	From Foundation to ILA (0 to 30 ft) (4.2.4*)	From ILA to Extent of SIZ (30 to 200 ft) (4.2.5*)
Fixed Fire Protection (NFPA 13, 13R, or 13D sprinkler systems)					
No Protection					
Protected	4.		0 {FP1}		
TOTALS	**27 (Moderate)**	**20 (Moderate)**	**9 (Slight)**	**4 (Slight)**	**10 (Slight)**
Hazard Rating Scale (Total the above individual ratings and compare the totals to scale below for an estimated structure ignition hazard (probability) from Wildland Fire.					
Slight	0-14	0-14	0-14	0-14	0-14
Moderate	15-29	15-29	15-29	15-29	15-29
Significant	30-49	30-49	30-49	30-49	30-49
Severe	≥50	≥50	≥50	≥50	≥50
Note: The estimated hazard rating of structure ignition should be used as a guide to aid in determining scenario/event frequency in the DSA hazard analysis. Each of the individual columns (areas of evaluation) above assess a group of features/controls that reduces the likelihood that a wildland fire will breach the facility external structure. The likelihood that the structure will be breached by the wildland fire is determined primarily by the most vulnerable feature (highest column value). For this example, the assessed hazard rating of structure ignition is Moderate. The hazard rating of structure ignition should be used as an input to the DSA HA qualitative selection of wildfire event frequency (unmitigated and mitigated) while considering other factors (e.g. location and containment of MAR, credited controls).					
‡ The gray shaded areas of the table are not applicable (NA) to the "Analyzed Parameters" listed in column 1. * Ref. NFPA 1144, 2013 Edition ** National Fire Rating Danger System (NFDRS) Fuel Models correspond to the type of vegetation/forest surrounding the facility. *** Additional information on roof ratings and the impacts of firebrands to facility roofs may be found in LA-UR-14-27684, *Analysis of Wildland Fire Hazard to the TWF at Los Alamos National Labs* (Gilbertson, 2014). †† The NFPA Table A.4.1.2 provides numerical and value rankings (low, medium, high). The user is urged to assign the value ranking of low, medium, or high based on the other ignition factors prevalent at the assessment site. For example, a deck made of combustible materials might rank low if it is small in size and the rest of the site is in a low fuel loading area that will not promote a large amount of firebrands. That same deck might rate high if it is in an area of high fuel loading that will promote numerous firebrands. Numeric values can be substituted as a local option. [Ref. NFPA 1144, 2013 Edition] For this Handbook, using a range of numerical values is presented as a means to address the evaluation of vulnerabilities in the fire resistance of the exterior construction; thus, incorporating the evaluation of vulnerabilities with the goal of improving DOE-complex wide consistency in the final hazard rating.					

The hazard rating results of Table 4-11 for the probability that a wildland fire in the vicinity of the facility will breach the structural barrier provides input into the DSA hazards analysis likelihood determinations. This evaluation should be performed for both the unmitigated (no controls) and mitigated (controls in place) cases to provide input and justification to the unmitigated and mitigated DSA hazard analysis wildland fire scenarios, respectively. If this is not performed in the facility FHA, it could be added to the DSA hazard evaluation.

As stated in the footnote to Table 4-11, additional information on roof ratings and the impacts of firebrands to facility roofs may be found in LA-UR-14-27684, *Analysis of Wildland Fire Hazard to the TWF at Los Alamos National Labs* (Gilbertson, 2014). That reference also provides guidance on assigning likelihoods based on whether the roof is combustible or noncombustible and consideration of the wildland fire separation distance.

The design features and controls (engineering and administrative) that are assumed in Table 4-11 for the reduction of the hazard rating are carried forward to the DSA as appropriately credited or defense-in-depth controls. The evaluated characteristics in the above example that may be considered as candidate controls include the fire resistance of the exterior walls, roof rating, and defensible space configuration control.

For the radiological consequence analysis, the damage ratio for the wildland fire is facility dependent, and considers the capability of other MAR containment components to withstand the fire. ARF and RF estimates are evaluated the same as those for operational facility fires as addressed in Section 4.2. The LPF is assumed to be 1 for an unmitigated wildland fire that results in a release of MAR from a facility because the facility structural boundary is assumed to be significantly breached.

The Table 4-11 example documents the results of the FHA assessment of wildland fire, which should be interpreted and included in the FHA or referenced to a supporting analysis. The DSA Chapter 3 hazard evaluation or accident analysis would then summarize the analysis and reference the FHA, add the mitigated analysis if not already included in the FHA, and expand on how the likelihood was assigned, identify protection features, and evaluate their safety significance.

4.7 MAN-MADE EXTERNAL EVENTS

Man-made external events can cause a breach in the structure of a facility and cause a release of radioactive or hazardous materials. The following events may be evaluated in a DSA accident analysis: (1) aircraft crashes, (2) vehicle crashes, and (3) loss of power to safety-related SSCs that provide a safety function to prevent or mitigate accidents.

Additional external events may also need to be evaluated for a DSA depending on:

- site characteristics, such as nearby facilities with accident potentials that can affect the facility being evaluated,
- nearby natural gas distribution lines or other gas lines not servicing the facility,
- explosion from a train derailment (for trains not related to facility operations),
- underground transformer explosions, and
- events involving storage tanks external to the facility that are not associated with facility operations.

Some of the methods presented in this section and in earlier sections of Chapter 4 regarding fires, explosions, and loss of confinement accidents assist in evaluating these other external events, although a special engineering analysis of the accident phenomena associated with the external event may also be needed.

4.7.1 AIRCRAFT CRASHES

The analysis of aircraft crash impact involves the following steps.

1. Performing a screening analysis based upon MAR, frequency, and consequences.
2. Defining the scenario.
3. Identifying the type of material involved and appropriate DR and LPF (for mitigated scenarios only).

4.7.1.1 SCREENING ANALYSIS

Guidance and criteria for evaluating airplane crashes are given in DOE-STD-3014-2006, *Accident Analysis for Aircraft Crash into Hazardous Facilities*. The assessment is presented in three phases:

1) determination if there is enough hazardous material in the facility to pose a threat to the public or workers;

2) determination of the estimated probability per year (i.e., frequency) of an aircraft crash into a facility with hazardous materials; and

3) determination if an aircraft crash into the facility would penetrate to the location of the hazardous materials and release it into the atmosphere.

If the relevant determination in any of these three phases falls below screening guidelines, the threat of an aircraft crash is considered insignificant for that facility.

For phase one, the screening guidelines are based on the assumption of the total release into the atmosphere of all of the hazardous material in the facility from an aircraft crash. The screening criteria for the public, for example, are a radiological dose to the MOI of less than 25-rem TED and a toxicological exposure of less than PAC level 2 (PAC/TEEL-2). Similar criteria apply to the worker. If the amount of hazardous material is insufficient to reach these levels, an aircraft crash into the facility is considered insignificant and phases two and three need not be evaluated as the scenario has been screened out.

For phase two, the screening criterion is a crash frequency of less than one crash per million years into the facility. Below this frequency, aircraft crashes are not considered significant and phase three need not be evaluated (see DOE-STD-3014-2006 and DOE-STD-3009).

For phase three, the screening criteria deal with the robustness of the facility. If an aircraft or any of its parts could not penetrate to the location of the hazardous material, an aircraft crash is not considered significant for that facility.

Refer to DOE-STD-3014-2006 for details on performing these analyses. The following observations are based on experience with applying that standard at multiple DOE sites.

1. Crash probabilities are estimated separately for airport operations (take-offs and landings) from nearby airports and from overflights from more distant airports and are then summed. A variety of aircraft types regularly operate near DOE sites. These include general aviation, commercial, and

military. There are typically no special restrictions in place for the air space around and above a DOE site, although sectional charts may carry an advisory relative to flights below a certain altitude, such as 1,000 feet. Overflights occur occasionally along predefined navigational pathways (Airways). Helicopter operations should also be considered, such as from hospital "Flight-For-Life" and spraying operations. Site-supervised overflights may also be performed by rotary-wing and fixed-wing aircraft for photographic and other purposes. In addition, a nearby airport may host air shows featuring military aircraft conducting displays and acrobatic activities. Small aircraft (those that weigh less than 12,500 pounds) operating from nearby airports are major contributors to the numbers of aircraft in the vicinity of a DOE site.

Although a pilot would be expected to attempt a minimal-impact landing, data show that the pilot has no control in approximately 76% of accidents and only limited control 19% of them (Cooper and Chira-Chavala, 1998). An aircraft-fuel fire may also accompany this accident. The estimation of the probability of an aircraft accident involving a site facility is based on the air traffic associated with the nearby airports and overflights, and the aircraft crash rate. The aircraft accident rate from airport operations is estimated as the product of the number of flights and the aircraft accident rate per square mile for airport operations (Boonin, 1974; DOE-STD-3014-2006). These data provide accident probabilities for impact locations as a function of distance from an airport. The aircraft crash rate from general aviation overflights is also significant and needs to be considered.

2. For fixed-wing aircraft, the estimated annual aircraft crash frequency from airport operations is calculated from aircraft crash rate for each flight phase (take-offs, landings, and in-flights), aircraft category (general aviation or commercial), flight source, and effective area of facility, including physical footprint, skid-in area, and shadow. The values of estimated number of site-specific airport operations, for each aircraft category and flight source, are found in airport operations data (http://www.airnav.com/airports/).
3. The crash rates from general aviation, commercial, and military *overflights* are provided in Appendix B of DOE-STD-3014-2006, *Accident Analysis for Aircraft Crash into Hazardous Facilities*, for each DOE site, as well as the maximum, minimum, and average rates for continental United States. The rates for a given site are added to the rate determined from operations at nearby airports to get the total rate. For general aviation, it was found that the overflight crash data may not be accurate for a given DOE site, as the database was limited by the paucity of crash data available when DOE-STD-3014-2006 was initially prepared in 1996. It would be appropriate for the safety analyst to do a reanalysis for a given DOE site. The National Transportation Safety Board (NTSB) database should be consulted to determine the total number of crashes within a certain distance from the site. The distance chosen should be small enough to be representative of the Site, but large enough to include a sufficient number of accidents so that meaningful statistics can be derived. For sites in more heavily populated areas, the "certain distance" could be as little as 25 miles, whereas for sites in less populated areas, it could be as much as 50 miles to obtain an adequate data sample.
4. Another parameter to calculate the likelihood of an aircraft cra*shing into* a facility is the aircraft crash location conditional probability at the facility location (x,y) relative to the runway. The coordinates x and y are relative to the runway, with the origin being at the center of the runway, positive x in the direction of takeoff or landing and positive y in the direction 90° counterclockwise from positive x (i.e., to the left). The bearing of the airport from the facility (θ) from geographic north, the bearing of the runway (φ) from magnetic north, and the distance (R) between the facility and runway are needed to calculate the (x,y) coordinates of the facility from the center of the runway.

   The coordinates of a facility relative to the runway are thus

$$\boldsymbol{x = -R\,cos(\theta - \varphi)}$$

$$\boldsymbol{y = R\,sin(\theta - \varphi)} \quad \textbf{Equation 4-53}$$

The calculation of *R* is based on the differences in latitude and longitude of the facility and the referenced airport.

Runway labels are expressed as degrees azimuth /10. Thus, runway 22 has a bearing of 220 degrees azimuth and runway 4 has a bearing of 40 degrees azimuth. Runways 4 and 22 are physically the same but differ in designation depending on the direction of motion of the aircraft, with 4 being to the northeast and 22 to the southwest. Runways may also have a left/right (L/R) designation if there are two runways side-by-side with the same orientation; sometimes, C is used for Central. The true runway bearing may differ slightly from its designation. For example, runway 22 might have a bearing anywhere between 215 degrees azimuth and 225 degrees azimuth from magnetic north. The difference between geographic north and magnetic north, the magnetic declination, needs to be considered and if it is smaller than the uncertainty in the runway bearing it may be ignored. The magnetic declination can be found at National Oceanic and Atmospheric Administration National Geophysical Data Center website http://www.ngdc.noaa.gov/ngdc.html and selecting Magnetic Field Calculators.

5. The values of effective area are dependent on the dimensions of the facility and aircraft type. As the effective area depends on the side of the building the aircraft crashes into, it should be evaluated for all reasonable approach directions and the largest value used. If two adjacent buildings are spaced apart less than the wingspan of the plane, the effective area will be the combination of the two buildings.
6. For buildings that are partially protected by other buildings or a hillside, the analyst should use the building dimensions appropriate for the direction of approach of the aircraft to the exposed walls. To be conservative, assume that the aircraft will approach from the side that gives the largest unprotected target area.
7. Do not assign conditional probabilities to different parts of the plane, such as the probability of the engine hitting the building versus the wings.
8. Helicopter crashes are treated differently from fixed-wing aircraft crashes. The helicopter crash frequency into a facility is given by:

$$F_H = N_H P_H A_H (2/L_H) \quad \textbf{Equation 4-54}$$

where N_H is the number of helicopter local overflights per year at the site,
P_H is the probability of a helicopter crash (2.5E-5 per operation),
A_H is the facility footprint area,
L_H is the average length of the flight path over the site.

The term $2/L_H$ arises from the conservative assumption that the helicopter crash takes place within 0.25 miles from the centerline of the flight path. This gives a total area in which the helicopter crashes of 0.5 miles wide and L_H miles long, for a conditional probability of $1/(0.5L_H) = 2/L_H$ per square mile. If the value of L_H is not available, it can be estimated as the distance to the nearest heliport.

4.7.1.2 AIRCRAFT CRASH DAMAGE ASSESSMENT

If an aircraft crashes into the portion of a facility housing radioactive or other hazardous materials, that material could be released by an ensuing fire (Section 4.2), explosion (Section 4.3), and/or by loss of containment (Section 4.4), or potentially may cause releases from chemical reactions (Section 4.5).

4.7.2 VEHICLE CRASHES

Two types of vehicle crashes need to be considered: (1) A vehicle crashing into a facility causing a release of hazardous material from that facility; and (2) A vehicle transporting hazardous materials is damaged en route and material is released from the vehicle.

4.7.2.1 VEHICLE CRASH INTO FACILITY

The accident analysis methodology for an external vehicle crash into a facility is:

1. Identify the scenario;
2. Identify whether a fire initiator is present;
3. Identify the type and quantity of hazardous materials involved and appropriate MAR, DR, and LPF (for mitigated scenarios only); and
4. Calculate the consequences of the accident.

If a vehicle crashes into the portion of a facility housing radioactive or other hazardous materials, that material could be released by a fire (Section 4.2), explosion (Section 4.3), and/or by loss of containment (Section 4.4). The analyst should determine the likelihood of such an accident based on the location of the MAR in the facility relative to the route the vehicle would take to impact that portion of the facility. Although it may not affect the likelihood of the vehicle crash causing a release, the location of SSCs should be considered if a vehicle crash into SSCs could initiate an accident progression. Vehicles to consider would include automobiles, trucks and vans, and railroad cars if a rail line passes near the facility.

The vehicle momentum, robustness of the facility walls, amount of fuel in the vehicle (assume the maximum), any combustibles it contains, and the facility combustibles at the crash site needs to be estimated. Then, following the guidance in Sections 4.2, 4.3, and 4.4, the source term can be estimated.

4.7.2.2 ONSITE TRANSPORTATION ACCIDENT

Transportation of radioactive and hazardous materials presents special hazards to operations and to personnel at the site due to the close proximity of these vehicles to facilities and the reduced level of containment of the materials while outside buildings. These types of materials include special nuclear material (SNM), residues, TRU waste, TRU mixed waste, low-level waste, low-level mixed waste, Resource Conservation and Recovery Act (RCRA)-regulated waste, Toxic Substances Control Act (TSCA)-regulated waste, mixed TSCA waste, samples, contaminated soil, incoming bulk shipments of fuels, acids, bases, miscellaneous chemicals, compressed gases, and laboratory reagents.

The accident analysis methodology for transportation accidents is:

1. Identify the scenario;
2. Identify whether a fire initiator is present (generally, one is present if the accident involves a motor vehicle);
3. Identify the type and quantity of hazardous materials involved and appropriate MAR, DRs, and LPFs (for mitigated scenarios only); and
4. Calculate the consequences of the accident.

The analyst should examine shipping records to determine the frequency, type of material, and quantity of shipping, both on-site and to/from off-site. The shipment of bulk fuels and toxic chemicals also needs to be quantified. This would include the type of material, the total amount shipped, the average and maximum delivery size, and which facilities are involved. Each site should have an on-site transportation manual that lists the packaging configurations currently approved for on-site and off-site use. For example, no package may be used for Pu or uranium unless it has received a criticality safety evaluation and has been determined to remain subcritical. It is not uncommon for transportation accidents to occur at a site. Most of these accidents involving radioactive material transfer would not be severe, and there could be minor releases. Loading and unloading accidents are the most common and could involve forklifts.

In estimating the MAR in a transportation accident, the maximum number of packages that can fit on a truck should be assumed, unless a specific justification is stated for a different number. An example of truck capacities is shown in Table 4-12, which provides the capacities of transport vehicles for a full load of each type of package that can be hauled. Different size vehicles used at a particular DOE site for transport of containers should be evaluated. Because of the requirement to keep radiation exposure levels in the truck cab below 5-mrem/hr, these capacities are conservative for SNM and waste drums. If analysis with these capacities provides unacceptable consequences, then the truck inventory should be limited by administrative controls.

For a single drum accident, the maximum amount of material allowed by criticality limits should be assumed to be in the drum. For large numbers of drums, where the actual inventories may be vastly different from the allowed inventories, it may be acceptable to use, inventory estimates from specific process knowledge (DOE-STD-5506-2007, Section 4.3.2). However, the importance of this assumption affects the need for an administrative control to preserve it. For container types other than drums, determine the maximum amount allowed by conditions imposed on that container type.

Table 4-12. Example of Transport Vehicle Package Capacities.

Transport	Truck Bed Size	SNM and Residues		
		Number of 10-Gallon Drums	**Number of 30-Gallon Drums**	**Number of 55-Gallon Drums**
Enclosed Metal Van	7’ 7” × 12’	54	28	18
Enclosed Metal Van	7’ 7” × 13’ 9”	66	32	21
Dump Truck	7’ 6” × 15’ 10”	72	36	24
Box Van	17’ 8” × 15’ 11”	168	90	72
		LLW and Hazardous Waste		
		Number of Half-Size Crates	**Number of Full-Size Crates**	**Number of 55-Gallon Drums**
Flat Bed Trailer (for on-site transfers)	8’ × 55’	10 (weight limited)	12 (weight limited)	112
Tractor Trailer Van (for off-site shipment)	8’ 6” × 53’ or two 25’ long in tandem	10 (weight limited)	12 (weight limited)	208

The MAR released by crash should be determined depending upon the result of the event, i.e., whether it results in a fire (see Section 4.2), explosion (see Section 4.3), or loss of containment (see Section 4.4).

4.7.3 LOSS OF POWER TO SAFETY-RELATED SSCs

The accident analysis methodology for loss of power to safety-related SSCs that may provide a safety function to prevent or mitigate accidents is:

1. Identify the scenario;
2. Identify the type and quantity of materials present;
3. Identify whether a fire initiator is present; and
4. Calculate the consequences of the accident.

The NRC has requirements and guidance for a “station blackout DBA” for a commercial nuclear reactor, where station blackout means loss of AC power within a facility (i.e., loss of all onsite and offsite sources), except that battery power may be credited for the duration analyzed to ensure safe shutdown. For a DOE nonreactor nuclear facility DSA, DOE-STD-3009 requires an unmitigated analysis that does not credit any active power sources, including battery power.

Loss of power scenarios are of interest in this Handbook in terms of the potential for releases of radioactive or hazardous materials. If the safety SSC is preventive, evaluate whether the failure of the safety SSC in question (upon loss of electrical power) could cause or initiate a hazardous condition or an accident involving the release of radioactive or hazardous materials. If the safety SSC is mitigative, the analyst could consider whether failure of the safety SSC in question could occur simultaneously with other existing analyzed accident scenarios (i.e., a common cause event like NPH).

The DSA loss-of-power scenario would include loss of building support systems such as ventilation system and GB inerting are lost. When the ventilation system loses power, the ventilation fans coast-down and there may be a slight pressure gradient that favors airflow from the GB out into the module. Such air reversal is postulated to draw some radioactive material from the GB into the module. In addition, with the loss of inerting atmosphere within the GBs, a small pyrophoric fire could also be initiated within a GB.

For the loss-of-power scenario, resuspension of holdup material and exposed inventories in GBs should be evaluated. The inventory of holdup material should include quantities in the facility GBs, and ventilation ducting. A loss-of-power is also a primary initiator for loss of GB inerting, which, while it occurs slowly, increases the probability of a pyrophoric fire involving vulnerable material that may be left unpacked. If a pyrophoric fire was considered credible in the fire analysis, then a pyrophoric fire should be considered in the loss-of-power scenario as well. The MAR for the pyrophoric fire during a loss-of-power scenario should be the same as the MAR for the pyrophoric fire from the fire analysis. Another progression is the loss of purge ventilation flow that sweeps away radiolysis gases. The loss of the purge flow could lead to an accumulation of flammable gases and then an explosion.

If a loss-of-power can initiate a release of hazardous material, then these scenarios and associated controls should be evaluated in the DSA hazard evaluation and the need to develop a specific DBA/EBA determined based on potential consequences. Even in cases where loss-of-power is not identified as a separate and specific DBA/EBA, the DSA (viz. chapters 3 and 4) evaluates the need for backup power for every active safety class and safety significant SSC.

5 SOURCE TERM ANALYSIS

5.1 INTRODUCTION

This chapter addresses development of source terms for accident analysis for the evaluation of consequences to the MOI, and also quantitative evaluation of consequences to the CW, when necessary. As noted in Footnote 4 for Table 2-8, Consequence Thresholds, consequences may be estimated using qualitative and/or semi-quantitative techniques for the hazard analysis. The source term is the amount of hazardous material released to the environment from a given confinement volume under the stress posed by a hypothetical phenomenological event. The source term initially released from confinement into process areas is also of interest for evaluation of consequences to FWs.

This chapter covers application of the five-factor formula presented in Figure 5-1: MAR, DR, ARF, RFs, and LPF, as described in the DOE-HDBK-3010-94. These parameters are evaluated in terms of the stresses imposed by internal events, external man-made events, and NPHs.

Examples of the type of thought processes, bounding assumptions, and overall methodologies used in parameter determination are also provided.

5.2 RADIOLOGICAL SOURCE TERM COMPONENTS

The amount of hazardous material released as a result of accident-imposed stresses is evaluated by a prescribed formula that considers the influence of those five factors. Figure 5-1 displays those factors and their relationships. The basic concept is as follows:

MARxDRxARF = Initial Source Term (IST)

ISTxLPF = Building Source Term (BST)

and

ISTxRF = IST that is respirable

IST (respirable) xLPF = BST that is respirable[40]

The material potentially available to be affected is the MAR. The DR represents that fraction of available material actually affected by the accident stresses. The ARF represents the fraction of material actually affected that is driven airborne, either as a gas or an aerosol. Together, these three factors define the amount of material in the air at the immediate point of release, or the IST. The airborne pathway is normally the exposure mechanism evaluated as it is the principle means by which exposures at a distance from the point of release can occur. Releases to large bodies of waters are a special case where the IST would reduce to simply the MARxDR, with the DR being expressed as a total fraction of material released or a leakage rate.

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[40] The "respirable BST" that represents the MARxDRxARF/RFxLPF has been called the "five-factor formula" and is generally presented as the "Source Term (ST)" when describing the input to the radiological consequence analysis for inhalation dose calculations.

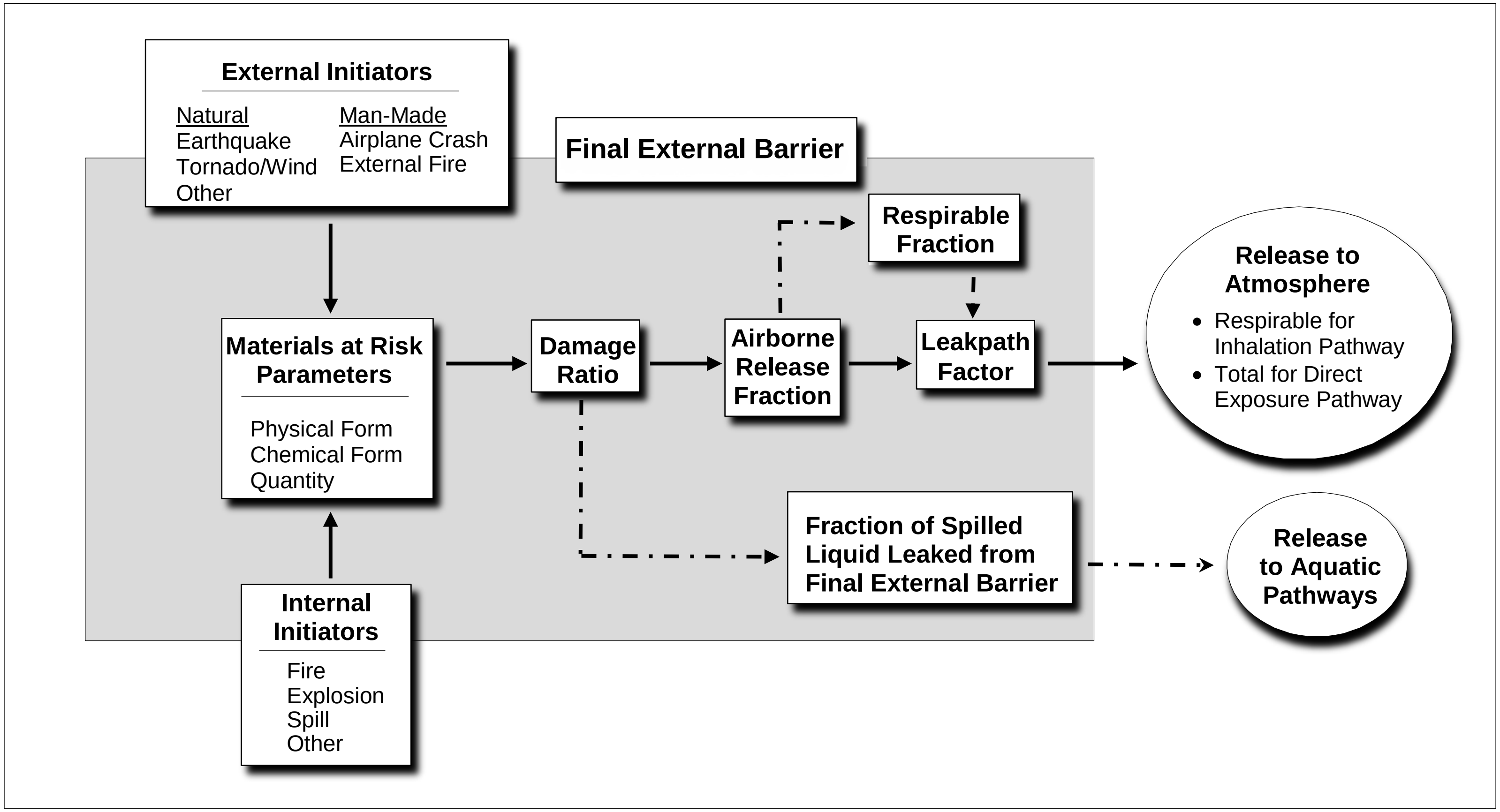

Figure 5-1. Five Factors Formula.

The RF identifies what fraction of the airborne aerosol can be inhaled and retained in the body. The responsible portion of the IST is of major interest for nuclear material handling operations as, with the exception of MAR such as tritium gas, fission products, or high energy gamma sources, most materials of concern (e.g., plutonium, uranium) are alpha-emitting radionuclides. These present no significant dose hazard outside the body. For gases, of course, the IST and the IST respirable amount are the same.

An LPF accounts for source term depletion due to filtration or deposition (“plateout”) as the source term migrates through various layers of confinement. By far the most common application of LPF is HEPA or sand filtration in exhaust ventilation. Applying all relevant LPFs yields the amount of material released to the environment, sometimes called the BST as most handling operations occur inside fixed facilities. The LPF is of interest for mitigated analysis, and is set to unity for unmitigated analysis.

5.2.1 MATERIAL AT RISK

5.2.1.1 OVERVIEW OF REQUIREMENTS, GUIDANCE, AND PRACTICES FOR IDENTIFYING MAR

DOE-STD-3009-2014, Section 3.2.4.1, provides the following direction regarding MAR:

> The MAR is the bounding quantity of radioactive material that is available to be acted upon by a given physical stress from a postulated accident. The MAR may be the total inventory in a facility or a portion of this inventory in one location or operation, depending on the event. MAR values used in hazard and accident analysis shall be consistent with the values noted in hazard identification/evaluation, and shall be bounding with respect to each accident being evaluated.

This concept is considered equally applicable to hazardous chemicals.

The MAR value assigned should be consistent with the DSA hazard identification[41] documented for a given facility or operation. That is, the DSA hazard identification used some basis to determine the maximum hazardous material accumulation foreseeable. The MAR should use that same basis. If it does not, absent some compelling explanation, the basis for either the hazard identification or the MAR designation, or both, becomes suspect. Therefore, if some compelling explanation for a discrepancy does exist, it is preferable to document the rationale for the discrepancy in both the summary section of the DSA hazard identification results and in the DSA hazard evaluation or accident analysis section.

Specifying the amount of a given material foreseeable is based on physical possibility, procedural or other administrative limits, or sampling/historical data. Physical possibility is most often used as a basis with regard to fixed volumes, such as storage vessels. In these cases, the maximum volume of material present can be precisely specified. However, there is still a need to specify the concentrations of the different radionuclides within that volume, in order to determine a bounding MAR.

Administrative limits dominate the assignment of MAR values for radioactive material handling in glovebox-type environments. These environments are constructed to allow operations within the confinement, as opposed to serving as simple holding volumes. Normal practice is to assess specific workstations, glovebox vessels, and storage containers, in terms of batch sizes, process parameters, and

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[41] Note that the DSA hazard identification values are is not necessarily the same as the initial data generated in the hazard identification activity itself. As noted in Section 2.2.2, Hazard Data Recording, the DSA hazard identification may identify bounding MAR values as opposed to maintaining a plethora of inventory limits.

criticality safety or other procedural limits.

Statistical sampling or historical data are primarily used for waste-handling and environmental cleanup activities. While some waste-handling operations will have physical upper limits for a given storage vessel such as a drum, much of the radioactive material of concern is mixed with debris, liquid or dirt and is present in very dilute concentrations. A vessel's inventory is estimated by specific process knowledge and is not exaggerated by using the full capacity with concentrated material. Likewise, the condition of residual material in cleanup efforts may not support precise specification of the quantities involved. A theoretical reconstruction based on historical data, measurement, sampling, or some combination of these is required. This is consistent with the statistical treatment of TRU waste allowed in DOE-STD-5506-2007, *Preparation of Safety Basis Documents for Transuranic (TRU) Waste Facilities*, as discussed later in this chapter.

Sometimes for simplification of accident analysis calculations it is beneficial to introduce the concept of surrogate compositions. For example, the concept can be used to establish a common inventory or tracking basis for a dose calculation. It can provide a process for accepting new material while remaining within the bounds of the accident analyses, thus allowing operational flexibility while complying with the safety basis and source strength administrative control limits. A DSA identifies and protects any significant assumptions used in deriving surrogate compositions (e.g., the fraction of combustible waste forms in TRU waste inventories, or the fraction of highly dispersible powders in glovebox operations). See Section 8.2.6, Plutonium Equivalent Curies (PE-Ci), for a further discussion of dose equivalent technique.

5.2.1.2 EXAMPLES FOR IDENTIFYING MAR

Figure 5–2 offers a simplified representation of a nuclear materials handling facility modeled off the example plutonium recovery facility in DOE-HDBK-3010-94. It consists of three glovebox processing rooms: a metal dissolution line, an ion exchange and precipitation room containing two gloveboxes, and a fuel fabrication room containing four gloveboxes. There are also two gloveboxes in a laboratory, one for handling solid samples and the other for handling liquids. Waste is stored in 55-gallon drums in a waste handling room. Finally, there are three storage vessels outside the facility: a chlorine gas supply to the laboratory, and sulfamic acid and nitric acid storage tanks. A MAR is developed for each of these operations. It is important to account for the potential accumulation of MAR throughout the process area, including piping.

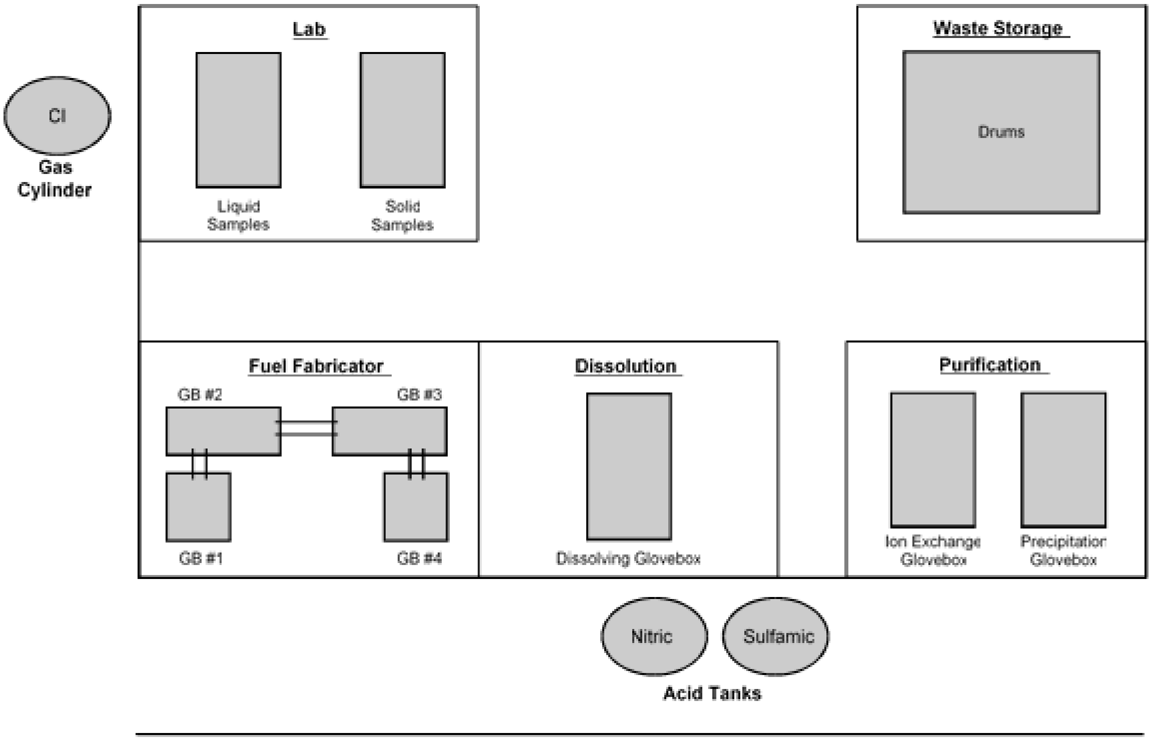

Figure 5-2. Example Nuclear Materials Handling Facility.

Note that the following discussion is for example only, and none of the fictitious quantities cited are intended to represent actual operations in any weapons complex facility.

MAR in External Storage Tanks

Simple physical possibility, with some reference to procedural limits, is used to identify the MAR for these operations. Suppose the chlorine source is a standard vendor-supplied compressed gas cylinder containing 30 pounds of chlorine. As the cylinder volume is fixed and its pressure is monitored by the supply manifold, it is not reasonable to presume a quantity of material greater than 30 pounds based on the unlikely possibility of the vendor overcharging the cylinder. Likewise, if the external acid supply tanks are sized to hold 3,000 gallons, that is maximum volume potentially present. Procedural limits factor into defining the operating concentrations desired. If 32 percent by weight nitric acid and 15 percent by weight sulfamic acid are what is supplied, these would be the values used to define density, and volatility.

Chlorine: 30 pounds in gaseous form

Nitric Acid: $3{,}000\text{gal} \times 1\text{ft}^3/7.48\text{gal} \times 74\text{lb/ft}^3 = 30{,}000$ lb of solution
$30{,}000$ lb of solution $\times 0.32 = 9{,}600$ lb of acid

Sulfamic Acid: $3{,}000\text{gal} \times 1\text{ft}^3/7.48\text{gal} \times 75\text{lb/ft}^3 = 30{,}000$ lb of solution
$30{,}000$ lb of solution $\times 0.15 = 4{,}500$ lb of acid

MAR for Dissolution Glovebox

The metal dissolution glovebox holds a small spray chamber, a 30-liter acid storage tank, a heat exchanger, a small pump, and various piping and valves. Single plutonium metal shapes are then placed in the spray chamber and dissolved by a heated acid spray recirculated from the slab tank via the following reaction:

$$Pu + 3NH_2SO_3H \rightarrow Pu^{+3} + 3NH_2SO_3^{-1} + 1.5H_2$$ **Equation 5-1**

In this case, the glovebox volume is capable of holding a great deal more material than practical operating considerations will allow. Therefore, the MAR is derived from administrative limits.

Suppose a criticality safety evaluation determined that the criticality limit for the acid storage tank is 100 g of plutonium per liter. A volume of 30 liters would then allow 3,000 g of plutonium. But further suppose that the actual pieces to be dissolved each individually contain a maximum plutonium inventory of 750 g. The critical discriminator would then be how the process is operated. If four 750 g pieces are allowed to be dissolved before the dissolving solution is sent out of the glovebox, the bounding MAR values would be as follows:

3,000 grams in liquid form, or

750 grams in solid form, or

whatever combination of both forms could result in the bounding radiological consequences.

On the other hand, if only one item can be dissolved at a time, after which the acid tank solution is sent out of the box, then 750 g of plutonium could represent a reasonable bounding value. For each accident scenario, the analyst would assume the material is in the form (liquid or solid) that maximizes the consequences for that scenario. Or the bounding value could be 1,000 grams if this limit is being normalized with the limits of other operations to provide for TSR consistency. Further, the limit might even be 2,000 grams for the entire glovebox to normalize glovebox TSR limits. There are multiple potential answers depending on how the operation is run and how material limits are apportioned.

Potential administrative burdens on facility management should be considered as well. Suppose the limit had been set at 750 g. If a campaign of unusual shapes ranging in mass up to 1,000 g becomes necessary, and there is no way to split the units into two pieces, a facility might again choose to assign a larger MAR limit for flexibility. The key point is that the limit allowed is the amount analyzed. Within reasonable bounds, there is flexibility to assume more MAR in the accident analysis than is expected to be present during operating campaigns with individual high process inventories.

MAR from Fuel Fabrication

This process takes as feedstock purified oxide powders from the ion exchange and precipitation process which takes the plutonium-bearing dissolution product. Fuel fabrication consists of four gloveboxes containing a variety of milling, blending, sintering, and fuel matrix formation stations. Assume there are 13 distinct operating stations with operating limits as follows:

Operating Limit	Number of Stations
1,000 grams	4
2,000 grams	3
3,000 grams	6

These limits yield a cumulative quantity of 28 kg of plutonium oxide for the overall room. The way in which the process is operated, however, could affect that conclusion. Suppose the process is a semi-batch operation run in campaigns. Three thousand grams (the feed of four dissolving operations) may be entered into glovebox #1, and 3,000 more grams entered when the first batch has progressed to glovebox #3. After the completion of this second batch, the process is then shut down for material control and accountability cleanup. If that is the case, then the overall MAR figure for the fabrication room could decrease to 6 kg of plutonium oxide. Again, the MAR assumed in accident analysis is a function of how facility management chooses to control the operation, and the MAR assumptions may require protection and coverage in the TSRs.

Note that to the degree individual accidents are sufficiently localized so as to affect only a subset of stations, the scenario-specific MAR might also be only a fraction of the overall total. Given the nature of the operation, there may also be a point in processing beyond which the material is no longer at risk from phenomena threatening the entire room, for example, after incorporation into a ceramic matrix. The accident analysis needs to consider station-specific form in order to fully assess vulnerability.

MAR for Waste Storage Area

The waste storage area provides temporary storage capacity for up to thirty 55-gallon drums of TRU waste. The drum limit for disposal is 80 PE-Ci. Based the fact that no drums from this facility have ever approached that level, the facility has an internal restriction of 10 PE-Ci/drum, but managed as 300 PE-Ci as a facility limit. The historical database for the facility, which covers a period of 15 years and includes a statistically significant amount of data, indicates the 95th percentile drum loading is 3.0 PE-Ci, the 50th percentile loading is 0.2 PE-Ci, and the mean loading is 0.4 PE-Ci.

Based on a maximum capacity of 30 drums, the MAR can range from a minimum of 6 PE-Ci (based on 50th percentile loading) to a maximum of 2,400 PE-Ci (based on disposal limit), while the mean loading is about 12 PE-Ci for the entire facility. That considerable range requires common sense parsing. At a minimum, the internal limit of 10 PE-Ci/drum or 300 PE-Ci for the facility is an acceptable MAR assumption for accident analysis. This is also a case where the use of statistical sampling or historical data should be considered. Even the 95th percentile drum loading is a factor of three less than the local facility limit, and the average loading is a factor of 25 less. DOE-STD-5506-2007, Table 4.3.2-1, Bounding MAR Limits for TRU Waste Operations 4, provides a statistical algorithm on how to address multiple drum accidents, except where drums with the highest inventories are commingled are segregated from the general population. Administrative controls may be (and generally are) required to protect the

MAR assumptions for a group of drums or other containers, if the analysis does not assume that every drum is loaded at the maximum allowable level. This applies to the use of the Standard 5506 statistical method, as well as other methods that do not assume the maximum inventory for each container.

The use of statistical sampling and historical data (acquired knowledge) is common in cases of old waste storage areas or environmental restoration where detailed nondestructive assay records do not exist. One such example is the case at Rocky Flats where plutonium residues had built up in ventilation ducting over many years. Prior to cleaning out this material, selected samples were taken to characterize the range of physical forms and chemical composition. This data was augmented by nondestructive assay measurements of radiation levels along the length of the ductwork to arrive at workable estimates of material holdup quantities. In such cases, reasonable conservatism is needed to provide a bounding estimate that is unrealistic.

5.2.2 DETERMINING THE DAMAGE RATIO (DR)

5.2.2.1 OVERVIEW OF REQUIREMENTS, GUIDANCE, AND PRACTICES

The DR is the fraction of material that is actually affected by the accident-generating conditions. DOE-HDBK-3010-94 notes that some degree of ambiguity can result from overlapping definitions of MAR and DR. A given DSA should use one consistent definition throughout. A DR of 1.0 is used unless there is an applicable standard or technical basis for a smaller value. For example, DOE-STD-5506-2007 contains specific DRs (and associated MAR guidance) that may be used in TRU waste operations.

If a qualified container is assessed to survive the postulated accident scenario (i.e., container test requirements exceed the accident environment) then a DR of zero is assigned since there is no release. If the qualified container does not survive the accident conditions, a DR of 1.0 is usually assigned, unless technical justification is provided for a lesser value.

There is an intrinsic interdependence between the definitions of MAR and DR. In simplest terms, the overall area impacted by an event, as well as the magnitude of any energy release, determines what material is impacted. But that can also be thought of as determining what materials are available to be acted upon.

This distinction is made clear by considering two cases. The first is an explosion that affects only one room in a large facility and does not have the capacity to generate a large fire. Most analyses will focus only on that one room. They will not consider material in other rooms, as by definition such material is not at risk, and thus not part of the MAR.

The second case is a seismic event that shakes the entire facility and topples various weak gloveboxes throughout the facility. In this case, analyses identify material in every room as MAR, specifying DRs over the range of zero (e.g., if seismically qualified) to one for each specific case. Because the event affects the entire facility, it is deemed necessary to demonstrate that every potential source of release has been considered. Or, in simpler terms, the practical limits of what could be MAR are not self-evident from the scenario definition itself.

This relationship between MAR and DR may seem trivial. There have, however, been multiple analyses that have stumbled over it. MAR has been defined imprecisely enough that DRs for a given form were credited when that form had already been stricken from the MAR, and DRs greater than zero were applied to material not ultimately at risk. In the former case, the DR is effectively credited twice, yielding a nonconservative source term; in the latter, it is effectively omitted so that the source term is excessively conservative. The relationship between MAR and DR is pointed out to emphasize the need for precise definition of each with reference to the other. Either unaffected material is not considered MAR, or it is and assigned a DR of zero. Likewise, material with a DR greater than zero should be identified as MAR. The simplest convention for avoiding confusion is to identify all material within the structural subdivision affected by the accident (e.g., glovebox, room, wing) as MAR. DR values of zero are then assigned for material not impacted in any significant fashion as justified in the scenario description.

DR values are based on the response of MAR form and available shielding to the stress imposed, as attenuated by any distances involved. In many cases, the nature of the stress-to-distance, stress-to-shielding, or stress-to-form relationship is simple enough to assign a DR from general engineering knowledge or historical experience. Ion exchange exotherms are a well-understood potential in certain operations, sufficiently so that many have been re-engineered to eliminate or minimize that possibility. If vitrified waste, or even hardened cement containing waste, waste is co-located in a room with an ion exchange glovebox, these can be quickly eliminated as MAR is significantly impacted by the exotherm for all but the most unusual of circumstances. Likewise, spilling a plutonium nitrate solution from one glovebox is not going to affect material in other gloveboxes.

When the nature of the stress relationship is not so simple, engineering estimates of type and level of stress are performed in conjunction with assessments of structural strength for available shielding and confinement. Seismic assessments determine whether a given glovebox will remain stable or fall over, and whether massive objects in the overhead will impact the glovebox either way. Fire modeling (see Section 4.2) can estimate whether or not temperatures necessary for combustion of bulk metal will occur for an extended period of time. Blast calculations (see Section 4.3) can determine if a steel vessel at a given distance will remain intact. All of this information may be needed to define a DR of zero, one, or any fraction in between.

5.2.2.2 EXAMPLES

Examples are provided in the following subsections to illustrate the thought process for determining DRs. These are not bounding default recommendations, and use in a DSA will require appropriate justification in context with the scenario being analyzed.

Fire Event

The hazard identification states that 100 g of Pu metal fines, a pyrophoric hazard, is the maximum amount of metal contamination anticipated in impure oxide received for processing. The nuclear criticality limit is 2,000 g if an entire feed can contain nothing but metal fines, but the maximum anticipated amount from historical records is 100 g. Therefore, the DR is 0.05. Note that this assumption may require protection by a TSR administrative control. It would also be acceptable to use a DR of 1.0 with a MAR of 100 g. Another potential hazard to analyze is whether the pyrophoric event could affect other MAR, such as bulk metal, if it is also allowed to be present in this process. For example, the pyrophoric event could ignite the bulk metal or ignite nearby combustibles, leading to a larger fire involving more MAR in nearby gloveboxes. In this case, different DRs would be developed for this additional MAR.

Explosion Event

Assume four liquid tanks holding plutonium nitrate solution. The location of the tanks is split, with two each being located on opposite sides of a large room. There is a significant amount of intervening equipment between them.

The tanks are physically sized to hold 200 liters of solution. At a nominal operating concentration of 30 g Pu/l, the tanks could physically hold 6 kg. The operational flow sheet for the process; however, indicates that each batch contains only 1 kg of plutonium. The operating limit specified in procedures is 1.5 kg.

Assume that under certain conditions, any tank can experience a runaway reaction that overpressures the tank to failure. However, each is operated independently, so that a common cause for multiple over-pressurizations simultaneously does not exist. How should the MAR and DR be defined?

The starting MAR would be 1.5 kg Pu per tank. This is the allowable limit, irrespective of the fact that only 1 kg of Pu is expected per tank. If facility management does not desire to analyze 1.5 kg of Pu per tank, the operational limit should be lowered. Facility management may also choose to analyze a higher value, say 2 kg of Pu per tank, for future flexibility. There is no obligation, however, to assume 6 kg of Pu per tank simply because one could physically do that. That conclusion is no different than a glovebox example, where one works with the practical limits established as opposed to calculating how much solid material could physically be crammed into the box at a given density. The important point is to establish a conservative bounding estimate that is not unrealistic. Since the 1.5 kg of Pu is much less than the physical limit of 6 kg, a TSR Administrative Control may be necessary to protect this assumption unless process upsets cannot exceed the 1.5 kg operating limit.

Accordingly, each tank contains 1.5 kg Pu for the DSA analysis. The next question to answer is what happens to that material? The liquid in the tank where the runaway reaction occurs will experience an over-pressurization release phenomena. What happens to the other tanks is a function of two variables: (1) location, and (2) the violence of the original tank failure.

There are two tanks on the same side of the room. If the first tank merely experiences a localized weld failure (DR of 1.0 for over-pressurization only), the second tank on that side of the room should not be damaged (DR of zero). On the other hand, if the first tank bursts violently into multiple pieces (DR of 1.0 for over-pressurization and DR of 1.0 for free-fall spill of the remaining solution), and the second tank is directly adjacent, it is reasonable to consider whether the second tank could be punctured (DR of 1.0 for free-fall spill). The answer to that question would be determined by mechanical engineering calculations. For example purposes, assume the second tank would be punctured if the engineering calculation is not performed.

The final matter to consider is the two tanks on the opposite side of the room. If the room is large, and the process equipment occupying the floor space between forms a natural barrier, assume that an engineering calculation has been performed that establishes that the remaining two tanks are unaffected; therefore, a DR of 0.0. That is an acceptable conclusion for an unmitigated analysis given that no specific preventive or mitigative capability is being credited. The relative locations of the tanks are physical facts, and the process they serve intrinsically requires equipment located on the intervening floor space.

Alternatively, as previously discussed, the analyst could choose to state that the tanks on the opposite side of the room are not MAR for this particular accident scenario. Other subtleties could come into play as well. If, for the purposes of this example, it is not physically possible to generate a puncture in the adjacent tank at low levels, because half the tank is located in a pit, then only 50 percent of the adjacent tank contents could spill. The spill release DR for that tank may then be given a value of 0.5.

In the mitigated scenario, of course, the DRs can change significantly. For example, if one credits a pressure relief system designed to handle the runaway reaction, there may be no release at all. Or there may be a smaller release depending on the ultimate destination of the pressure relief outlet.

A final consideration is human error. That is not a consideration in this scenario as developed, but suppose the potential for human error to drain one of these tanks in a spill scenario was examined. At only two hundred liters, if there is a plausible way to initiate a spill by erroneous draining, the entire tank is usually assumed to spill. This is because although it might be noticed and the process stopped, the available volume relative to typical pump capacities can result in emptying the tank relatively quickly. A DR less than 1.0 would thus be inappropriate. On the opposite extreme, assume one is evaluating a legacy liquid waste storage tank holding over two million liters of solution. At some point, the cumulative level of human error required to drain the entire tank can become willfully egregious. There is no requirement to analyze scenarios that become physically ridiculous, so a reasoned basis for the maximum portion of the tank that might be drained is acceptable.

Determining DR for Spill Event – Powder Spill from example 7.3.1 in DOE-HDBK-3010-94: As discussed in that Handbook, the DR for a powder spill event is usually 1.

Liquid Spill from example 7.3.2 DOE-HDBK-3010-94: A spill can occur from a piping or vessel leak due to corrosion, or inadvertent damage from an activity such as maintenance or an unrelated accident. If the leak in a line is small, or a leak in a vessel is above the vessel bottom, not all of the material would be spilled. For the sake of simplicity, a leak large enough and situated so as to allow all of the liquid to drain from confinement is postulated (i.e., DR = 1.0).

Liquid Spray: The use of a centrifugal pump for liquid circulation generates positive pressure. While the pressure is not high in this small process, it is sufficient to produce liquid spray and thus a different release stress than the vacuum transfer systems in other dissolution lines. A pump seal, flange failure, or even a piping leak could cause spray generation. The maximum amount of material available in solution is 1,200 g of plutonium if all of the metal is dissolved. The DR will probably not be 1.0 even if no operator intervention occurs as the pump eventually shuts off from loss of net positive suction head after sufficient liquid is lost. The distinction, however, could be minor; therefore a DR of 1.0 is used for the sake of simplicity in this example.

Exothermic Event

The ion exchange process is located in the purification room shown in Figure 5-2, receiving feed solutions from the dissolving tanks and sending the processed liquid streams to annular holding tanks; both sets of tanks being located in other rooms. The process consists of three ion exchange columns in series in a glovebox with support equipment and piping. The columns themselves are 6-inch diameter, 5.5-foot tall Pyrex cylinders with flanged heads on the top and bottom. Each column holds approximately 24 liters of Dowex 21-K anion resin, or equivalent. This activity involves liquid plutonium solutions and plutonium absorbed on solid resins. The source term for the ion exchange exotherm is a function of MAR distribution as DRs are variable and there are competing release mechanisms for solid and liquid phases, with no constant ratio of plutonium between the phases depending on whether in the loading or eluting cycle. At the completion of a loading cycle almost 6,000 g of plutonium are absorbed in the beds with a maximum of 6,500 g allowed. Assume that no other MAR in the adjacent precipitation glovebox is affected by an explosion in the ion exchange glovebox.

First, if the temperature of the liquid flowing from the affected column to the next column in line is sufficiently high, it may initiate a resin exotherm in the next column. Secondly, when the affected column ruptures, historical experience and understanding of the phenomena indicate that at least some of the resin from the damaged column will continue to burn on the glovebox floor.

How much will burn depends on whether the spilled resin is piled on the glovebox floor to maintain local temperature above the autoignition temperature. If a large amount of resin burns, the heat generated may be sufficient to initiate resin exotherm reactions in the undamaged columns. This effect is not certain and there are historical incidents where an exotherm in one column was followed by a fire with no subsequent exotherm in adjacent columns. With respect to the Hanford exotherm incident discussed in Section 4.5 above, the presence of a significant amount of uncharred resin was reported after the incident. Finally, the other columns may be damaged in the initial explosion, shattered by shrapnel from the damaged column, in which case spilled resin may burn, but pressurization of multiple columns is not possible.

Therefore, depending on how many columns are assumed to be affected by a given stress, the first potential factor of the DR is 0.33, 0.67, or 1.0. A second potential factor is, at least for solids, how far the process is into a loading or elution cycle. For example, if only 2,000 g are loaded per operational limits that are protected by a TSR AC, the DR is 2,000/6,500 = 0.31. If both potential factors are used, they need to be defined together so that “double-counting” does not occur.

Earthquake Event

Figure 5–3 is a reproduction of Figure 5–2 with the additional designation of a structural collapse zone along the south wall vulnerable to a seismic event. The affected equipment includes half of the dissolution glovebox and the final glovebox (No. 4) in the fuel fabrication line. A seismic study indicates all other gloveboxes and major equipment have sufficient margin to survive the seismic stress.

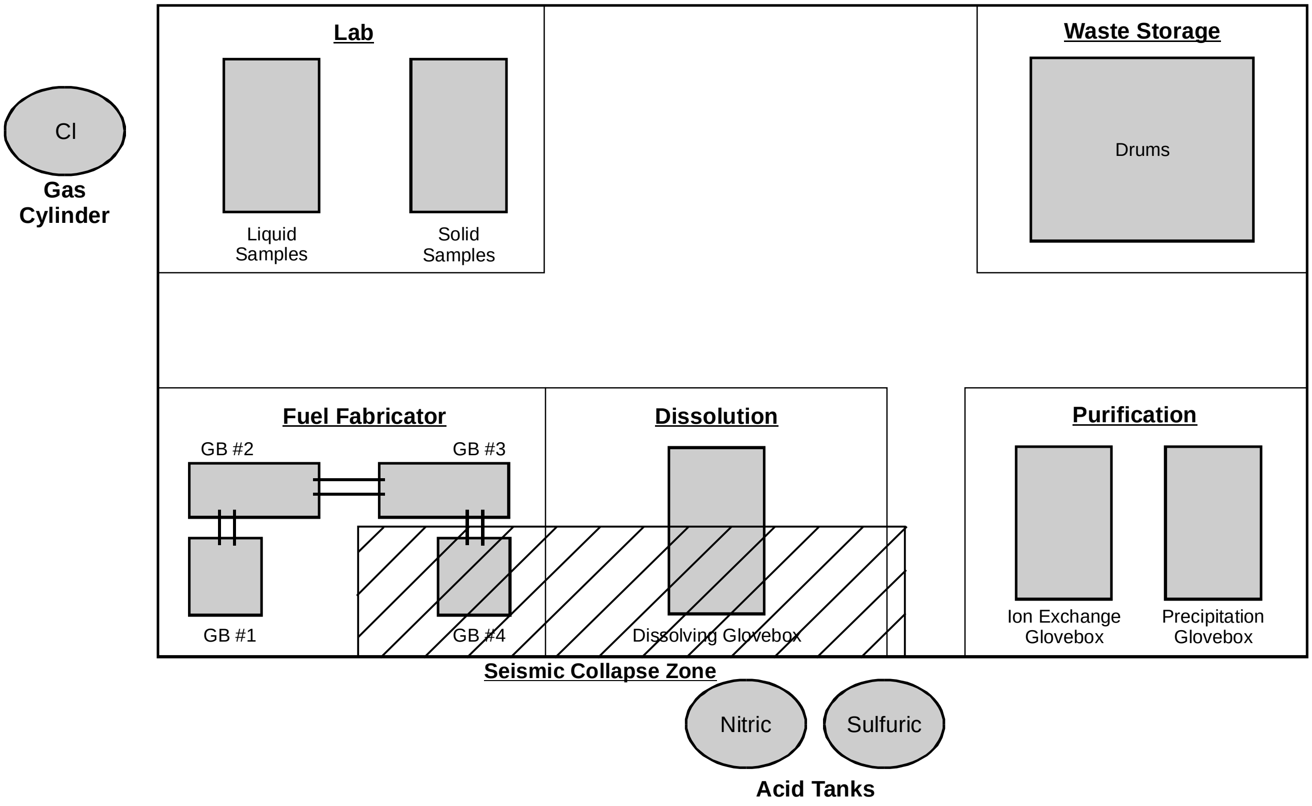

Figure 5-3. Seismic Collapse Zone.

Based on the batch operation discussions for this example in the MAR section, 3,000 g of material can be in the dissolution glovebox. Six thousand grams of powder from the precipitation operation can be in the fuel fabricator line, with 3,000 grams in the front end (i.e., glovebox #1), and 3,000 grams in the back end (gloveboxes #3 and #4).

At first glance, the largest source term of concern would occur if 3,000 g of powder is in glovebox #4, which is impacted by falling debris. A DR of 0.5 (3,000 of available 6,000 g) would be assigned to this material, with a DR of 0.5 for the powder in undamaged gloveboxes # 1 and #2. Moreover, it would be equally acceptable to use a DR of 1.0 with a MAR of 3,000 g for each of these locations.

But suppose by the time the material reaches glovebox #4 that it has been rendered into a ceramic state impervious to the stresses offered by the structural collapse. The ARF for the stress imposed upon ceramic components would be significantly less than the ARF for the stress imposed upon powder. It is conceivable that the bounding release scenario might now move the 3,000 grams of material from glovebox #4 to glovebox #3, where it would still be powder and experience the limited release from seismic shock. These are the types of considerations that come into play when generating source term estimates.

Another possible source of airborne material would be the seismic vibration experienced by surface contamination in all four gloveboxes. This material might contribute in a minor way for the first three gloveboxes as it could have a larger ARF (for smaller quantities) than bulk powder contained in cans or equipment. It could even prove the dominant source term from glovebox #4 if the ceramic fuel forms in question truly are undamaged in the post-seismic state. This drives home again the point that the source term analysis assesses multiple factors. While individual factors should not be unrealistically exaggerated, no potential contributor should be dismissed without consideration.

Moving to the issue of the dissolution glovebox, consider two cases. In the first, the spray chamber and acid storage tank are located at the south end of the glovebox in the collapse zone. Both should be considered structurally compromised in the aftermath of such an event. The question is what value to assign for what MAR? In this case, the ARF for liquids will exceed that for metal. The accident analysis should therefore assume a full dissolution run of four items has finished and the liquid tank contains 3,000 grams of material in solution. The DR for this MAR is 1.0.

The second case is one where the spray chamber and acid storage tank are located at the north end of the glovebox, outside of the collapse zone. This would initially lead to an assumed DR of zero. If, however, the piping that transfers liquid out of the glovebox passes through the collapse zone, some release is possible. If the pipe is one inch in diameter, and the affected length is ten feet, with an additional twenty feet in the next room over that might drain back to this new low point, a total of 4.6 liters might be available to spill. This yields a DR of 0.15 (4.6 liters out of 30). Likewise, if the acid storage tank survived, but seismic analysis indicated failure of a penetration on the tank at the 15-liter level, 15 liters could be assumed to spill from the tank and 15 liters remain, yielding a DR of 0.5.

As a final note, analysts should realize that the structural strength of the majority of the facility, and the seismic capacity of the gloveboxes, is an initial condition of analysis. That is why the hypothetical analysis discussed above focused on areas of potential facility damage. See discussions in Chapters 2 and 3 of this Handbook regarding initial conditions and protection as design features in the DSA and TSRs.

5.2.3 AIRBORNE RELEASE FRACTION AND RESPIRABLE FRACTION

5.2.3.1 OVERVIEW OF REQUIREMENTS, GUIDANCE, AND PRACTICES FOR DETERMINING ARF/RF

DOE-STD-3009-2014, Section 3.2.4.1, provides the following information/directions related to ARF and RF:

> The ARF is the coefficient used to estimate the amount of a radioactive material that can be suspended in air and made available for airborne transport under a specific set of induced physical stresses. The RF is the fraction of airborne radionuclide particles that can be transported through air and inhaled into the human respiratory system. The RF is commonly assumed to include particles of 10-μm Aerodynamic Equivalent Diameter and less. Bounding estimates, and in many cases median estimates, for radionuclide ARFs and RFs for a wide variety of MAR and release phenomena are presented in DOE-HDBK-3010. The bounding estimates shall be used unless a different value is provided in an applicable standard or is otherwise technically justified. In cases where direct shine may contribute significantly to dose, that contribution should be evaluated without the use of the RF, and without the use of the ARF if due to a spill release resulting in exposure to a pool. ARFs and RFs are selected based on physical conditions and stresses anticipated during accidents. DOE-HDBK-3010 defines bounding ARFs and RF mechanisms and airborne release rates based on physical context.

The ARF and RF are evaluated together except in circumstances where it is desired to know the total release of a given material, or when the RF is one, such as is the case with gases. Defining these two parameters generally presents the greatest difficulty in source term analysis. Historically, available information on the subject was extremely limited. As a result, whatever information could be found was used regardless of its true applicability. Little quality control was applied either: different ARFs were assigned by different analysts based on the same information, best guesses became quasi-facts with sufficient repetition, numbers were transposed in copying and passed down. In response to this state of affairs, the DOE set in motion a project to collect the available data on ARF/RFs for material at nonreactor nuclear facilities, test its application in real life circumstance, and attempt to define bounding values for various phenomena. This effort culminated in the development of DOE-HDBK-3010-94. The estimates from that document have since been reproduced in NUREG/CR-6410 and ANSI/ANS-5.10, *Airborne Release Fractions at Non-Reactor Nuclear Facilities*. Both of the documents cited were subject to significant peer review.

In the development of DOE-HDBK-3010-94, available experiments and other data were correlated with the major types of material forms present at materials handling facilities, as well as the normal accidents of concern for such facilities. The major types of material were considered to be: (1) gases, most specifically tritium; (2) liquid solutions, both organic and aqueous; (3) solids, including metals, bulk powders, aggregates, spent fuel and other special forms; and (4) surface contamination, whether in the form of holdup in processes, material entrained in waste, or soil contamination. The major types of accidents considered included spills, fires, explosions, seismically induced vibrations and impacts, and criticalities. The latter, while included in DOE-HDBK-3010-94, represent a special case whose potential MAR is directly defined by the physics of the phenomena itself.

The net result of correlating data to material and accidents was a general categorization of ARFs by four categories: (1) explosive, (2) thermal, (3) mechanical, and (4) aerodynamic entrainment (i.e., suspension in air or resuspension). Explosive stresses of interest are shock effects, blast effects, and venting effects associated with detonation (e.g., high explosive), deflagration (e.g., most gas explosions), and over-pressurization (e.g., heating confined material to rupture pressure). Thermal stresses include evaporation of liquids and combustion of organic liquids, combustion of solids and contaminated waste, and intense heating of noncombustible material. Mechanical stresses of concern include free-fall spill to impact, vibration/shock induced by events such as an earthquake, and impact or crushing of material and containers by falling debris. Aerodynamic entrainment relates to the special case of material freshly deposited on surfaces in the immediate aftermath of an accident or other releases as evaluated in DOE-HDBK-3010-94 Chapter 5, and for wind suspension from a bed of powders or aged contaminated soils as evaluated in the DOE-HDBK-3010 Chapter 4.

Along with ARF values, associated RFs were assigned whenever possible. The size distribution of accident generated aerosols is a particularly complex issue, as most experiments cannot be designed so as to capture a truly representative sample. The logistical requirements of sampling typically result in a skewed sample. Either a sample is obtained where the larger size particles have already deposited due to sampling at a distance or engineered features of the sampling device itself, or the size distribution is affected by the physical chaos of the event itself on in-close sampling equipment. Further, this most basic of problems does not even address detailed physics interaction problems, such as the attractive forces between particles (inter-particle attractive forces) or between particles and the surface (including the effect of surface roughness and the presence of other materials that increase the adhesion of the particles to the surface).

Table 5-1, taken from ANSI/ANS-5.10-1998 (R2013), *Airborne Release Fractions at Non-Reactor Nuclear Facilities*, Table A-1, “Bounding ARFs and Applicable Experimentally Measured RFs,” presents a brief summary of ARF and RF values currently available. This table is an update to a similar summary Table 3-1, “Bounding ARFs and Applicable Experimentally Measured RFs,” initially developed for

NUREG/CR-6410 in 1998. This is only a summary, and the discussion of ARF selection to follow is both brief and general in nature. ARF and RF values should be chosen using DOE-HDBK-3010-94, DOE-STD-5506-2007, NUREG/CR-6410, technical journal articles, from other approved DSA's for unique situations, or derived from physics/chemistry principles. The source of the values needs to be cited and technically justified for use. As stated in the quote above, alternate values to the DOE-HDBK-3010-94 bounding values may be technically justified. Qualitative engineering judgment should not be used as the sole basis for departing from DOE-HDBK-3010-94 bounding values, without substantial technical basis from data that can be appropriately extrapolated or used as an analogy − see Section 5.4.1 below.

An ARF value is selected on the basis of the scenario postulated, the type and level of stress presumed to impact the MAR, and the characteristics of the MAR. Both volatile and nonvolatile materials can be suspended. To suspend a stable material at rest, it is necessary to impact the material sufficiently to convert it to a dispersible form and to provide sufficient air flow to carry the suspended material into the local flow field. In the case of volatile materials, the physicochemical environment to convert the material to its gaseous form needs to be present. If the conversion is due to a chemical reaction, sufficient reactant needs to be available to convert all the affected MAR to its gaseous phase. If the quantity of reactant necessary for conversion is limited and only converts a portion of the volatile material to its gaseous phase, the fraction converted becomes the ARF. In the case of material in the gaseous phase, no RF can be assigned, since, all the material can be transported and inhaled as long as the material remains in the gaseous phase. Airborne reactions, however, can either convert some gaseous materials to solid particles (e.g., reaction of NO_2^- with NH_4^+ to produce NH_4NO_3), attach them to existing airborne particles (e.g., attachment of I_2), or result in adhesion to surfaces (e.g., I_2).

Table 5-1. Summary of Bounding ARF and RF Values.

(Extracted from American National Standard ANSI/ANS-5.10-1998 (R2013)
with permission of the publisher, the American Nuclear Society;
with addition of Clark, 2015, uranium thermal ARF/RFs)

NOTES:
The codes in the column titled “TSL” (Technical Support Level) indicate the following:

1 - supported by experimental data from more than one independent source of the stated range with experimental support for particle generation mechanism;

2 - experimental support over that stated range;

3 - single experimental datum or inferred from other studies.

In the “ARF (RF)” column, the value for the ARF is given in exponential form, and the value for the RF, where used , is given in decimal form, and in parentheses. If no RF is given, it is set to 1.0. Letters in square brackets ([a], [b]) refer to notes at the end of the Table A1 as presented in ANSI/ANS-5.10-1998 (R2013). Other minor formatting and editing changes were also made to the original Table A1, and any non-editorial changes to Table A1 are shown in *{italicized text}*. “DOE Handbook” refers to DOE-HDBK-3010-94.

Stress/Material	ARF (RF)	TSL	Reference*,#	Comments
Explosive Forces: Detonation				
Reactive Metal Implosion, Pu surrounded by and in intimate contact with high explosives (HE), HE:Pu ratio > 1 to 10, single point detonation	1E+0 (0.2)	2	Mensing et al., 1995, Shreve and Thomas, 1965	Calculated from airborne sampling data for operation “Roller Coaster” 1965 (experiments to determine the dispersal of nuclear materials by explosives).
Implosion, metal surrounded by and in intimate contact with high explosives (HE); HE:metal ratio >1 to 10, single point detonation	2E-1	3	ANSI/ANS-5.10-1998	Based on small scale experiments on the dispersal of metal hemisphere by explosives. Applicable to metals less reactive than Pu. Release of any Pu is estimated by ARF/RF values shown.
Metal or Solution – Explosion, metal or aqueous solution, high explosive in intimate contact with material, HE:material ratio 0.07 to <1	TNT Eq. [a]	2	DOE Handbook, Sections 3.2.2.1 and 4.2.2.1	
Powder – Explosion, High Explosives lying on surface, HE:powder ratio 1 to 100	ARF/RF = 0.2 x TNT Eq. [b]	2	DOE Handbook, Section 4.4.2.1	From soil lofted during field tests where HE (bare and as artillery shells) were placed directly on the soil surface.
HEPA Filters *{Shock pulse}*	2E-6	2	DOE Handbook, Section 5.4.2.1	Small pieces of glass fiber medium were dislodged from a few locations on the creases in the downwind region of the filter.

Stress/Material	ARF (RF)	TSL	Reference*,#	Comments
Explosive Forces: Deflagration				
Powder Unshielded, directly under or in blast volume of large explosion with high confinement pressure	1E+0 [c]	2	DOE Handbook, Section 4.4.2.2.1	
In containers or at a distance of meters from the blast volume, aerodynamic entrainment by accelerated gas velocities	5E-3 (0.3)	2	DOE Handbook, Section 4.4.2.2.2	
HEPA Filters *{Venting by pressurized gases}*	1E-2	2	DOE Handbook, Section 5.4.2.2	
Explosive Forces: Over-pressurization to Rupture				
Liquid, confined in vessel or container Slow buildup of pressure [d], vented above the surface level of liquid, failure <0.35 MPa$_g$	5E-5 (0.8)	2	DOE Handbook, Section 3.2.2.3.2.A	
Slow buildup of pressure, vented above the surface level of liquid, failure pressure >0.35 up to 3.5 MPa$_g$	2E-3 (1.0)		DOE Handbook, Section 3.2.2.3.2.A	
Rapid buildup of pressure, vented above the surface level of liquid	NVA [e]		DOE Handbook, Section 3.2.2.3.2.B	
Rapid buildup of pressure, vented below the surface level of liquid [f]	1E-4	2	DOE Handbook, Section 3.2.2.3.1	
Superheated liquids (“flashing spray”), <50 °C superheat	1E-2 (0.6)	2	DOE Handbook, Section 3.2.2.3.3.A	
Superheated liquids (“flashing spray”), 50 °C – 100 °C superheat	1E-1 (0.7)	2	Mishima et al., 1968, Borkowski et al., 1986, and Kataoka and Ishii, 1983, DOE Handbook, Section 3.2.2.3.3.4	
Powder Confined in vessel or container, release pressure < 0.17 Mpa$_g$ (< 25 psig)	5E-3 (0.4)	2	DOE Handbook, Section 4.4.3.3.2	
Confined in vessel or container, release pressure > 0.17 < 3.5 Mpa$_g$ (25–500 psig)	1E-1 (0.7)	2	DOE Handbook, Section 4.4.2.3.1	
Vitrified High Level Waste Canisters High pressure sufficient to dissolve the plug	3E-5	3	DOE Handbook, Section 4.3.1.1	Based on a measured value of 3.5E-4 of inventory as particles in the upper plenum of canister and ARF/RF of 1E-1/0.7.
Thermal Stress				
Volatile compounds	1E+0	1	Brereton et al., 1997	AP AC Spills Report.
Liquid, aqueous solutions Simmering, no visible bubbles	3E-5	2	DOE Handbook, Section 3.2.1.1	

Stress/Material	ARF (RF)	TSL	Reference*,#	Comments
Boiling [g]	2E-3	1	Mishima et al., 1968, Borkowski et al., 1986, and Kataoka and Ishii, 1983, DOE Handbook, Section 3.2.1.3	
Liquid, organic combustible Volatile compounds	1E+0	2	DOE Handbook, Section 3.3.1, 3.3.7	
Non-volatile compounds, burns to self-extinguishment, no significant surface turbulence	1E-2	2	DOE Handbook, Sections 3.3.1, 3.3.7	
Non-volatile compounds, vigorous burning with surface turbulence, burns to self-extinguishment	3E-2	2	DOE Handbook, Sections 3.3.3, 3.3.4, 3.3.5, 3.3.7	
Non-volatile compounds, vigorous burning with surface turbulence, to complete dryness	1E-1	2	DOE Handbook, Sections 3.3.3, 3.3.7	
Burning of combustible liquid over air-dried residue from solution on porous, non-heat-conducting surface	5E-3 (0.4)	2	DOE Handbook, Sections 3.3.6, 3.3.7	
Burning of combustible liquid over air-dried residue from solution on heat-conducting surface	2E-1 (0.3)	2	DOE Handbook, Sections 3.3.6, 3.3.7	
Solid reactive metal				
Plutonium, < ignition temperature [h] of oxide formed	3E-5 (0.04)	2	DOE Handbook, Section 4.2.1.1.2	
Plutonium, > ignition temperature	5E-4 (0.5)	1	Mishima, 1966, 1967; Luna, 1994; Carter and Stewart, 1970; Eidson et. al., 1988; Eidson and Kanapilly, 1983, DOE Handbook, Section 4.2.1.1.3	
Plutonium, free-fall spill of molten metal into air, small fall distance	1E-2	2	Stewart, 1963, DOE Handbook Section 4.2.1.1.4	
Plutonium, small drops of molten metal violently dispersed that travel greater than 1 m in air	1E+0 (0.5)	1	Raabe et. al., 1978, Chatfield, 1969, DOE Handbook Section 4.2.1.1.5	
Uranium, less than ignition temperature [i], greater than 500 ˚C	1E-3	2	DOE Handbook, Section 4.2.1.2.1	
Ignitable forms of β-phase Uranium Alloys, greater than 500 °C	1E-3	2	DOE Handbook, Section 4.2.1.2.1	Elder and Tinkle (1980) and experiments using Staballoy DU penetrators.

Stress/Material	ARF (RF)	TSL	Reference[*,#]	Comments
Ignitable forms of pure-Uranium and α-phase Uranium Alloys, greater than 500 °C	1E-4	2	Carter and Stewart (1970)	Discussion of Carter and Stewart Experiments in DOE Handbook Section 4.2.1.2.1 for Median ARF/RF value.
Non-ignitable forms (e.g., bulk/large pieces) of pure-Uranium and/or α-phase Uranium Alloys, below ignition temperature	1E-6	2	Clark (2015)	Note: Median ARF/RF rounded to nearest order of magnitude. From Table 5 in Clark (2015), 5E-7 is rounded up to 1E-6.
Non-ignitable forms (e.g., bulk/large pieces) of β-phase Uranium Alloys, below ignition temperature	1E-5	2	Clark (2015)	Note: From Table 5 in Clark (2015), arithmetic mean is rounded down to 1E-5, same as the geometric mean.
Non-ignitable forms (e.g., bulk/large pieces) of γ-phase Uranium Alloys, below ignition temperature	1E-7	2	Clark (2015)	Note: From Table 5 in Clark (2015), 5E-8 is rounded up to 1E-7.
Uranium, free-fall spill of molten metal greater than 1 m	1E-2	2	DOE Handbook, Section 4.2.1.2.2	
Uranium, explosive dispersal of thin sheets of metal	1E+0	2	DOE Handbook, Section 4.2.1.2.3	
Concrete				
Tritium (^{3}H) as water, > 20 ˚C to 200 ˚C	5E-1	2	DOE Handbook, Section 4.3.1.2	
Tritium (^{3}H) as water, > 200 ˚C to 600 ˚C	1E+0	2	DOE Handbook, Section 4.3.1.2	May also suspend radionuclides held in cement matrix if cement is decomposed and particles of CaO can be suspended.
Solid, powder				
Nonreactive [j], up to 1,000 ˚C, upflow around powder to 100 cm/s	6E-3 (0.01)	2	DOE Handbook, Section 4.4.1.1	
Reactive, plutonium compounds, up to 100 ˚C, upflow around powder to 100 cm/s: Plutonium fluoride	1E-3 (0.001)	2	DOE Handbook, Section 4.4.1.2	
Solid, Compounds				
Reactive, plutonium compounds, up to 100 ˚C, upflow around powder to 100 cm/s: Plutonium oxalate, nitrate	1E-2 (0.001)	2	DOE Handbook, Section 4.4.1.2	
Solid, contaminated combustible				
Packaged waste, burns to self-extinguishment	5E-4	2	DOE Handbook, Section 5.2.1.1	

Stress/Material	ARF (RF)	TSL	Reference*,#	Comments
Loose cellulosic material, burns to self-extinguishment	1E-2	2	DOE Handbook, Section 5.2.1.2	
Loose polystyrene	1E-2	2	DOE Handbook, Section 5.2.1.4.3	
Loose, other plastics	5E-2	2	DOE Handbook, Section 5.2.1.4	
Light cellulosic material remaining suspended during complete combustion (i.e., ash)				
UO$_2$ preformed particle	4E-1	2	DOE Handbook, Section 5.2.1.3	
Contaminated with air-dried residues from solution	8E-2	2	DOE Handbook, Section 5.2.1.3	
Solid, contaminated HEPA filters passage of heated air up to 400 ˚C [k]	1E-4		DOE Handbook, Section 5.4.1	
Aerodynamic Entrainment/Resuspension [l]				
Homogeneous Deposit	ARR:			
Liquid, indoors, shallow pool on heterogeneous surface (e.g., stainless steel, glass, concrete), normal building ventilation flow/low airspeed (< 2 m/s, ~5 mph)	4E-7/hr	3	DOE Handbook, Section 3.2.4.5	
Liquid, indoors, as above, covered with substantial layer of debris or indoor static conditions	ARR: 4E-8/hr	3	DOE Handbook, Section 3.2.4.5	
Liquid, outdoors, large pool, up to 13.6 m/s (~30 mph)	ARR: 4E-6/hr	3	DOE Handbook, Section 3.2.4.5	
Powder, pile on heterogeneous surface (e.g., concrete, stainless steel, glass), normal building ventilation flow/slow airspeed (< 2 m/s, ~5 mph)	ARR: 4E-5/hr	3	DOE Handbook, Section 4.4.4.1	
Powder, indoors, as above covered with substantial layer of debris or indoor static conditions	ARR: 4E-6/hr	3	DOE Handbook, Section 4.4.4.1	
Powder, dispersed into flowing air, airspeed up to 9.1 m/s (20 mph)	[m]	2	DOE Handbook, Section 4.4.3.2	
Heterogeneous Deposit	ARR:			
Liquid, outdoors, absorbed on soil, no large standing pools of free liquid, up to 22.7 m/s (50 mph)	9E-5/hr	2	DOE Handbook, Section 3.2.4.4	
Powder, indoors, loose surface contamination [n], normal building ventilation flow, low airspeed (<2 m/s, 5 mph)	ARR: 4E-5/hr	3	DOE Handbook, Section 5.3.4	

Stress/Material	ARF (RF)	TSL	Reference*,#	Comments
Powder, outdoors, due to the passage of vehicular traffic across or by loose powder on road, up to 22.7 m/s (50 mph)	ARR: 1E-2/ pass	2	DOE Handbook, Section 4.4.4.2	
Mechanical Stress [o]				
Free-Fall Spill				
Liquid, aqueous solution, spill distance < 3 m	2E-4 (0.5)	2	DOE Handbook, Section 3.2.3.1	
Liquid, slurry (<40 percent solids), spill distance < 3 m	5E-5 (0.8)	2	DOE Handbook, Section 3.2.3.2	
Liquid, viscous solution, spill distance < 3 m	7E-6 (0.8)	2	DOE Handbook, Section 3.2.3.3	
Liquid, spill distance > 3 m (see reference)			DOE Handbook, Section 3.2.3.1	
Powder, spill distance < 3 m	2E-3 (0.3)	1	Sutter et al., 1981, Ballinger et al., 1988, Plinke et al., 1991, Heitbrink et al. 1992, DOE Handbook, Section 4.4.3.1.2	
Powder, spill distance > 3 m (see reference)		2	DOE Handbook, Section 4.4.3.1.3	
Powder, shock impact due to falling debris	1E-2 (0.2)		DOE Handbook, Section 4.4.3.3.2	
Powder, dispersed into flowing air, to 9.1 m/s (20 mph) (see reference)			DOE Handbook, Section 4.4.3.2	
HEPA filter, object strikes encased [p] filter or encased filter impacts unyielding surface after fall	5E-4	3	DOE Handbook, Section 5.4.4.1	
HEPA filter, object strikes unencased filter or unencased filter impacts unyielding surface after fall	1E-2	3	DOE Handbook, Section 5.4.4.2	
Spent nuclear fuel				
Noble gases	5E-2	2	Soffer, 1993	
Iodine (I_2)	2.3E-3	3	Mishima, 1995	
Cesium vapor	2.5E-4	3	Mishima, 1995	
Fines	2.4E-4 (7E-5)	2	Mishima, 1995	
Crush/Impact				
{Vitrified} Glass	[q]	2	DOE Handbook, Section 4.3.3	
Aggregate	[r]	2	Owczarski and Mishima, 1996	

Stress/Material	ARF (RF)	TSL	Reference*,#	Comments
Spent nuclear fuel				
noble gases	7E-2 [s]	2	Kent, et al., 1995	For the degree of fragmentation in experimental program.
iodine (I_2)	2E-3	2		
^{3}H (as HTO)	1E-2	2		
Ffuel	2E-3 (7E-5)	2		Bounding for energy density (crushing force) imparted to material in the range of 10 to 100 J/cm^3.
Encapsulated ceramic oxide pellets, particles generated but not released, impact velocities of steel to 188 mph, concrete to 99 mph, and soil to 550 mph	5E-3 (0.6) *{[t]}*	2	Mishima, 1995	
Shock/Vibration				
Loose surface contamination	1E-3	2	DOE Handbook, Section 4.4.3.3.1	
{powder}	(0.1)			
{contaminated noncombustible materials}	*{(1.0)}*		*{Sections 5.2.3.2, 5.3.3.2.2}*	
{Bulk powder]	*{1E-3* *(0.1)}*	*{2}*	*{DOE Handbook, Section 4.4.3.3.1}*	
{Loose surface contamination, substrate packaged in container such as pail or drum}	*{1E-3* *(0.1)}*	*{2}*	*{DOE Handbook, Section 5.2.3.2}*	

[a] A very conservative assumption of mass airborne in respirable size range (10 μm AED) is equal to the TNT Equivalent calculated for the explosion.

[b] Particles in the respirable size range of initial inventory made airborne, provided that this value does not exceed the fraction of *{respirable}*particles in the size range in the source material.

[c] RF for these events cannot exceed the fraction of *{respirable}* particles in the source material.

[d] Absorption and equilibration of gases in liquids is a function of chemical composition of the solution, the surface area and depth of the liquid, and the volume of the gas. Equilibrium may take minutes to hours dependent upon conditions.

[e] NVA = No value currently available.

[f] Generation of RF liquid droplets can be greater than the values shown here that bound circular, knife-edge orifices of 0.125-in diameter and greater with upstream pressures up to 200 psig. The “worst case” for RF droplets of solutions is a crack 50 micrometers wide. The longer the length, the more liquid that can be vented for a given upstream pressure. This type of crack is not a common nor typical occurrence for faults in pipes or vessels, and, at higher pressure, would probably propagate into a wider, longer crack.

[g] Only applies to bubbly flow (distinct bubbles visible, <30 percent liquid in form of bubbles). Does not apply to churn turbulent nor chaotic boiling regimes.

[h] Ignition temperature for plutonium metal is a function of surface to mass ratio (S:M). At S:M of 100 cm^2/g, the measured ignition temperature for plutonium metal is in the range of 160 °C. The ignition temperature rises rapidly after S:M 10 cm^2/g and ranges from 480 to 520 °C for bulk pieces.

Stress/Material	ARF (RF)	TSL	Reference[*,#]	Comments

[i] Like plutonium, the ignition temperature for uranium metal is a function of the Surface to Mass ratio (S:M). At S:M of 100 cm^2/g, the uranium ignition temperature is in the range of 200 ° C to 300 °C. Like plutonium it rises rapidly in the region of S:M 10 cm^2/g and reaches temperatures in excess of 700 °C or more. There is some doubt that bulk pieces of uranium can attain ignition conditions except for very special circumstances.

[j] Does not react chemically to change form under accident conditions postulated.

[k] Assumes HEPA filter medium (glass fiber) softens and melts at higher temperatures and thus retains particles accumulated on the fiber surfaces. *{This should not be taken as a presumption that filters will remain functional for prolonged exposure to temperatures up to 400 ˚C.}*

[l] In this part of the table (the next nine items), the second column is the Airborne Release Rate (ARR), rather than ARF and RF.

[m] ARF = 0.0134[U] + 0.00543, where U is local windspeed in m/s.

[n] Loose surface contamination that can be removed by swiping or by low air speeds such as blowing across the deposit.

[o] From here to the end of the table, the second column is again ARF (RF).

[p] Encased denotes a container that does not £ail due to impact of falling objects nor impact with unyielding surface after fall of the container.

[q] Formula for crush/impact forces on brittle solids is shown on pg. 4-52 of DOE-HDBK-3010-94. For vitrified HLW, the empirical correlation 2E-11[J/cm^2] shown is applicable. The user should be cautious in application of this formula since the value calculated is an energy density applied to the material. If the crush/impact force is applied to all the material, the energy density is simply the force/volume. If the crush/impact force is only applied to a portion of the object (e.g., the object impacts just a portion of the surface of the brittle material), the formula only applies to the volume being crushed.

[r] For aggregate materials such as cement and sandstone, the correlation factor for use in the formula on pg. 4-52 of DOE-HDBK-3010-94 is 3E-11.

Stress/Material	ARF (RF)	TSL	Reference*,#	Comments

[s] For spent nuclear fuel, the empirical correlation is found in the NRC Safeguards Report (Kent, et al., 1995)

{[t] Care should be taken in use of this value. It is based on extreme impact energies.}

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* Original sources cited in Section A3 of ANSI/ANS-5.10-1998 for Table 5-1 above are as follows:

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Stress/Material	ARF (RF)	TSL	Reference$^{*,\#}$	Comments

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In the case of liquids and solids, the material is either subdivided into droplets or particles, or, in the case of powders, is de-agglomerated. De-agglomeration of a powder at rest is not readily accomplished. This is especially true for stored powders, where the smaller particles have had time to settle into the interstices between larger particles. De-agglomeration/separation is difficult due to the small surface areas of small particles and the limited space for gas flow between them. Even in a heavier medium, such as a liquid, the application of sonic agitation for long periods (30 minutes or more) is necessary to restore a size distribution approximating the original distribution. All phenomena (including detonations with minimal stand-off distances) do not fragment small particles (<100 μm). Thus, the amount of particles in the respirable size range that can be suspended is limited by the amount of material of this size found in the original source powder. Thus, the amount of particles in the respirable size range that can be suspended is limited by the amount of material of this size found in the original source powder. See Section 4.4, Powders, of DOE-HDBK-3010-94 for further discussion of the difficulty of de-agglomerating powders.

Bulk solids and liquids require more energy to fracture the bonds that hold the form together. In the case of liquids, the material is drawn into a fine filament or sheet that breaks when the tensile strength of the material is exceeded. This can occur in many ways. If the liquid forms bubbles at the surface from boiling or the passage of a gas through the liquid, breakup of the bubbles generates fragments that can be suspended or result in secondary droplets when condensation of the liquid vapors. A mechanism that can form significant amounts of fine liquid droplets is a "flashing spray" that forms upon the venting to lower pressures of a liquid that is super-heated. The liquid initially forms a column approximately the shape of the opening. Then, bulk vaporization of the liquid (a significant fraction of the liquid is "flashed" into a vapor) within the column results in rapid subdivision of the remaining liquid. The greater the superheat, the smaller the diameter of the liquid droplets. In all cases of heated liquids, additional evaporation of the liquid occurs during airborne transport and, depending on the temperature, environmental factors, the distance traveled, and solute concentration, the droplet diameter decreases.

Bulk solids of various categories have different physical characteristics. For brittle materials (e.g., glass-like materials, aggregate, composites), crush-impact forces (including shock waves from explosions) can result in fragmentation. The level of force and the material tensile/compressive strength are factors that influence the particle size distribution of the fragments formed. Materials that have elastic-plastic response to the application of forces (e.g., metals) require greater forces and are generally fragmented only by the pressures generated by the detonation of solid explosives in contact with the surface of the metal. Crush-impact forces generally result in deformation and tearing of metals; unless, the metal is embrittled.

One feature in particular of the data analysis is noted. ARF and RF values are assigned by physical context. That is, the physical context of the material determines the stress it experiences. For example, consider the case of powder spills. The bounding ARF/RF specified in DOE-HDBK-3010-94 (page 4-77) for plutonium oxide powder falling freely (< 3 m) through air is 6E-4. The bounding ARF/RF assigned if plutonium oxide falls inside a container is 1E-4. The difference is that the physics of release for the free-fall spill are driven by shear stress from air currents moving through the powder. That phenomenon physically does not exist inside a container. Release in the latter case is driven primarily by flexing of the container substrate upon impact with the ground, with some self-acting mitigation in the form of a powder’s physical tendency to agglomerate. Therefore, if powder falls inside a can, acknowledging that point does not constitute improper crediting of a can in unmitigated analysis. For the perspective of DOE-HDBK-3010-94, the pedigree and capability of the can is irrelevant. The physical fact of it defines the stress being experienced by material. Further, it is not reasonable to assume personnel carry plutonium powder about cupped in their hands. In unmitigated analysis, however, if the can is not to be credited, it should assume to open upon impact with the ground and release the appropriate source term (i.e., can inventory * 1E-4, per DOE-HDBK-3010-94, page 4-85).

The treatment of TRU waste is another such example. The respirable release fraction for loosely strewn waste in a fire is 1E-2. But packaged waste, even in as primitive a form as plastic bags or pails, is assigned a respirable release fraction of 5E-4. The experimental data supports that distinction due to the physical fact that a clumped mass traps particles in a self-filtering effect.

5.2.3.2 EXAMPLES FOR DETERMINING ARF/RF

Given that it is not desired to use this document as a primary reference for selecting release fractions, the reader is referred to the extensive examples in Chapter 7 of DOE-HDBK-3010-94. Only a brief discussion is provided regarding one aspect of the example previously cited in Section 5.2.1.2 above. It is intended to demonstrate the basic thought process for ARF selection.

A. Case One

Consider the example facility of Figures 5–2 and 5–3, specifically the fuel fabrication line. Presume for the moment that the structural collapse depicted in Figure 5–3 does not occur and all four gloveboxes remain intact (i.e., upright in a largely undamaged state) during a seismic event. What stress is then being imposed on any powder contained in the glovebox?

The four main categories of potential stress are explosive, thermal, mechanical, and aerodynamic entrainment. No explosion or fire is postulated for this event. No debris impacts either the powder or its outer glovebox confinement. This could lead an analyst to dismiss mechanical impact as well, but that would be a mistake, because even intact gloveboxes will experience transitory movement of structural members and an associated seismic vibration. If the gloveboxes held only solid metal, such a stress would present no significant force. For the much more fragmented powders, however, that force is sufficient to produce a small amount of aerosolization.

Examining Table 5-1 for mechanical stresses indicates that an ARF and RF of 1E-3 and 0.1, respectively, are assigned for shock/vibration of bulk powders. Previous examinations of this case have indicated the maximum MAR is 6,000 g of plutonium oxide powder for all four gloveboxes. The initial source term would therefore be 6 g, and the initial respirable source term 0.6 g.

Given this 0.6 gram respirable release, could surface contamination produce a significant contribution? Table 5-1 indicates that the ARF and RF for shock/vibration of loose surface contamination is assigned an ARF and RF of 1E-3 and 1.0, respectively, thus yielding a combined ARF/RF one order of magnitude greater than that for bulk powder. For the purpose of discussion in this example, if significant contribution is defined as 10 percent of the 0.6 gram source term, then surface contamination would have to contribute 0.06 g of airborne material to be significant. Working backward with the ARF/RF of 1E-3 yields a required surface contamination MAR of 60 g. That is certainly possible given that historical surface contamination levels for representative gloveboxes can range up to 50 g. Using a value of 0.1 g/ft^2 for powder handling gloveboxes (from historical experience), and assuming each glovebox is 12 feet by 4 feet by 4 feet (with a factor of 1.3 applied for equipment inside the gloveboxes) yields a total MAR of 116 g for all four gloveboxes. It can be concluded, therefore, that surface contamination is a nontrivial contributor. Both of these approaches to determine the level of surface contamination (MAR) and potential airborne release, are appropriate application of DOE-HDBK-3010.

This last result points out another question that an analyst should always keep in mind: when is a result real, and when is it an artifact of analysis? Examining the specifics of DOE-HDBK-3010-94 indicates that the main reason the ARF/RF for surface contamination is assigned a higher value than for bulk powder is because no real confidence existed as to a generic size distribution for surface contamination residues. It is, in essence, simply a conservative assumption. DOE-HDBK-3010-94 contains multiple cautions against taking its bounding recommendations as absolute statements of reality, or as a starting point for extrapolating ever more extreme circumstances that could theoretically exacerbate the physics of release. Either of these approaches can quickly tumble over into analytical gamesmanship, defeating the cited purpose of DOE-HDBK-3010-94, which is “to provide information to support general bases for decision making.”

B. Case Two

Consider again the example facility of Figures 5-1 and 5-2, specifically the fuel fabrication line. Presume for the moment that the structural collapse depicted in Figure 5-3 does occur, but is sufficiently severe to collapse all four gloveboxes. What additional stresses are then being imposed on any powder contained in the glovebox?

Depending on how the powder is contained, and the nature and orientation of the debris impacting gloveboxes, it may not experience much in the way of additional stress. In the interests of conservatism, however, that is not presumed for the type of gloveboxes common in the DOE weapons complex. The collapse is instead broken down into the sequence of distinct events occurring. First, the glovebox is experiencing a fall of some kind, more so if it tips over than if it simply slumps downward, but the latter is considered equal to the former given that it is difficult to specify the exact nature of the collapse. Second, the glovebox is impacted by debris. Windows can break or contents can be spilled out of the glovebox. Either case raises the possibility of debris impacting powder.

For spill distances less than three meters, Table 5-1 specifies an ARF and RF of 2E-3 and 0.3, respectively, for the free-fall spill of powders. This circumstance is not, in fact, a free-fall spill, but the experimental data on free-fall spills is the closest equivalent available. Any conservatism involved in the use of this ARF/RF is simply accepted. Table 5-1 also lists an ARF and RF of 1E-2 and 0.2, respectively, for debris impacting powder. This might not be considered if the nature of the debris is small fragments or if the gloveboxes are shielded by slumping installations in the overhead. That will not be presumed to be the case. If the box contains loose powder that falls and is heavily impacted by debris, the cumulative ARF/RF could be as high as 6E-4 + 2E-3 = 2.6E-3.

Conversely, suppose all powder in the glovebox is held in cans or other metallic containers. The overall effect might then be characterized as two similar events. The can falls with the glovebox and is impacted by debris as it lands. As noted, DOE-HDBK-3010-94, the ARF/RF for shock impact and falling debris on confined bulk powder is 1E-4. The cumulative ARF/RF could therefore be as low as 1E-4 + 1E-4 = 2E-4. In this case, however, the idea of powder being outside of a container while in a glovebox is not an absurd construct similar to personnel carrying plutonium cupped in their hands outside of a glovebox. If the operation naturally lends itself to the powder being confined, that initial condition should be preserved in the TSR control set.

5.2.4 AIRBORNE RELEASE RATE

Sometimes ARFs are expressed as a function of time. The parameter is then identified as an airborne release rate (ARR). This is, in fact, the norm for chemical releases. Gas escaping from a damaged cylinder will leak at a rate of so many pounds per second. Liquids spilled into a bermed area or as a shallow pool dispersing to its limits will evaporate at a rate of pounds per minute, depending on the surface area of the pool, its temperature, and the specific physical properties of the liquid.

Radionuclides are treated in a more overall fashion, as noted in the examples of Section 5.2.3, Airborne Release Fractions and Respirable Fractions. Most radioactive material releases occur due to momentary chaotic stresses. Therefore, even when the release might occur over a minute or several minutes, the total quantity airborne is assumed to exit the facility at one moment in time. That is often the case even for an event such as a fire, which occurs over an interval of tens of minutes, sometimes even hours. In these cases, unlike with the leak rate of a gas of a given pressure or the evaporation of a pool of a given liquid, there is no simple physical principle from which to compute reasonable time dependence. The most common exceptions to this are solution criticalities (whose time for a complete set of pulses is part of the event definition) and aerodynamic entrainment, which is defined as a rate. Chemical releases are discussed further in Section 5.3.

Example

It is not unreasonable to assume that an event as severe as the earthquake assessed in the Case Two example from the previous section could result in cleanup activities being delayed for some period of time. Aerodynamic entrainment will suspend more material during that period. How should that release be estimated?

An assumption is that for long duration releases, DOE-STD-3009 limits the unmitigated consequence analysis to eight hours. Table 5-1 defines an ARR of 4E-6 per hour for “powder, indoors ... covered with substantial, layer of debris or indoor static conditions.” Using that value, the ARR for 6,000 g of spilled oxide powder would be 2.4E-2 g/hr, or a total of 0.2 g/8 hr. If this figure were trivial compared to the overall facility release, it could either be ignored or lumped in with the immediate release.

5.2.5 LEAKPATH FACTOR

The term "leak path" refers to the path taken by material released in a facility on its way to the outdoor atmosphere. Common leak paths of a building are air ventilation ducts, door gaps, and various building leaks. The "leakpath factor" (LPF) is the "fraction of the radionuclides in the aerosol transported through some confinement deposition of filtration mechanism" (DOE-HDBK-3010-94, page 1-6). The LPF used in the common five-factor formula is the total fraction of respirable airborne material released during the accident that escapes from the building to the environment. Once an aerosol is formed, it continuously depletes (in concentration) due to natural mechanisms such as gravitational settling and other lesser important mechanisms such as impaction, agglomeration (a subset of gravitational settling), diffusion to surfaces, and possibly mechanical filtration. The LPF is of interest because it has the potential for reducing the initial source term (IST) at the point of generation before it exits the facility, thus producing a much smaller release to the external environment.

The DSA analysis does not allow credit for a facility LPF for unmitigated analysis. Unmitigated analyses necessarily start with LPF of 1.0. For mitigated analysis, the LPF is dependent on the physical characteristics and configuration of the facility as it is estimated to exist under the postulated accident conditions.

Assignment of an LPF of 1.0 is the general practice for most low consequence facility DSAs. As accident consequences from bounding events increase into the rem range for the offsite public, LPF determinations become important and a process and strategy for estimation of a LPF < 1.0 generally becomes appropriate, such as crediting filtration or other natural depletion mechanisms. An active confinement ventilation system with filtration is the preferred mitigative control as required by DOE Order O 420.1C, and discussed further in DOE-STD-3009-2014, Section A.8, Hierarchy of Controls. However, sometimes a passive confinement strategy may be justified that credits other natural depletion mechanisms.

Other than for filtration systems, LPFs are functions of building ventilation, building leak-tightness, atmospheric conditions (e.g., wind speed), building pressurization by a fire, the length of the leakpath, floor area for deposition of particulates, and other factors. They are specific to the building and the location of the source within that building, and are specifically estimated for each scenario and building. Therefore, the effort in estimating the LPF is significant and the analyst should consider that there may be limited benefit for refinement of LPF below 1.0 for facilities with a small MAR.

Historically, some DSAs have been developed applying complicated in-facility transport analyses using the MELCOR or CONTAIN codes.[42] Egress doors being open during evacuation have been considered for both normal ventilation and loss of ventilation scenarios. Also, based on these types of computer code analyses, and/or hand calculations, DSAs have credited an in-facility transport LPF for loss of power concurrent with radioactive material release within the facility. Under such scenarios, doors open during evacuation and otherwise closed doors with some assumed leakage past the door seals have been considered. The adequacy of those LPF justifications has been determined based on facility-specific ventilation designs, specific circumstances and postulated accident environments; approved by the DOE Safety Basis Approval Authorities.

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[42] These codes were not designed for modeling dozens of volumes. The uncertainty increases with the number of nodes and junctions.

Many LPF estimates are assumption-driven, can be challenging to defend, and should be carefully applied. Therefore, it is always important to remain cognizant of the inherent uncertainty in the LPF due to analytical variances in all of the parameters used in the assignment, which applies to both active and passive confinement strategies. As is the case with all safety analysis calculations, sufficient conservatism is factored into the overall determination by reasonably conservative assignment of the respective input parameters. Also, assumptions used in LPF analysis are required to be identified and evaluated so that the need for TSR controls can be decided for a facility-specific situation.

5.2.5.1 FILTRATION LPF

If a release passes through filtration before reaching the atmosphere, a conservative LPF assumption based on filter efficiency (i.e., LPF = 1 – efficiency) for the accident conditions being evaluated should be made. This is appropriate if active ventilation filters releases that do not breach primary confinement systems (e.g., gloveboxes). However, this does not represent a bounding LPF for energetic releases that breach primary confinement systems if active secondary confinement ventilation pressure differentials are not maintained during full building evacuations over several minutes. Moreover, the measured filter efficiency may not directly lead to the LPF determination if there are unfiltered leak pathways in the system or through building penetrations that need to be evaluated.

General guidance on HEPA filter design, installation, testing, and service life is provided in Chapters 3 and 8 of the DOE-HDBK-1169-2003. HEPA filters, by definition, have a minimum filtration efficiency of 99.97% for 0.3 µm particles (the most penetrating size). For accident analysis, DOE-HDBK-1169-2003 (page 2-31) states the following:

> Accident analysis typically assumes a first stage credit of 99.9 percent efficiency (DF of 10^3) for removal of plutonium aerosols. Second and subsequent stages typically assume an efficiency of 99.8 (DF of 5×10^2). [DF = Decontamination Factor] These assumed efficiencies are based on the premises that: (1) the HEPA filters have successfully been through the DOE Filter Test Facility (FTF) at Oak Ridge; (2) they are installed and in-place leak tested to at least 99.95 percent; (3) they are installed in a system built to the specifications of AG-1; and (4) are tested in accordance with national standards.

This assumption is predicated upon the filters in question having been leak tested upon installation and tested thereafter in accordance with national standards. The efficiencies assigned translate to LPF values of 1×10^{-3} for 99.9 percent and 2×10^{-3} for 99.8 percent. Thus, one stage of HEPA filtration has an LPF of 1×10^{-3}; two stages of HEPA filtration have an LPF of 2×10^{-6}. Assuming HEPA filter efficiency of 99.9% for the first HEPA filter stage and 99.8% for the second stage (in series) is appropriate if both HEPA filters are credited in the analysis to reduce consequences, and are designated and maintained as safety SSCs.

Section F.2.1.3 of NUREG/CR-6410 provides the following additional guidance regarding HEPA filter efficiencies to mitigate accidents:

> … HEPA filters must demonstrate a particle collection efficiency of >99.97 percent for 0.3-µm diameter particles and have a particle collection efficiency of >99.95 percent for similar sized particles in-situ (installed in the system). For accidents in which conditions at the HEPA filter are unchanged from normal operating conditions, use of the in-situ tested efficiency is recommended for analysis (Elder et al., 1986). If a series of HEPA filters is protected by pre-filters, sprinklers, and demisters, efficiencies of 99.9 percent for the first filter and 99.8 percent for all subsequent filters is recommended for accident analysis (Elder et al., 1986). If conditions are severe or the filters are

> unprotected, efficiencies as low as 99 to 95 percent are recommended (USNRC 1978).

Even if tested after installation and periodically to meet industry standards, some DSA mitigated analyses have credited a smaller LPF (e.g., 0.01 or 0.1) since that was sufficient to reduce the unmitigated offsite and CW doses to low consequences (see Table 2-8, Consequence Thresholds. However), if unprotected, the filter may be breached by flame impingement, which will open up the leak path to near unity or it may be located remote from flame but be plugged by soot or other factors (as specified in DOE-HDBK-1169, Chapter 10); further discussion on this topic is found in Section 4.2.3.2 of this Handbook. Any modeling of LPF (e.g., through the use of computer codes such as MELCOR) will have to account conservatively for the damage to HEPA filters by fire conditions.

5.2.5.2 LPF MODELING

A more realistic estimation of the LPFs associated with complex pathways (e.g., rooms, corridors, stagnant supply and exhaust ducting) other than HEPA filtration also have the potential to significantly reduce release estimates for the DSA mitigated analysis (Ma, 2006). If the release passes through long passageways, cracks, or torturous routes before exiting to the atmosphere, fall-out and plate-out can be considered in determining LPF. It is possible to calculate how much material of a given size range will deposit out in the time it takes to navigate the available release paths. When multiple paths are present, LPFs may be specified individually for each path, or may be summed into one overall LPF. In more complex cases, each path normally is assigned its own LPF. As the LPF for aerosol particles depends on particle size, multiple LPFs may be assigned for various size ranges as well.

Determination of LPFs less than unity takes a variety of forms. Quantitative LPFs can be performed by hand calculations or by using a variety of computer codes, each dependent upon the complexity of the facility, the specific release parameters and the magnitude of unmitigated accident consequences. As would be expected, small LPFs require substantial justification, particularly if the LPF is the dominant parameter and necessary in the reduction of accident consequences below the safety classification guidelines discussed in Chapter 10.

Because of this strong dependency on the facility and phenomenology of the release, default LPF values are not recommended. There are several hand-calculation methods to calculate the parameters that go into developing a LPF. One method is NUREG/CR-6189, *A Simplified Model of Aerosol Removal by Natural Processes in Reactor Containments*, developed by Sandia National Laboratories for the NRC.

NUREG/CR-6410, Chapter 4, also provides guidance on calculating LPFs. It describes the phenomena that control transport through buildings. Such phenomena include ventilation and other flows of air, filters that remove particulates, and various effects such as gravitational settling, impaction on surfaces, thermophoresis. A portion of the introduction to that chapter is reproduced as follows:

> This chapter describes in-facility transport and deposition of gases, heavy gases, vapors, and particles, together with controlling parameters, basic aerosol physics, and airborne chemical reactions. The chapter emphasizes airborne particles, because such aerosols seem to predominate in accidents that might occur in fuel cycle facilities. The quantitative value that expresses the fraction of initially airborne material that successfully escapes the facility is called the Leakpath Factor (LPF). For particles, the LPF primarily depends on three parameters: the flow rate of the aerosol through the facility, the particle sizes, and the areas available for deposition of contaminants.
>
> The objective of this chapter is to provide the tools necessary for defining the fraction of accident generated airborne material that escapes the facility and, if desired, the concentrations of airborne material throughout the facility as well as the amount of initially airborne material that has deposited

> within the facility.
>
> This chapter continues the accident analysis process whereby the source term provided in Chapter 3 is carried through and out of the facility. The primary final output is the fraction (for particles, the RF) of the source term that escapes the facility, the LPF. Secondary outputs are the concentrations and amounts deposited in the facility of the initial source term. To obtain these outputs, Chapter 4 provides guidance to help the user: (1) identify the facility barriers that define the flow path of the airborne material in the facility; (2) quantify the driving forces moving material along the flow path; (3) quantify the flow rates along the path; (4) quantify the effects of any mitigating engineered safeguards (e.g., filters); (5) quantify the roles of deposition processes along the flow path; and (6) estimate facility concentrations during the movement of the airborne source term.

Computer codes can be used to support LPF calculation for the mitigated analysis. Computer code calculations should be considered for highly complex facility configurations where multiple release paths exist and the relative importance of the various leak paths is not obvious. The computer codes are also extremely beneficial in the cases of time-dependent phenomena (e.g., propagating fires) and when the contaminant transport processes are complex, such as is the case where wide particle size distributions and coupled transport and deposition (e.g., agglomeration) processes exist.

The DOE Central Registry Toolbox code, MELCOR (Methods for Estimation of Leakages and Consequences of Releases), has been applied for some DOE nonreactor nuclear facilities and DOE has established code guidance supporting its use. MELCOR is a fully-integrated, engineering-level computer code whose primary purpose is to model the progression of accidents in light water reactor nuclear power plants. Major uses of MELCOR for nonreactor facilities include estimation of confinement behavior due to radiological source terms under postulated accident conditions, and their sensitivities and uncertainties in a variety of applications, evaluation of LPFs, and survivability of fans, filters, and other engineering safety features. A conservative LPF analysis should be consistent with the guidance provided in *MELCOR Computer Code Application Guidance for Leak Path Factor in DSA Final Report* (DOE, 2004d) that has been issued identifying applicable regimes in accident analysis, default inputs, and special conditions for using the code.

5.3 CHEMICAL RELEASE SOURCE TERMS

The MAR is the bounding quantity of a toxic chemical or mixture of toxic chemicals that is available to be acted upon by a single or series of physical stresses or insults from a postulated accident. Toxic chemical source terms may be evaluated using DOE-HDBK-3010-94, if appropriate, for a non-reactive toxic chemical release phenomenology or non-volatile liquid.[43] These source terms include airborne particulates suspended from accident stresses on solids, as well as the particulates (i.e., aerosols) from the non-flashed portion of pressurized liquids, aerosols from heating of liquids or free-fall spills, and aerosols aerodynamically entrained over time; all using the five-factor formula. However, the burden of proof is on the analyst to establish whether the bounding value or formula presented in that reference is an accurate representation of the particular accident phenomenology. Additional guidance related to the application of DOE-HDBK-3010-94 for chemical source terms is provided in “Applicability of Airborne Release Fraction and Respirable Fraction Values to Particulate Toxic Chemical Material Releases at DOE Sites” (Laul et al., 2006).

An alternative to the five-factor formula to calculate toxic chemical liquid and gas release source terms is

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[43] Liquid that does not readily evaporate at normal ambient temperature and pressure due to its very low vapor pressure.

the EPA 40 CFR Part 68 methodology for worst-case scenario development provided in EPA-550-B-99-009. Detailed guidance, in Chapter 3 of that reference, is generally an appropriate starting point for determining release rates and release quantities for a full spectrum of releases of toxic chemical gases and liquids. However, that EPA reference is silent with respect to releases of airborne particulates suspended from accident stresses on solids, and for non-volatile liquids where vapor pressures are very small or where vapor pressure data are not available. In most cases, an RF value less than 1.0 should not be applied for chemicals given that chemical particulates larger than respirable that have not deposited out of the plume at the CW or MOI location may pose a health risk. For example, a particulate needs only be inhalable to have a health impact, and skin absorption can play a role in a chemical's toxicity although it is not specifically addressed in the derivation of concentration guidelines.

ARFs and RFs, which are highly dependent on particle size distributions and evaporative effects on aerosols, are selected based on physical conditions and stresses anticipated during accidents. For calculating toxic chemical releases from gases and liquid evaporation, the above more current EPA methodology is preferred. However, if EPA methodology does not provide relevant guidance for the accident scenario, DOE-HDBK-3010-94 defines bounding ARF and RF mechanisms based on the physical context of the accident stress. These include phenomena affecting liquids and powders such as a free-fall spill, fire or heating of a substance, and shock or blast effects (e.g., overpressures) from an explosion or detonation. These energetic phenomenologies are described in more detail in Chapter 4 (Section 4.3, Explosion Analysis), and in Section 9.5, Toxic Chemical Release Phenomenology and Subsequent Atmospheric Transport and Diffusion.

Section 5.2.4 and Table 5-1 summarize airborne release rate recommendations from DOE-HDBK-3010-94 that are applicable to aerodynamic entrainment of radioactive materials as a function of time. Those recommendations may also be applicable to toxic chemical releases involving suspension of toxic chemical powders or aerosols from heating of liquids.

The toxic chemical source term calculation generally results in a constant (i.e., linear) release rate in units of mass per unit time, or total release quantity in units of mass coupled with a specified release duration in units of time. For pressurized gas and pressurized liquid releases or evaporation of volatile liquids, the release rate is non-linear, varying over time, as indicated in Section 9.5. If the toxic chemical source term is not calculated as a constant release rate over the accident duration for solids, or as a pool evaporation rate for liquids and gases, the total airborne release quantity should be divided by the release duration consistent with the postulated scenario assumptions, or by recommended conservative estimates from the aforementioned guidance documents that appropriately address non-linear release phenomenologies.

For the calculation of toxic chemical releases from a chemical process, if dilution is inherent in the release pathway, dilution effects may be incorporated into the analysis by determining the concentration of the chemicals in the total stream flow that includes the offgas generation and a carrier gas such as fresh air. This stream flow concentration at the exhaust stack discharge is used to establish the toxic chemical release rates to the atmosphere. The stack discharge rate accounts for dilution effects of a carrier gas in the exhaust path starting above the liquid surface of the chemical reactions and ending at the exhaust stack discharge location. This can be calculated as a volume of toxic chemicals generated per unit time, as adjusted by the density of the toxic chemicals mixed with the carrier gas at the point of release from the facility.

This type of analysis accounts for fresh air entrainment in the process ventilation system due to ambient air exchanges with the environment for the unmitigated analysis, or the active process ventilation system for the mitigated analysis. These quantities represent the source term of the toxic chemicals in units of mass per time (e.g., mg/s) that are input to the 95th percentile dispersion conditions as discussed in

Section 9.7, Toxic Chemical Atmospheric Transport and Diffusion Models, for the determination of concentrations and resulting consequences to the CW and MOI.

For the unmitigated analysis, this adjustment may consider the mixing volume of the toxic chemicals generated at the chemical process location, diluted with ambient air exchange as driven by the outside environment. The dilution of the toxic chemicals from the process generation location, which is a function of the volume of the release path and ambient air exchange with the outside environment, may be performed using methodologies discussed in Section 5.2.5. Accounting for in-facility dilution effects is not the same as a LPF; it is considered to be a phenomenological component of the source term determination. The analyst, with the assistance of a HVAC engineer and chemical engineer, can establish the ambient air exchange factor based on the specific design of the process and the ventilation system. Another factor that may affect the unmitigated analysis is the stoichiometry of toxic chemical generation that may rapidly decay with the limited amount of air available since active ventilation is not credited, that is, the source term release rate would be nonlinear. See Chapter 6 discussions regarding an unmitigated analysis crediting an effective stack height due to a passive physical feature (i.e., discharge from an elevated stack), and/or may credit buoyancy effects due to a conservative estimate of offgas temperature at the point of release to the environment. Both of these effects would result in improved atmospheric dispersion. The assumptions of no active ventilation and crediting of the release from a stack with plume buoyancy due to the high temperature of the offgas are consistent with unmitigated analysis guidance in DOE-STD-3009-2014.

For the mitigated analysis, the analyst may consider crediting active ventilation. The ventilation flow will dilute the toxic chemical releases before discharge to the atmosphere (i.e., the source term release rate), and it may also drive a momentum flux at that release point, as discussed in the plume rise discussion in Chapter 6. For a chemical process, the toxic chemical reaction rate may be linear or nonlinear. Therefore, the first 15-minute release rate may be the most bounding unmitigated estimate and could be affected by other factors such as combustion/reactant air supply. A conservative estimate for the 15-minute decay period could be made if the release rate drops rapidly.

To illustrate the above discussion, consider an example release of nitrous oxide (NO) from a chemical process in a vessel provided with 1,000 cfm of process ventilation (air as the carrier gas) that is discharged to the atmosphere. An unmitigated analysis does not credit depletion due to filtration and an offgas treatment system. To simplify the illustration, although many species may be generated in the vessel offgas that are in the form of gases or aqueous vapors, this example evaluates a single toxic chemical. The NO has a mass generation rate of 11.7 kg/hr (3,250 mg/s) that is one of the constituents in the stream that has a total mass flow rate of 1,700 kg/hr. Therefore, NO contributes approximately 0.7% to the mass release rate from the stack (without considering the effect of the ventilation flow which would not substantially add to the mass flow rate). The stream density (NO mixed with other constituents at the point of generation) is 0.366 kg/m^3. For this density, the volume NO flow is 19 cfm and the total gas flow of 1,700 kg/hr has a volume flow of 2,700 cfm. Further assume that the total gas flow is mixed prior to entering a stack with an air flow of 1,000 cfm. To credit dilution, the ratio of NO flow to total stream flow is used to adjust the NO mass generation rate (3,250 mg/s) in the vessel. If the total stream flow is composed only of NO, the fraction is one and the NO leaving the stack is 3,250 mg/s. When the total gas stream (NO + remaining offgas parameters) is credited, the fraction is 19 cfm / 2,700 cfm = 0.0069 and the diluted NO leaving the stack is 22.4 mg/s. Similarly when the air dilution of 1,000 cfm is credited, the fraction is 19 cfm / 3700 cfm = 0.0050 and the diluted NO leaving the stack is 16.4 mg/s.

5.4 APPROPRIATENESS OF SOURCE TERMS

The brief discussions and associated examples in Section 5.2 should serve to clarify that source term determination is not an exact science. Instead, it involves a reasonable definition of circumstance, which is then broken down into a sequence of oversimplified parameters. This limited representation of reality demands a certain degree of conservatism to overcome the uncertainties introduced by the simplification.

No source term can account for all of the parameters introduced by first engineering principles, and this process may be subject to abuse. As an example, consider a glovebox with plutonium-239 powder collapsed by a seismic event and associated falling debris. It is possible to define the event so as to eliminate any consideration of the ARF/RF of 2E-3 associated with debris impacting the powder even if the actual facility configuration does not support such an assumption. This can be done by making poor assumptions relative to shielding effects or the nature of the debris falling, or by probability arguments that are not defendable. This can be minimized by standardization, expert elicitation and independent review. DOE-HDBK-3010-94 was prepared to facilitate the development of some consensus among DOE oversight and facility operators regarding a conservative estimate of consequence potentials. That consensus is necessary to effectively implement integrated safety management by minimizing the subjectivity in source term assessment.

The basis for determining source term appropriateness is to use a combination of parameters on the upper end of any potential uncertainty. That does not mean an average value, or even a 95th percentile value, since meaningful informed statistical distributions cannot be generated for most of the accidents under consideration. Instead, it means that a general consensus exists on upper and lower bounds for the cumulative scenario definition and associated parameter specifications, which should yield a source term in excess of the actual event that is not excessively conservative.

5.4.1 ADEQUATE TECHNICAL BASIS TO DEPART FROM DEFAULT OR BOUNDING VALUES

Section 3.2.4 of DOE-STD-3009-2014 states:

> Calculations shall be made based on technically-justified input parameters and underlying assumptions such that the overall consequence calculation is conservative. Conservatism is assured by the selection of bounding accident scenarios, the use of a conservative analysis methodology, and the selection of source term and input parameters that are consistent with that methodology.
>
> For some input parameters, this section identifies default or bounding values that may be used without further justification. Unless otherwise stated for a particular input value, this section allows use of alternative values when supported by an adequate technical basis. When an input parameter used is not a default or bounding value, an acceptable technical basis of the value describes why the value selected is appropriate for the physical situation being analyzed, and references relevant data, analysis, or technical standards. The completeness and level of detail in the technical basis should increase as the parameters depart from default or bounding values.

Additional guidance to develop an adequate technical basis that departs from default or bounding values is the focus of this subsection. There are two fundamental reasons for departing from default or bounding values:

1. It may be expedient to use clearly bounding and conservative values to demonstrate that no controls are necessary, which will result in a simplified analysis; and

2. Default values for a specific site may be too conservative leading to unnecessary burdensome controls.

For expediency, the analyst may perform a consequence calculation by simply using clearly bounding assumptions along with bounding and/or default input parameters provided in DOE-STD-3009-2014, DOE-HDBK-3010-94, or other sources such as NUREG/CR-6410, because the values to be used are easily identified and readily defended as bounding and conservative. The dispersion analysis Option 2 discussed in Section 6.10 of DOE-STD-3009-2014 is an example using this approach. If such a consequence calculation shows that no controls need to be SC or SS, then no refined or more complicated calculation is needed to classify controls. However, this approach generally results in an overestimate of consequences and likelihoods, sometimes by orders of magnitude. If this very conservative calculation yields consequences that exceed thresholds for control classification, a more refined analysis is performed unless implementing and protecting the controls derived from the simplistic analysis has a small impact on schedule and cost, especially lifecycle cost.

As calculations are refined, conservatism in the analysis is reduced, with appropriate technical justification, but no further than the point where either: (1) individual input parameters and underlying assumptions are less conservative than a best estimate (i.e., mean value) of their expected values during the accident scenario; or (2) the overall result of the consequence calculation is not conservative. Option 3 in Section 6.10 is an example using this approach to refine calculations after the required approvals are obtained.

Another example would include testing model results against a large and varied experimental database which includes data points measured under bounding circumstances. The analyst would then show, for every measured data point, whether the overall result of the model was bounding of the measured data point. The model inputs would have to be “fair and reasonable” in that the input parameters used while testing the model would have to be applicable to the conditions of each experimental data point. For example, it would not be reasonable to input a bounding temperature or flow rate into the model if the bounding temperature or flow rate is not representative of the measured data point used to test the model. This type of model-data test could be used to demonstrate overall conservatism of a modeling strategy.

Three requirements in DOE-STD-3009-2014 are important to providing assurance that consequence calculations are conservative for plausible accident scenarios, NPH events, and external man made events:

1. MAR values used in hazard and accident analysis shall be consistent with the values noted in hazard identification/evaluation, and shall be bounding with respect to each accident being evaluated.[7] [Section 3.2.4.1]

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    [7] For facilities that provide retrieval, handling, storage or processing of TRU waste containers, a bounding MAR may be determined in accordance with DOE-STD-5506-2007.

2. Radiological consequences are presented as a TED based on integrated committed dose to all target organs, accounting for direct exposures as well as a 50-yr commitment. [Section 3.2.4.2]

3. While the three options allow for alternative methods to calculate the χ/Q values, all three options shall evaluate the dose at the MOI using either a 95th percentile for a directionally independent method or a 99.5th percentile for a directionally dependent. Conservatism of the X/Q value is ensured by using 95th or 99.5th percentile site-specific meteorology. All other values in the X/Q analysis do not need to be bounding to ensure a conservative result; past analyses have shown that piling up a number of conservative assumptions can lead to results representing a higher percentile above the 95th or 99.5th. This is also true for the overall accident consequence evaluation if all the other input values were selected at their maximum measured or theoretical values, hence, the reason for establishing the original bounding or default values in DOE-HDBK-3010-94 and DOE-STD-3009. [Section 3.2.4.2]

When default values are too conservative, resulting in unnecessary controls for unrealistic scenarios, input parameters can be adjusted if there is sufficient technical justification to show that the new parameters are still bounding. The rationale could be based on new representative experimental data on release fractions, or based on evaluation of the experimental data used to recommend bounding ARFs/RFs in DOE-HDBK-3010-94. For example, a bounding value for a free-fall spill of powders is based on a drop at a 3-m height. Typical glovebox operations in nonreactor nuclear facilities requiring manual operations could be evaluated based on a 1-m fall height for either a spill within the glovebox, or a seismic-induced toppling of the glovebox[44] based on the experimental data that provided the basis for the 3-m spill. Considerations should include the following factors:

- Representativeness of the data to the accident scenario being evaluated;
- Statistical completeness of the data (e.g., based only on a few samples?);
- Pedigree of the data; and
- Available data on particle sizes within the application domain of the calculation.

Regarding representativeness of the data, consider whether the data is applicable to the conditions of the bounding design basis accident being analyzed. Examples include drop height, explosion energy, fire severity, and other environmental considerations.

As a matter of practice, detailed statistical analyses are not necessary, nor expected. A review of the experimental data and what percentile ranking the selected alternate value is may provide some insights for the decision. However, DOE-HDBK-3010-94, Section 1.3, provides cautions regarding interpretations of the experimental data and that the experimental data should not be used as a basis for an ARF statistical distribution.

In some instances, the data available to support selection of input parameters are not prototypic of the situation being analyzed, or there is large uncertainty. Hence, sound technical judgment is essential in selecting appropriate input values, considering the range of possible values given the physical and chemical conditions involved with the accident scenario and the relevant uncertainty. Although some degree of subjective engineering judgment may be necessary, the rationale needs to have a technical basis and not just opinions. Expert elicitation is essential to the success of this process.

The completeness and level of detail of the rationale used in technically justifying individual input parameters increases as the parameters approach more realistic values. The methodology used in

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[44] Other release mechanisms are also applicable as discussed in the DOE-HDBK-3010-94, Chapter 7.0, Application Examples.

selection of input parameters and analysis should not lead to unrealistic accident scenarios and concomitant consequence estimates, nor an overall realistic estimate of consequences that may be appropriate for a comprehensive probabilistic risk assessment (PRA). An example of an approach previously justified in a DSA is related to a facility-wide seismic evaluation where median ARF/RF values were applied for a large facility with MAR in many locations that would be acted upon by a common stressor such as a spill. Applying the bounding ARF/RFs with the maximum MAR and DRs would have resulted in an overly conservative estimate due to compounding conservatisms that could have resulted in unnecessary SS controls and potential physical upgrading of the structure and equipment to meet current seismic standards. The burden is on the safety analyst to justify that the overall consequence estimates will be sufficiently conservative for the purpose of determining the need for safety SSC or SACs. The following quote from DOE-STD-3009-94 CN3 (Section 3.4.2.X.2) should be kept in mind: “The degree of conservatism believed to be present in the calculation needs to be consistent with the Evaluation Guideline definition.” As alternate values depart from the bounding or default values, at some point the calculation will not meet the original intent of the Evaluation Guideline based on a conservative analysis.

It is plausible to discern if there is a lesser or greater degree of conservatism in a calculation, but it will always be difficult and require judgment to determine the adequate level of conservatism. Another consideration regarding conservatism is from DOE-HDBK-3010-94 Section 7.3.6.2, Release Estimation,” that states:

> In the examples in this handbook, DRs are typically bounded by assuming a value of 1.0 for the sake of simplicity. The above discussion indicates how conservative such a bound can be. It is important not to lose sight of the fact that the phenomena being examined are generally unlikely to highly unlikely. By the time a maximum MAR has been assumed, the DR has been maximized as 1.0, the bounding ARFs and RFs of this document have been applied, no leakpath is accounted for, and 95% or greater meteorology has been used for dispersion, the answer obtained is extreme. Objectivity must be retained in the evaluation process so that a rote conception does not distract available resources from areas where greater real gains in safety can be made. As previously cautioned in this handbook, answers obtained are only as good as the decisions they lead to.

6 ATMOSPHERIC DISPERSION

6.1 INTRODUCTION

Radiological and/or chemically hazardous materials released into the environment can be transported to potential receptors through air and water pathways. This chapter discusses the mechanisms of atmospheric transport and diffusion, collectively referred to as *dispersion*, of such pollutants. Chapter 8 discusses the consequences of exposure to radioactive materials and Chapter 9 discusses dispersion principles specific to chemical releases (such as dense gas dispersion).

The basic equation for the calculation of radiological inhalation dose to a downwind receptor is:

$$Dose\ (rem) = ST \times \chi/Q \times BR \times DCF \qquad \textbf{Equation 6-1}$$

where

ST = source term (Ci), as discussed in Chapter 5

χ/Q = atmospheric dispersion factor (s/m^3), discussed below

BR = breathing rate (m^3/s), and

DCF = dose conversion factor (rem/Ci)

This chapter and Chapter 8 address the recommended approach to evaluating the terms in the above equation. This discussion is intended to be a practical guide and thus discusses these topics only to the extent needed to support a given topic in order to calculate potential consequences to receptors downwind for the DSA accident analysis. Only atmospheric (airborne) dispersion is addressed in this chapter, as DOE-STD-3009 excludes waterborne pathways from consideration in a DSA, except when the water pathway could significantly contribute to the overall radiological consequences. However, Chapter 7 does provide some guidance on aquatic dispersion principles with respect to infrequent releases of radioactive materials into water bodies. That chapter also briefly addresses groundwater transport.

For in-depth background on atmospheric dispersion, consult these references:

- *Workbook of Atmospheric Dispersion Estimates, An Introduction to Dispersion Modeling* (Turner, 1994), which is based on *Meteorology and Atomic Energy (*Slade, 1968);
- *Atmospheric Science and Power Production* (Randerson, 1984);
- *Atmospheric Diffusion, Study of the Dispersion of Windborne Material from Industrial and Other Sources* (Pasquill and Smith, 1983);
- *Radiological Assessment: A Textbook on Environmental Dose Analysis* (NRC, 1983);
- *Radiological Risk Assessment and Environmental Analysis* (Till and Grogan, 2008); and
- DOE Central Registry "Toolbox Code"[45] guidance documents listed in the Chapter 11, *References*.

In addition, *Directory of Atmospheric Transport and Diffusion Models, Equipment, and Projects*, is an excellent background source for 64 dispersion models (OFCM, 1998).

6.2 KEY RECEPTORS

The concentrations of pollutants at selected downwind distances are estimated in order to calculate the consequences to hypothetical receptors. DOE-STD-3009-2014 identifies two generic receptors[46] to be considered in accident analyses involving atmospheric dispersion, the CW and the MOI.

> **CW**: A hypothetical worker located at a distance of 100 m from a facility (building perimeter) or estimated release point, defined to allow dose comparison with numerical criteria for selection of Safety Significant (SS) controls described in Chapter 2. The CW may be located at a farther distance if an elevated or buoyant radioactive plume causes a higher exposure beyond the 100 m distance. For ground level releases, DOE-STD-3009-2014, Section 3.2.4.2, specifies the CW χ/Q value as 3.5E-03 s/m^3 (based on NSRD-2015-01, Technical Report for Calculations of Atmospheric Dispersion at Onsite Locations for Department of Energy Nuclear Facilities [DOE/ONS, 2015]).[47] For situations

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[45] "Toolbox code" is a term used to identify software qualified to be listed in the DOE Safety Software Central Registry (http://energy.gov/ehss/safety-software-quality-assurance-central-registry) that is used primarily for DOE safety analyses. The toolbox codes for atmospheric dispersion are discussed later in this section.

[46] A third generic receptor, the facility worker (FW), is also considered in the DSA hazard evaluation. The FW is a worker within a facility boundary and located less than 100 m from the release point. Atmospheric dispersion is not considered for this worker.

[47] DOE-STD-3009-2014 Section 3.2.4.2 does not specify the CW χ/Q value for elevated or buoyant releases. It does allow a value other than 3.5E-03 s/m^3, if technically justified. See Section 6.13 for more discussion and methods to calculate an alternative value and for a justification of the 3.5E-03 s/m^3 value.

where a release is from a facility significantly smaller than that assumed in the default parameter (i.e., a 10-meter tall by 36-meter wide building), or if a building is not present, the default χ/Q value may not provide a conservative estimate of dispersion.

MOI: A hypothetical individual representing the public, defined to allow dose comparison with an EG for selection of SC controls described in Chapter 2. The MOI is located at the point of maximum exposure on the DOE site boundary of the facility in question for a ground level release, or at some farther distance if an elevated or buoyant radioactive plume produces a higher exposure (elevated release) beyond the site boundary. Although this definition is specifically for radiological exposures, it can be extended to toxic chemical exposures as well for selection of SS controls as described in Chapter 10, Hazard Control Selection and Classification.

Per DOE-STD-3009, “the DOE site boundary is a geographic boundary within which public access is controlled and activities are governed by DOE and its contractors, and not by local authorities. A public road or waterway traversing a DOE site is considered to be within the DOE site boundary if DOE or the site contractor has the capability to control, when necessary, the road or waterway during accident or emergency conditions.”

Radiological exposure is treated differently than exposure to toxic chemical emissions. For radiological exposures, the total time-integrated effective dose (primarily due to inhalation dose) is normally of interest because it is bounding for most radionuclide releases. To be conservative, the receptor is assumed to remain in the plume centerline during the entire period of plume passage, although evaluations for mitigated analysis may consider engineered safety features and emergency management dose-reduction measures (evacuation, sheltering) for the CW. For toxic chemical exposures, on the other hand, a TWA, or peak concentration during some exposure period (such as 15 minutes) is normally of greatest interest. This is addressed further in Chapter 9.

6.3 METEOROLOGICAL PARAMETERS AFFECTING DISPERSION

Once released into the atmosphere, radiological and toxic chemical emissions are transported in the direction of the wind and diffused by atmospheric turbulence[48] in the horizontal and vertical planes. This atmospheric turbulence consists of random, chaotic air motion in the form of countless whirling eddies. These eddies have a great range of size, from millimeters to tens or even hundreds of meters in diameter, with the smaller eddies being embedded within the larger ones (Richardson, 1927). When a plume of radiological or toxic chemical material is released into the atmosphere, the smaller eddies cause the material to diffuse within the plume, while the larger ones cause the plume to meander, mostly in the horizontal plane. These turbulent eddies are formed by surface frictional effects (mechanical turbulence) and by vertical gradients in both the velocity and the temperature of the air (mechanical turbulence and buoyancy), as discussed below.

A puff or plume that is released at the ground level grows vertically due to vertical diffusion. It reflects vertically from the ground surface and from the top of the mixed layer, which act as vertical boundaries. This is discussed more fully below.

Figure 6-1 displays the atmospheric and terrestrial processes determining the ultimate fate of a radionuclide or chemical pollutant after it is released to the environment. These highly complex

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[48] Molecular diffusion is much slower than turbulent diffusion in dispersing materials, and much smaller in scale, and thus may be ignored.

interactions of physical phenomena with underlying topography and foliar populations are extremely difficult to describe mathematically. In order to approximate the effects of such phenomena, a Gaussian plume model has found wide application.

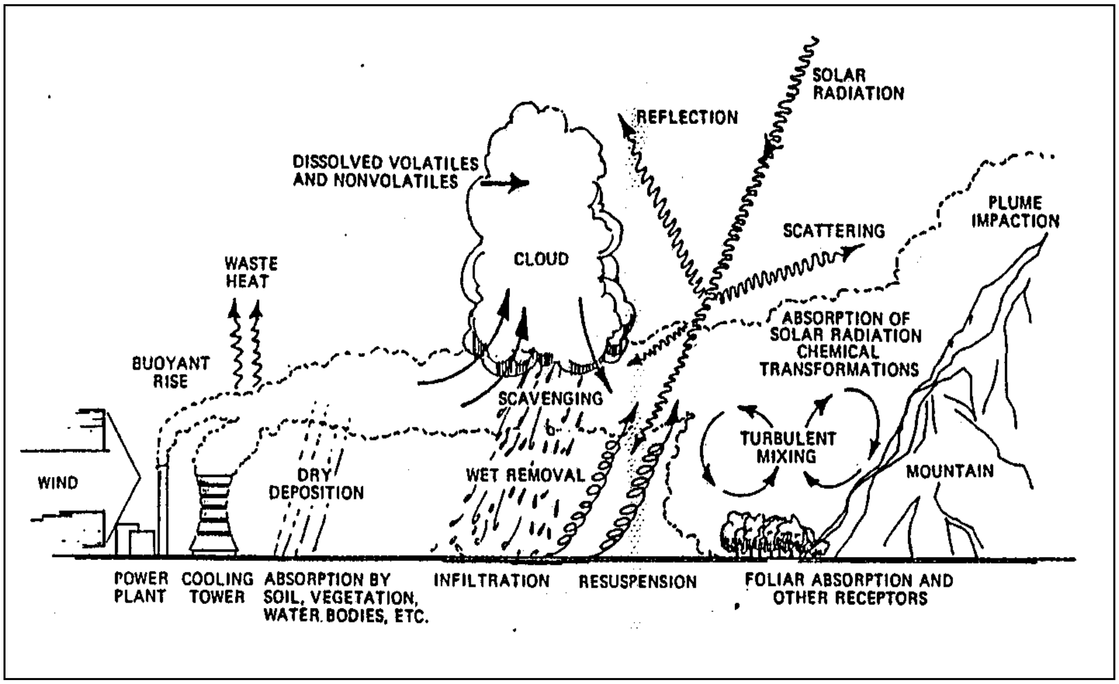

Figure 6-1. Atmospheric and terrestrial processes involved in determining the ultimate fate of a radionuclide or chemical pollutant.

The meteorological parameters affecting dispersion are discussed in the following subsections.

6.3.1 WIND SPEED, WIND DIRECTION, AND WIND DIRECTION STANDARD DEVIATIONS

Wind velocity is a vector quantity, having both magnitude and direction. Its magnitude is the wind speed. Variations in both magnitude and direction are important in dispersion.

6.3.1.1 WIND SPEED

The wind speed at the height of the release determines the travel time to reach a given downwind receptor and the amount of *initial* dilution from the point of release. The greater the wind speed, the more "stretched out" the plume will be and the more surrounding air will be mixed in. It is also a factor in determining the magnitude of atmospheric stability, which is discussed below. Mechanical turbulence is generated in the air when adjacent parcels of air move at different velocities, either at different speeds or in different directions; this is termed wind shear. Thus, a change in wind speed with height above the ground, or a variation in wind direction at different heights above the ground, causes mechanical turbulence. Mechanical turbulence is also generated when air interacts with some fixed object, such as the ground, described by roughness length, or with a building, described by aerodynamic effects (wake, cavity).

Short-lived radionuclides may decay appreciably if the transport time of the puff or plume to a receptor is long. The horizontal wind speed used in Gaussian models is based on the average wind speed over a selected time, usually fifteen minutes or one hour. Gaussian models are very conservative under light wind speed conditions (<1 m/s) since such conditions are too variable to be accurately approximated by a steady-state code. See Section 6.5.4.

6.3.1.2 WIND DIRECTION

The horizontal wind direction at the height of the release determines the initial direction of transport. The horizontal wind direction used in Gaussian modeling is the average, or first moment, of a series of "instantaneous" wind direction measurements. In meteorology, wind direction has traditionally been defined as the direction *from which* the wind blows, which is of interest to weather forecasters. However, most computer models for dispersion and consequence applications use wind direction to mean the direction *toward which* the wind blows. For example, a SE wind (as termed by meteorologists) will transport the plume to the NW. For a steady-state straight-line Gaussian model, once a plume segment is released, its direction of transport typically remains the same in time and space, as do the wind speed, turbulence intensities, and release rate. The MACCS2 code allows different segments to move in different directions.

6.3.1.3 WIND DIRECTION STANDARD DEVIATIONS

Atmospheric turbulence is directly related to the variability of the instantaneous wind speed and direction. This variability is normally expressed in terms of the standard deviation of a series of "instantaneous" wind direction measurements over a selected observation period, normally 15 minutes. The standard deviation, or second moment, of the horizontal wind direction (σ_θ) is commonly used to type atmospheric turbulence into stability classes. Some DOE sites also include the standard deviation of the vertical wind component (σ_φ) to type atmospheric turbulence, as discussed further in Section 6.4.2.2.

6.3.2 WIND SPEED PROFILE WITH HEIGHT

Wind speed varies with height in the Planetary Boundary Layer (PBL). It is often characterized with an equation known as the wind profile power law, which is a relationship between the wind speed at one height, and wind speed at another height. Winds generally increase with height as the frictional effects of the Earth's surface decrease as the distance from the surface increases. When the frictional effects of the surface are no longer felt, the upper boundary of the PBL, and bottom of the free atmosphere, is reached and the winds are termed geostrophic.

The wind profile of the PBL is generally logarithmic in nature (see PNNL-14584) and is best approximated using the logarithmic wind profile equation that accounts for surface roughness and atmospheric stability. However, the wind profile power law relationship is often used as a substitute for the logarithmic wind profile when surface roughness or stability information is available. Figure 6-2 presents a simplified representation of the logarithmic wind profile in the PBL, showing how wind speed increases with the height above the ground due to the reduction in the ground's frictional effect with height above the ground level.

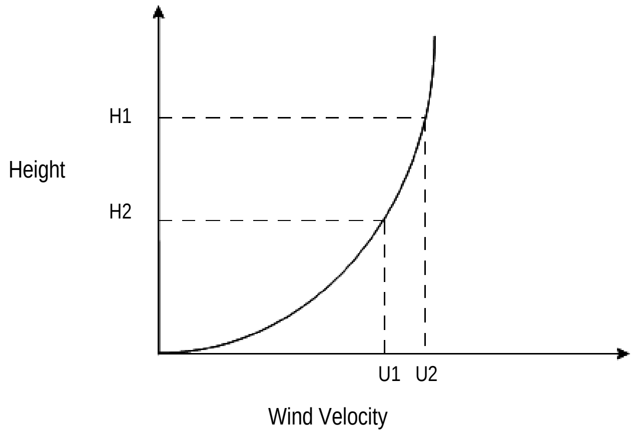

Figure 6-2. Logarithmic Wind Profile.

The wind profile power law relationship is described by:

$$u/u_r = (z/z_r)^{\alpha} \qquad \textbf{Equation 6-2}$$

where

u = wind speed (m/s) at height z (m);

u_r = known wind speed at a reference height z_r; and,

α = empirically derived coefficient that is dependent upon stability of the atmosphere. For neutral stability conditions and a rural environment, α is approximately 1/7, or 0.143. For urban environments it is somewhat larger (EPA, 2000).

6.3.3 MIXING LAYER HEIGHT

For an evaluation of χ/Q that includes reflections from the ground and the top of the mixing layer, knowledge of the height of the top of the mixing layer at the site is required. Mixing height is the height above which relatively vigorous vertical mixing essentially stops; the layer from the ground to mixing height (mixing depth) is where vigorous vertical mixing occurs. Low mixing heights are related to a meteorological circumstance where air is generally stagnant with very little vertical motion and where radiological and toxic chemical emissions are usually trapped in a narrow layer near the ground surface. Under very stable conditions (F or G stability), the temperature inversion that is common to this stability class is typical of a low mixing height. Correspondingly, high mixing heights allow vigorous vertical mixing within a deep layer of the atmosphere and accordingly a good dispersion capacity.

Mixing heights can be used to estimate how far plumes rise in the vertical. The actual rise of a plume, however, considers complex interactions between atmospheric stability, wind shear, and heat release rate, density differences between the plume and ambient air, and radiant heat loss. Accordingly, an estimate of mixing height provides only an initial estimate of plume height, but with respect to DSAs, it is sufficient.

Mixing height varies throughout the day and throughout the seasons, since it is directly related to the amount of insolation that reaches the ground level. Mixing heights are usually lowest late at night or early morning and highest during mid- to late-afternoon. Average morning mixing heights range from

300 m to over 900 m above ground level (EPA Publication No. AP-101) for many locations in the United States. The highest morning mixing heights occur in coastal areas that are influenced by moist marine air and cloudiness that inhibit radiation cooling at night. Average afternoon mixing heights are higher than morning mixing heights and vary from less than 600 m to over 1400 m above ground level. The lowest afternoon mixing heights occur during winter and along coastal locations. Mixing heights vary considerably between locations and from day to day. *Smoke Dispersion Prediction Systems* (Ferguson, 2001) generated detailed maps and statistics of mixing heights in the United States that can be useful to the analyst.

The actual magnitude of the mixing heights can be obtained from Rawinsonde balloon soundings or from remote sensing techniques, such as sound detection and ranging (SODAR) and light detection and ranging (LIDAR). These remote sensing systems are becoming more commonly used at DOE sites and provide real-time data on the vertical structure of the atmosphere; whereas Rawinsonde data are discrete and specific to the time of each balloon release; usually at 12-hour intervals and perhaps at distances far from the DOE site. In the absence of such data, regional tables can be consulted, such as those in *Mixing Heights, Wind Speeds, and Potential for Urban Air Pollution throughout the Contiguous United States* (EPA Publication No. AP-101). Each DOE site needs to technically justify its selection of mixing layer height in a dispersion modeling protocol (see Section 6.11).

6.3.4 VERTICAL TEMPERATURE PROFILES

Atmospheric turbulence can also be produced by temperature gradients, especially vertical temperature gradients. The pressure of the atmosphere decreases with height. Therefore, when a parcel of air is displaced vertically, it will expand if rising or contract if sinking to adjust its pressure to that of the surrounding atmosphere. The expansion or contraction is accompanied by an adiabatic (no gain or loss of heat) temperature change. Accordingly, as a parcel rises, it cools. If the surrounding air is warmer, the parcel will be heavier than its surroundings and sink back toward its original position until it reaches equilibrium. On the other hand, if the surrounding air is cooler, the parcel will be lighter and continue to move upward and its vertical motion is enhanced. Similarly, if the air parcel sinks, it warms up as it contracts. If the surrounding air is cooler, the parcel will be lighter and rise back toward its original position until it reaches equilibrium. However, if the surrounding air is warmer, the parcel will be heavier and continue to sink. Thus, turbulence is suppressed if the temperature profile of the air, termed the lapse rate, is less than adiabatic (subadiabatic), and enhanced if greater than adiabatic (superadiabatic). The dry adiabatic lapse rate near ground is about -9.8 °C/km (-5.4 °F/1,000 feet), while the moist adiabatic lapse rate, which depends on temperature, is about -5.8 °C/km (-3.2 °F/1,000 feet); the difference is due to heat required to overcome latent heat of the moisture in the air parcel (Wallace and Hobbs, 1977).

The atmospheric layer near the ground is termed the mixed layer, as this is where atmospheric turbulence is most common. During daylight, the ground heats up, warming the air near the surface through convective eddy transport. The lapse rate near the surface thus becomes superadiabatic and positive buoyancy forces enhance any existing mechanical turbulence caused by ground roughness or wind shear. At night, the ground cools due to release of long-wave radiation, causing the air near the surface to cool, and the lapse rate becomes subadiabatic and frequently inverted, suppressing much of the existing mechanical turbulence. At greater heights, a few hundred to a few thousand meters in altitude, the lapse rate may change. It is common for a turbulent lower atmosphere to be capped by a lapse rate that is subadiabatic so that turbulent eddies rising from below are suppressed. Vertical plume expansion is thus limited, reflecting off the top of the mixed layer, as well as off of the ground.

6.3.5 PRECIPITATION

With regard to precipitation scavenging (rainout, snowout, hailout), the rate of precipitation is needed as an input to models that address this atmospheric phenomenon. Rainout can cause major local deposition of radionuclides leading to radioactive "hot spots" at locations that receive rainfall. However, DOE-STD-3009-2014 does not require, nor does modeling code guidance recommend, the consideration of precipitation scavenging in DSAs. If the analyst wants to include wet deposition, a dispersion modeling protocol should be developed and approved as discussed in Section 6.11 below.

6.3.6 TEMPERATURE AND RELATIVE HUMIDITY

Temperature and relative humidity are not important parameters with respect to the calculation of radiological consequences. However, it is quite important with respect to calculation consequences from toxic chemical releases, which is addressed in Section 9.6.

6.4 GAUSSIAN PLUME MODEL FOR NEUTRALLY BUOYANT PLUMES

6.4.1 BASIC GAUSSIAN EQUATIONS

If pollutants are neutrally buoyant, as in the release of trace amounts of very fine particulates or gases, plume dispersion approximates a Gaussian distribution in both the crosswind (lateral) and vertical directions. As the plume moves downwind, it gets progressively larger and less concentrated. The Gaussian approximation of atmospheric dispersion assumes that as a plume is transported downwind, its horizontal expansion is essentially unlimited[49]. Vertical expansion is limited by the earth's surface and aloft under inversion conditions. The downward expansion of the plume stops at the ground, while upward expansion may be stopped if there is a stable layer (a "cap") at the top of the mixed layer. This cap acts as a lid to rising "thermals" of air, thus restricting the range and magnitude of vertical turbulence. The plume is often considered to "reflect" off both the ground and the top of the mixed layer, causing the *vertical* profile to become increasingly uniform as the plume proceeds downwind. For low level mixing heights, multiple reflections can occur from the ground and lid, especially for far-field receptors.

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[49] Horizontal, or lateral, plume expansion may be somewhat limited by physical barriers, such as buildings and topographic obstacles, but these are normally treated as special cases. Vertical plume expansion is enhanced by these barriers but can also be limited by mixing depth.

Figure 6-3 (Turner, 1994) illustrates the general shape of a Gaussian plume as released from a stack. The coordinate system used in Gaussian equations is shown, in which *x* is defined as the downwind direction, *y* is the horizontal cross-wind direction, *z* is vertical direction, and *h* is the height of release. The height of the plume after release, or effective stack height, is *H*.[50]

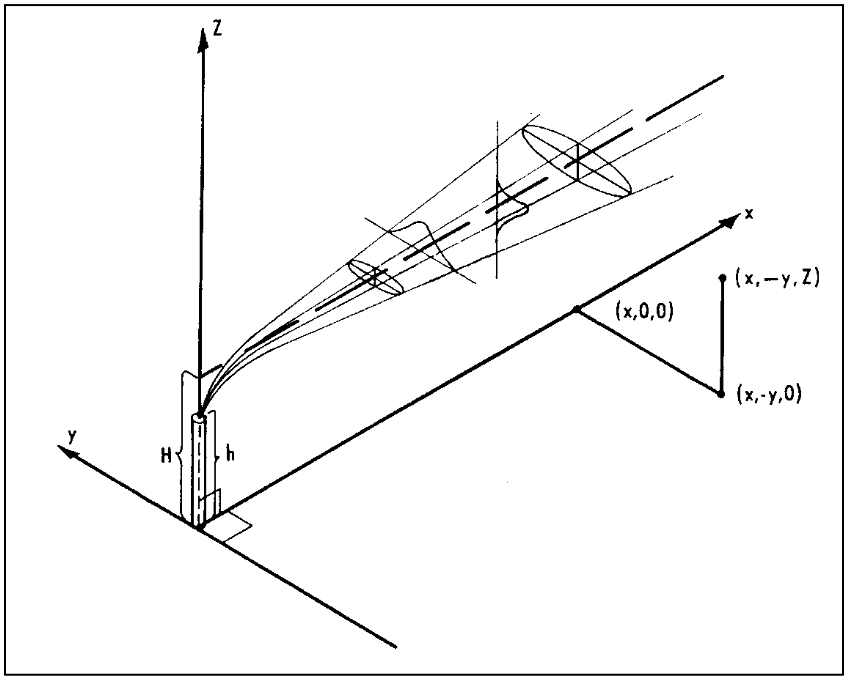

Figure 6-3. Coordinate System of Gaussian Plume.

The amount of atmospheric dispersion is usually expressed in terms of normalized concentration, or χ/Q, where:

χ = the concentration of the radionuclides or toxic chemical in air at some downwind (x, y, z) location; this can be either the instantaneous concentration (e.g., Bq/m^3 or mg/m^3) or the time-integrated concentration (e.g., Bq-s/m^3 or mg-s/m^3), and

Q = the constant rate of radionuclide or toxic chemical release (e.g., Bq/s or g/s), if χ is taken to be the instantaneous concentration, or total source strength (e.g., Bq or g), if χ is taken to be the time-integrated concentration.

The units of χ/Q are s/m^3 whether the instantaneous or time-integrated releases are considered or whether radioactive or toxic chemical releases are being evaluated. Thus, χ/Q is the concentration of the radionuclides or toxic chemical in air at the receptor per unit source rate, or time-integrated concentration per unit source release. The actual concentration of the radionuclides or toxic chemical in air (χ) at the receptor is thus the product of χ/Q and the rate of release of the radionuclides or toxic chemical (Q), as determined by the source term calculations from Chapter 5, Chapter 8, and Section 9.5 of this Handbook.

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[50] The symbol "H" in this figure is shown as "h" in the remainder of this chapter.

When accounting for reflection off the ground, but not constrained by the top of the mixed layer, the Gaussian plume model (Slade, 1968) is expressed as:

$$\frac{\chi(x,y,z,h)}{Q} = \frac{1}{2\pi u \sigma_y \sigma_z} e^{-y^2/2\sigma_y^2} \left[e^{-(z-h)^2/2\sigma_z^2} + e^{-(z+h)^2/2\sigma_z^2} \right]$$ **Equation 6-3**

where

x = downwind distance of the receptor from the point of release (m),

y = horizontal cross wind distance of the receptor from the centerline of the plume (m),

z = distance of the receptor above the ground (m),

h = height of the plume centerline above the ground (m) (same as H in Figure 6-3),

σ_y = standard deviation of the horizontal Gaussian distribution (m) (converted from the “half width” of a rectangular cross-section of a plume),

σ_z = standard deviation of the vertical Gaussian distribution (m) (converted from the “half thickness” or “half depth” of a rectangular cross-section of a plume),

u = wind speed at a representative height (m/s).

With respect to ground-level releases, the analysis usually begins with the wind speed measured at a height of 10-m, which is the lowest standard height for measuring wind speed (NRC, 2007). The standard measurement height is the measurement level of winds at First-Order National Weather Service stations and the lowest level of measurement at most DOE sites and commercial nuclear facilities. The 2π in this equation is implicit in a Gaussian distribution, in which the lateral (*y*) and vertical (z) components each contribute $(2\pi)^{½}$. Physically, the wind speed, *u*, represents the initial dilution of the plume caused by the “stretching out” of the plume when it is released into clean air moving about the release. Note that the downwind distance (*x)* does not appear explicitly in this equation. The x dependence is implicit, as the σ_y and σ_z are functions of x only, for a given stability class. The choice of what wind speed is input into Equation 6-3 for ground-level releases is discussed further in Section 6.5, Characterization of Meteorological and Site Data.

The bracketed term in Eq. 6-3 defines the vertical distribution. If the radionuclides or toxic chemicals are reflected from the ground and from the top of the mixed layer, this term is to be modified. This is done mathematically by adding multiple mirror source terms. The bracketed term in Eq. 6-3 thus is replaced with:

$$\Big[e^{-(z-h)^2/2\sigma_z^2} + e^{-(z+h)^2/2\sigma_z^2} + \sum_{n=1}^{N} \Big(e^{-(z-h-2nL)^2/2\sigma_z^2} + e^{-(z+h-2nL)^2/2\sigma_z^2} + e^{-(z-h+2nL)^2/2\sigma_z^2} + e^{-(z+h+2nL)^2/2\sigma_z^2} \Big) \Big]$$ **Equation 6-4**

The term before the summation in Eq. 6-4 is the ground reflection component since perfect reflection is assumed. The series of terms after the summation represent multiple reflections from the top of the mixed layer and the ground. *L* represents the height of the top of the mixed layer and the summation is over the number (*N*) of reflections to be considered. The contribution of the summation term is a function of distance from the source and mixing height. This contribution is generally minor, especially for distances close to the source and for larger values of *L*. The higher-order terms contribute progressively less and the series is normally terminated after only a few terms. For example, in the MACCS code (NUREG/CR-

4691), the series is terminated at $N = 5$. As the plume travels and spreads, Equation 6-4 will eventually result in a plume that is fully mixed vertically, between the ground and height L. In order to simplify the computations, several codes switch from using an equation like 6-3 to using an expression that assumes a vertically mixed plume. Detailed information on this transition for the codes that perform it are available in the documentation for each code.

For a ground-level release ($h = 0$) when the receptor is at ground level ($z = 0$) (general assumption), the first two exponential terms become equivalent as each of the z-h terms is equal to 1. In this case, the “2” in the denominator of Eq. 6-3 cancels out with the “2” in the numerator, if the summation term is ignored, as is often done in hand calculations and in some software codes.

The maximum concentration occurs on the plume centerline ($y = 0$). Thus, if the summation term is ignored, the Gaussian equation simplifies to:

$$\frac{\chi(x, y=0, z=0, h=0)}{Q} = \frac{1}{\pi u \sigma_y \sigma_z} \qquad \textbf{Equation 6-5}$$

If the summation term had not been ignored, the numerator in the above expression would have been greater than one. The numerator in the above expression is slightly greater than one because of the contribution of the summation term. Eq. 6-5, which is now only a function of downwind distance of the receptor, is often used in hand calculations for the CW and MOI, as plume centerline represents a conservative value.

6.4.2 GAUSSIAN PLUME WIDTHS AND DEPTHS

The horizontal and vertical spread of pollutants within a Gaussian plume is a function of the diffusion parameters, σ_y and σ_z, respectively. As representations of plume boundary spread, σ_y and σ_z are often referred to as the “half width” and “half thickness,” respectively.

The most widely used sets of dispersion parameters are known as the Pasquill-Gifford curves (Pasquill, 1961; Gifford, 1961). These parameters have a varied basis. At shorter distances, some of the sigma-z parameters are based on the results of field experiments known as Project Prairie Grass that were performed on flat fields in Nebraska (Barad, 1958). Gifford adapted the original work by Pasquill and published the curves in graphical form (Gifford, 1961). The curves can also be found in NRC Regulatory Guide 1.145, and are shown in Figure 6-4. They are found in *Workbook of Atmospheric Dispersion Estimates, An Introduction to Dispersion Modeling* (Turner, 1994), Slade (1968), and Randerson (1984). These curves became known as the Pasquill-Gifford (P-G) dispersion curves[51], and the set of parameters represented by them are the P-G dispersion parameters. In Figure 6-4, the curves beyond 1,000 m are dashed because of lower confidence in those curves at the longer distances; Pasquill described some of the curves beyond 1,000 m as being speculative extrapolations. For distances less than about 50 m, these dispersion parameters did not provide a good fit to the observations. Moreover, building wake effects further complicated near-field dispersion. This situation led to a lower confidence in curves below 100 m, which is why the curves begin at 100-m. This limitation was a factor that influenced the choice of the selected distance for evaluating the exposure to a CW as 100-m. NUREG-1140 provides some insight into the decision to not use conventional Gaussian models at distances within 100 m.

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[51] These curves are sometimes also referred to as the Pasquill-Gifford-Turner (P-G-T) curves, given their publication by Turner in a workbook initially developed in 1970 for the EPA (current version is the 2nd edition, Turner 1994).

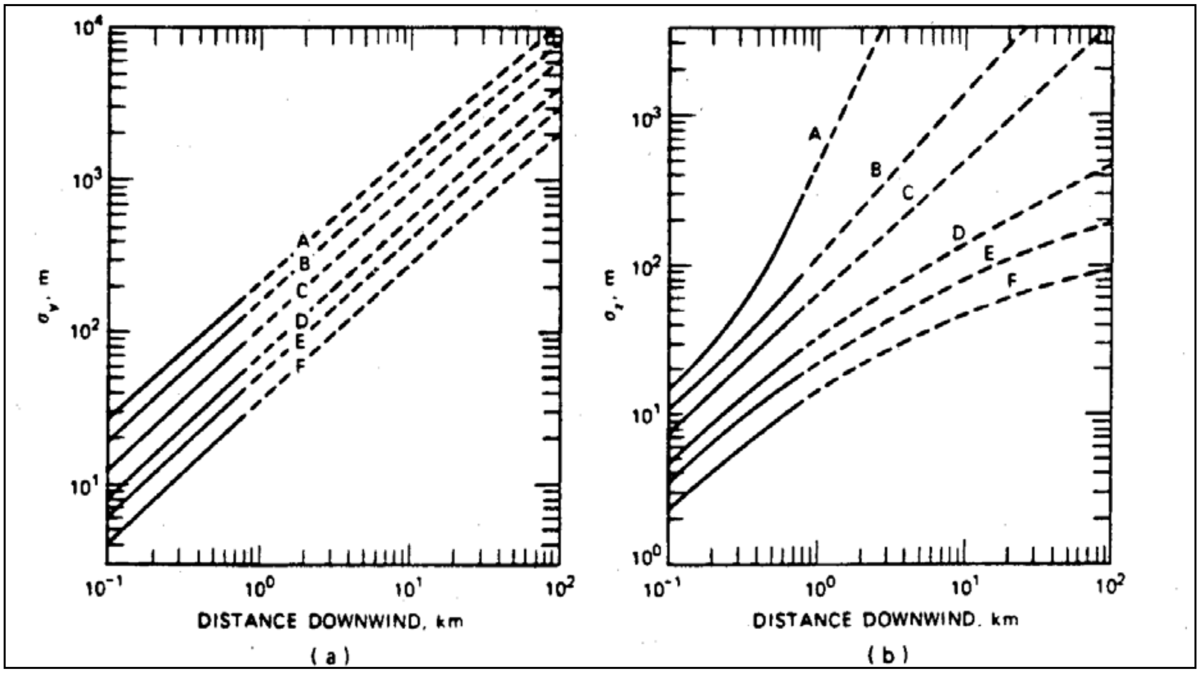

Figure 6-4. Variations of Horizontal and Vertical Plume Dimensions with Distance. The curve labels refer to atmospheric stability classes.

6.4.2.1 ATMOSPHERIC STABILITY CLASSES

Because atmospheric dispersion is so complex and turbulence is so random and chaotic, mathematical descriptions of atmospheric phenomena are, in most cases, developed from empirical data. One method defines distinct atmospheric stability classes and associates a magnitude of lateral and vertical diffusion with each stability class as a function of downwind distance only. Although these computations provide only a rough approximation to reality, they have proven extremely useful and are still in use, although treatments that are more accurate are available. The most common measurements employed in typing stability class are wind direction variability and vertical temperature gradients. The wind direction variability provides the best approximation of the mechanical turbulence component and the vertical temperature gradient provides the best approximation of the buoyancy component. The following subsections provide some definitions associated with stability class and the methods to type it in order to approximate the turbulence intensities that drive atmospheric diffusion. Schemes like that shown in Figure 6-4 are then used with the stability class to determine σ_y, and σ_z as a function of downwind distance. As seen in Figure 6-4, the σ_y, and σ_z curves are represented in graphical form. For computational purposes, there is a need for curve-fits, of which several have been developed. This is discussed further in Section 6.4.2.4.

The rate at which turbulence diffuses radioactive and toxic chemical releases depends upon the stability of the atmosphere. Seven distinct stability classes, namely, the Pasquill-Gifford-Turner (P-G-T) classes, have been defined. These classes, with their relationship to measured temperature gradient, and the conditions of occurrence, are defined below. The P-G curves use six stability classes (i.e., Classes A through F), although some schemes for assigning stability class use a seventh stability class (i.e., Class G). Therefore, from the results of the Project Prairie Grass atmospheric tracer tests, Pasquill and Gifford developed an atmospheric dispersion stability class scheme that is still used today, which is similar to Table II in Pasquill (1961).

A: Extremely Unstable (strong superadiabatic). Normally occurs during bright sunshine with relatively low wind speed (< 3 m/s).

B: Moderately Unstable (moderate superadiabatic). Normally occurs during conditions that range from bright sunshine, with wind speeds in the 3 to 5 m/s range, to dim sunshine, with wind speeds < 2 m/s.

C: Slightly Unstable (slight superadiabatic). Normally occurs during conditions that range from bright sunshine with wind speeds in the 5 to 6 m/s range, to dim sunshine with wind speed in the 2 to 3 m/s range.

D: Neutral (adiabatic). Normally occurs with moderate to dim sunshine, cloudy conditions, and at night, with wind speeds > 3 m/s. It also occurs with very strong wind speeds on either sunny or cloudy days. It usually is the most frequent of the stability classes.

E: Slightly Stable (slight subadiabatic with or without inversion). Normally occurs at night or early morning with some cloud cover and with wind speeds in 2 to 5 m/s range.

F: Moderately Stable (moderate subadiabatic with inversion). Normally occurs at night or early morning with little cloud cover and with relatively low wind speeds (< 3 m/s).

G: Extremely Stable (strong subadiabatic with inversion)[52]. Normally occurs at night or early morning with very light to nearly zero wind speed (calm wind conditions).

The G stability class, as well as the F stability class, is associated with inversion breakup fumigation conditions, occurring in early morning, in which an elevated plume is rapidly forced to the ground. Due to the stable conditions (slow lateral and vertical diffusion) and the low wind speed (slow dilution), the plume concentrations from an elevated release are rapidly brought to the ground can be high. Fumigation represents the worst case scenario for near-field immersion doses associated with elevated releases.

Unstable conditions result in rapid-spreading lateral and vertical diffusion of pollutants (wide plumes), whereas stable conditions result in slow-spreading lateral and vertical diffusion (narrow plumes).

Although Class A stability is not rare, it is not as common as Classes B through F. Class D is the most common stability class because of the large number of combinations of meteorological conditions that can result in Class D stability. For example, high-wind conditions and/or cloudy conditions during the day or at night are normally Class D. During periods of extended rainfall and overcast conditions, as many as 100 consecutive hours of Class D stability have been recorded. Classes E and F most commonly occur at night. Class G is less common and it is often ignored in computer models based on the Gaussian equations.

6.4.2.2 METHODS OF CALCULATING STABILITY CLASSES

Many schemes have been proposed for determining stability class from measured meteorological parameters. The conditions listed above are dependent on wind speed and amount of incoming solar radiation, the latter a function of opaque cloud cover. These stability class definitions are not practical for many DOE sites because the amount of opaque cloud cover is a visually observed condition and not normally recorded by automated weather instrumentation. In addition, opaque cloud cover is somewhat

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[52] The NRC uses class G in licensing all civilian nuclear power plants. In the RSAC code used at Idaho National Laboratory, an additional class, referred to as “class F fumigation”, is introduced. It is similar to class G but in the RSAC code is distinct from class G. Hotspot and GENII both include class G stability.

subjective, varying from observer to observer. Alternative methods have therefore been developed based on measured data.

Several methods exist to convert measured or observed meteorological data into atmospheric stability class data. Two methods are recommended given their regulatory support by the NRC and U.S. Environmental Protection Agency (EPA) and their use across DOE sites based on available meteorological data. Note that the NRC guidance for stability classification extends the original P-G scheme by subdividing P-G class F to create a seventh stability class (class G) for extremely stable condition. In contrast, the EPA guidance combines classes F and G into a single class F. The implications for atmospheric transport and diffusion modeling are addressed below.

The method that is prescribed by the NRC for supporting licensing of nuclear power plants makes use of measurements of vertical temperature difference (ΔT_z) to determine atmospheric stability as shown in Table 6-1 (NRC Regulatory Guide 1.145). In this method, ΔT_z is expressed in terms of the vertical temperature difference over a 100-meter layer of the atmosphere (termed ΔT_{100m}), with the lowest measurement 10-m above the ground. ΔT_{100m} is determined by doubling the difference in temperature measurements over a 50-meter layer at 60 m and 10 m, which are common temperature measurement heights at DOE sites, or by normalizing the difference to a 100-meter depth if the lower height is not 10m.

Table 6-1. Classification of Atmospheric Stability Based on Vertical Temperature Difference.

Stability Classification	Stability Class	Ambient Temperature Change with Height (°C/100 m)
Extremely unstable	A	$\Delta T_{100m} \leq -1.9$
Moderately unstable	B	$-1.9 < \Delta T_{100m} \leq -1.7$
Slightly unstable	C	$-1.7 < \Delta T_{100m} \leq -1.5$
Neutral	D	$-1.5 < \Delta T_{100m} \leq -0.5$
Slightly stable	E	$-0.5 < \Delta T_{100m} \leq 1.5$
Moderately stable	F	$1.5 < \Delta T_{100m} \leq 4.0$
Extremely stable	G	$\Delta T_{100m} > 4.0$

Example: If the temperature at 10 m was 10°C and at 60 m it was 9.5°C, the temperature difference would be -0.5°C/50 m (ΔT_{100m} = -1.0°C/100 m); a stability Class D.

DOE site meteorologists have observed that turbulence typing based on PBL temperature gradients tend to produce a distribution of stability categories that is more skewed toward the strongly stable (F and G) and strongly unstable (A and B) categories; especially if the upper measurement level is much lower than 60 m.

A method recommended by EPA calculates the stability in a two-step process based on turbulence measurements. The first step makes an initial estimate and the second makes a correction to the initial estimate. The initial categorization is based on the standard deviation of wind direction fluctuation in the azimuth (horizontal) plane (σ_θ) as shown in Table 6-2 (EPA-450/4-87-013).

Table 6-2. Initial Estimates of Stability Class, EPA Method.

Stability Class	Standard Deviation of Wind Direction, σ_θ
A	$22.5° \leq \sigma_\theta$
B	$17.5° \leq \sigma_\theta < 22.5°$
C	$12.5° \leq \sigma_\theta < 17.5°$
D	$7.5° \leq \sigma_\theta < 12.5°$
E	$3.8° \leq \sigma_\theta < 7.5°$
F	$\sigma_\theta < 3.8°$

The final categorization is then made by combining this initial estimate with the wind speed and time of day, specifically whether it is “day” or “night”, as shown in Table 6-3. “Day” is defined here as being the period between one hour after sunrise and one hour before sunset. The remainder of the time is defined as “night.”[53] The measurement height of the standard deviation of wind direction should be at the 10-m level.

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[53] For some DOE sites that are located nearby large bodies of water and subject to sea breezes and lake breezes (such as Brookhaven National Laboratory, Argonne National Laboratory), it may be necessary to adjust the definition of “day” to account for the later onset of more stable conditions during morning and afternoon lake breeze and sea breeze conditions.

Table 6-3. Final Estimates of Stability Class, EPA Method.

Time of Day	Initial P-G Stability Class Estimate	Wind Speed Range, WS (m/s)	Final P-G Stability Class
Daytime	A	$WS < 3$	A
		$3 \le WS < 4$	B
		$4 \le WS < 6$	C
		$6 \le WS$	D
	B	$WS < 4$	B
		$4 \le WS < 6$	C
		$6 \le WS$	D
	C	$WS < 6$	C
		$6 \le WS$	D
	D, E, or F	ANY WS	D
Nighttime	A	$WS < 2.9$	F
		$2.9 \le WS < 3.6$	E
		$3.6 \le WS$	D
	B	$WS < 2.4$	F
		$2.4 \le WS < 3.0$	E
		$3.0 \le WS$	D
	C	$WS < 2.4$	E
		$2.4 \le WS$	D
	D	ANY	D
	E	$WS < 5.0$	E
		$5.0 \le WS$	D
	F	$WS < 3.0$	F
		$3.0 \le WS < 5.0$	E
		$5.0 \le WS$	D

Example: If the value of σ_θ was measured to be 3.0° azimuth, the initial classification would be Class F. Then if the wind speed was measured to be 4.0 m/s and it was nighttime, the final stability class would be Class E.

6.4.2.3 ADDITIONAL STABILITY CLASSIFICATION TECHNIQUES

Two additional methodologies are occasionally used: (1) the σ_E-σ_A method; and, (2) the SRDT method.

The σ_E-σ_A Classification Method is based on the direct measurement using three-dimensional mechanical or sonic anemometers of either the horizontal wind fluctuation, or azimuth angle (σ_A) or vertical wind fluctuation, or elevation angle (σ_E). The initial estimates for both the σ_E and σ_A methods, based on the standard deviation of turbulence measurements are shown in Table 6-4, EPA-454/R-99-005, *Meteorological Monitoring Guidance for Regulatory Modeling Applications* (EPA, 2000).

Table 6-4. Initial Estimates of Stability Class Based on Elevation Angle and Azimuth Angle Turbulence Measurements (EPA-454/R-99-005).

P-G Stability Class	Standard Deviation of Horizontal Wind Fluctuation (σ_E)	Standard Deviation of Vertical Wind Fluctuation (σ_A)
A	$11.5° \leq \sigma_E$	$22.5° \leq \sigma_A$
B	$10.0° \leq \sigma_E < 11.5°$	$17.5° \leq \sigma_A < 22.5°$
C	$7.8° \leq \sigma_E < 10.0°$	$12.5° \leq \sigma_A < 17.5°$
D	$5.0° \leq \sigma_E < 7.8°$	$7.5° \leq \sigma_A < 12.5°$
E	$2.4° \leq \sigma_E < 5.0°$	$3.8° \leq \sigma_A < 7.5°$
F	$\sigma_E < 2.4°$	$\sigma_A < 3.8°$

In addition, EPA-454/R-99-005 recommends two possible additional adjustments to the σ_E-σ_A method since the turbulence typing criteria are based on measurements at the standard height (Z) of 10 m and for locations with a terrain roughness length (z_o) of 15 cm. For sites with rougher terrain and/or measurement heights different from 10 m, the category boundaries should be adjusted by wind speed measurement height and terrain roughness factors:

$$\textit{Measurement Height Adjustment Factor} = (Z/10)^p \qquad \textbf{Equation 6-6}$$

The exponent p is a function of P-G stability class and has different values for the σ_E and σ_A methods as shown in Table 6-5.

Table 6-5. Measurement Height Adjustment Factor for σ_E and σ_A Methods as a Function of Stability Class.

P-G Stability Class	σ_E Method p-value	σ_A Method p-value
A	0.02	-0.06
B	0.04	-0.15
C	0.01	-0.17
D	-0.14	-0.23
E	-0.31	-0.38

$$\textit{Roughness Adjustment Factor} = (z_0/15)^{0.2} \qquad \textbf{Equation 6-7}$$

The SRDT Method involves the use of total solar radiation and surface wind speed data during the day to determine atmospheric stability. During the night, ΔT_z data and surface wind speed data are used (EPA-454/R-99-005). In this method, the wind speed is measured at or near the 10-m level or adjusted to this reference height. The SRDT method is outlined in Table 6-6 (EPA-454/R-99-005).

Table 6-6. Classification of Atmospheric Stability Based on SRDT Method.

	DAYTIME			
Wind Speed (m/s)	**Solar Radiation (W/m^2)**			
	≥ 925	925 - 675	675 - 175	< 175
< 2	A	A	B	D
2 - 3	A	B	C	D
3 - 5	B	B	C	D
5 - 6	C	C	D	D
≥ 6	C	D	D	D
	NIGHTTIME			
Wind Speed (m/s)	**Vertical Temperature Gradient**			
	< 0	≥ 0		
< 2.0	E	F		
2.0 - 2.5	D	E		
≥ 2.5	D	D		

6.4.2.4 METHODS OF CALCULATING PLUME WIDTH AND PLUME THICKNESS

Once the stability class has been determined for a given weather condition, the plume widths and depths (σ_y and σ_z) are estimated in order to calculate χ/Q. This is needed for each hour of the year for five years or more, to be compliant with DOE-STD-3009-2014. Depending on completeness of the data record, consecutive years of recent meteorological data is preferred (EPA, 2000). Data is also needed for selected distances from the point of release, out to the MOI, or beyond if the plume is lofted. The calculational method is chosen depending on distance and terrain roughness.

> Example: If the stability class is determined to be Class E, and the Tadmor-Gur method is chosen, the values of σ_y and σ_z at 1,000 m would be calculated from $\sigma = a\,x^b$, where $a_y = 0.1046$, $b_y = 0.9031$, $a_z = 0.4$, and $b_z = 0.6021$. This gives $\sigma_y = 0.1046\times1000^{0.9031} = 53.6$ m and $\sigma_z = 0.4\times1000^{0.6021} = 25.6$ m. The width (σ_y) is then adjusted by the plume meander factor and the depth (σ_z) by the surface roughness factor. For a one hour plume duration and a 10-minute time base, the plume meander factor would be $(60\text{ min}/10\text{ min})^{0.2} = 1.43$, yielding $\sigma_y = 76.7$ m. For a surface roughness of 100 cm (such as in a forested region), the roughness factor would be 2.02, yielding $\sigma_z = 51.7$ m.

Calculations such as in this example, are performed within the various dispersion codes, such as MACCS2 (discussed in Section 6.9.1). They can also be calculated manually using a spreadsheet but this is normally done only for spot checking and scoping calculations.

Numerous methods of calculating plume dimensions for the different stability classes have been developed over the past 60 years. Many of these schemes attempt to determine the magnitude of atmospheric dispersion by relating σ_y and σ_z to stability classes, based on curve fitting of data that were taken during tracer experiments over flat grassland (Barad, 1958), and downwind distance.
One commonly used curve-fitting method is that of *Analytical Expressions for the Vertical and Lateral Dispersion Coefficients in Atmospheric Diffusion* (Tadmor and Gur, 1969), in which each σ value is expressed as a power law:

$$\sigma = a\, x^{b} \qquad \textbf{Equation 6-8}$$

where a and b are empirical constants, given in Table 6-7 (a_y and b_y for horizontal, and a_z and b_z for vertical), as used in the MACCS2 code, with the Tadmor-Gur typographical errors corrected (see Dobbins, 1979); the units of x and σ are in meters. There are two sets of vertical diffusion values as they depend on distance from the source.[54]

Example: For stability class D and a distance of 1 km (1000 m), the Tadmor-Gur formulation gives $\sigma_y = 0.1474 \times 1000^{0.9031} = 75.5$ m and $\sigma_z = 0.3 \times 1000^{0.6532-} = 27.3$ m.

A power law expression, when graphed on logarithmic coordinates, appears to be linear. Examination of the Pasquill-Gifford curves reveals that σ_y can be described by a power law, but σ_z cannot. Tadmor and Gur attempted to address this difficulty by performing different power law fits over different ranges of distance. It should be noted that Tadmor and Gur did not specify constants that are appropriate at distances less than 500 m. However, Eimutis and Konicek (1972) determined that a curve-fit with better fidelity to the Pasquill-Gifford σ_z can be achieved with a third fitted constant.

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[54] In some formulations, a third empirical constant, c, is added (as in Eq. 6-9) but in MACCS2, the c term of σ_z has been set to zero for mathematical convenience, which has required an adjustment to the values of a and b.

Table 6-7. Fitting Constants for σ_y and σ_z from Tadmor and Gur.

Stability Class	σ_y		σ_z (0.5 to 5 km)		σ_z (5 to 50 km)	
	a_y	b_y	a_z	b_z	a_z	b_z
A	0.3658	0.9031	2.5E-04	2.1250	NA*	NA*
B	0.2751	0.9031	1.9E-03	1.6021	NA*	NA*
C	0.2089	0.9031	0.2	0.8543	0.5742	0.7160
D	0.1474	0.9031	0.3	0.6532	0.9605	0.5409
E	0.1046	0.9031	0.4	0.6021	2.1250	0.3979
F	0.0722	0.9031	0.2	0.6020	2.1820	0.3310

* NA - Not available. Power-law constants for stability class C are applied, per recommendation of the MACCS2 code developer (DOE, 2004a).

Eimutis and Konicek adopted three sets of power-law expressions to cover three downwind distance regimes: (i) < 100 m, (ii) 100 m to 1000 m, and (iii) > 1000 m (Eimutis and Konicek, 1972). This parameterization is widely used in NRC dispersion models.

$$\sigma_j = a_j \cdot x^{bj} + c_j$$ **Equation 6-9**

For $j = y$ (horizontal), $b_y = 0.9031$ and $c_y = 0$. The other constants a_j, b_j, and c_j are given in Table 6-8; a_z, b_z, and c_z are with respect to the vertical. Note that in the Table 6-8, typographical errors in Eimutis and Konicek have been corrected.

Table 6-8. Fitting Constants for σ_y and σ_z (from Eimutis and Konicek, 1972).

		ATMOSPHERIC STABILITY CLASS						
	Distance	**A**	**B**	**C**	**D**	**E**	**F**	**G**
a_y	all	0.3658	0.2751	0.2089	0.1471	0.1046	0.0722	0.0481
a_z	< 100 m	0.192	0.156	0.116	0.079	0.063	0.053	0.032
	100 to 1000 m	0.00066	0.0382	0.113	0.222	0.211	0.086	0.052
	>1000 m	0.00024	0.055	0.113	1.26	6.73	18.05	10.83
b_z	< 100 m	0.936	0.922	0.905	0.881	0.871	0.814	0.814
	100 to 1000 m	1.941	1.149	0.911	0.725	0.678	0.74	0.74
	>1000 m	2.094	1.098	0.911	0.516	0.305	0.18	0.18
c_z	< 100 m	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	100 to 1000 m	9.27	3.3	0.0	-1.7	-1.3	-0.35	-0.21
	>1000 m	-9.6	2.0	0.0	-13.0	-34.0	-48.6	-29.2

Example: For stability class D and a distance of 1000 m, the Eimutis-Konicek formulation gives $\sigma_y = 0.1471 \times 1000^{0.9031} = 75.5$ m and $\sigma_z = 0.222 \times 1000^{0.725} - 1.7 = 31.5$ m.

In addition to the Pasquill-Gifford curves, there are two other sources of atmospheric dispersion parameters available in some DOE Toolbox codes from *Diffusion Estimates for Small Emissions* (Briggs, 1973; as updated in Griffiths, 1994): (1) Briggs open-country curves; and,(2) Briggs urban curves. Just like the Pasquill-Gifford curves, the open-country curves are applicable to rural conditions. The Briggs urban curves are based on additional data from an atmospheric dispersion experiment in St. Louis (Hanna, 1982). In the Briggs expressions each σ is expressed as:

$$\sigma = a\,x\,(1 + bx)^{c} \qquad \textbf{Equation 6-10}$$

where *a*, *b*, and *c* are constants, given in Table 6-9. Note that the Briggs-urban curves are not correct for rough rural conditions because of the lack of urban thermal effects on the scale of a large city.

Example: For stability class D, open country, and a distance of 1000 m, the Briggs formulation gives
$\sigma_y = 0.08 \times 1000 \times (1 + 0.0001\times1000)^{½} = 76.3$ m; and,
$\sigma_z = 0.06 \times 1000 \times (1 + 0.0015\times1000)^{½} = 37.9$ m.

Table 6-9. Fitting Constants for σ_y and σ_z from Briggs.

Curve Fitting Constant	ATMOSPHERIC STABILITY CLASS					
	A	B	C	D	E	F
	Open-Country Conditions					
a_y	0.22	0.16	0.11	0.08	0.06	0.04
a_z	0.20	0.12	0.08	0.06	0.03	0.016
b_y	0.0001	0.0001	0.0001	0.0001	0.00001	0.0001
b_z	0	0	0.0002	0.0015	0.0003	0.0003
c_y	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5
c_z	1	1	-0.5	-0.5	-1	-1
	Urban Conditions					
a_y	0.32	0.32	0.22	0.16	0.11	0.11
a_z	0.24	0.24	0.20	0.14	0.08	0.08
b_y	0.0004	0.0004	0.0004	0.0004	0.0004	0.0004
b_z	0.001	0.001	0	0.0003	0.0015	0.0015
c_y	-0.5	-0.5	-0.5	-0.5	-0.5	-0.5
c_z	0.5	0.5	1	-0.5	-0.5	-0.5

Note: An incorrect b_z value of 0.00015 has been presented in many references in the literature for the stability classes E and F urban dispersion parameter equations, based on conversion of half-widths and half-depths of a rectangular plume with uniform concentration in the original Briggs, 1973 reference to lateral and vertical standard deviations of the Gaussian plume. Table 6-9 shows the correct value, 0.0015, as reported in Griffiths, 1994.

The Tadmor-Gur and Briggs Open-Country formulations give results that are nearly the same for some distance ranges and stability classes. However, they may differ by a factor of two or more for other distance ranges and stability classes. The fitting constants given in the above tables, and in other Gaussian models, are based on fitting curves to observational data of plumes released over flat grassland.

Pacific Northwest National Laboratory (PNNL) evaluated the various sets of dispersion parameters available with MACCS2 and GENII2 for rural terrain (Napier et al., 2011). Even though the evaluation was performed for Savannah River Site (SRS) morphology, the general conclusions summarized below are expected to be applicable to other DOE sites.

1. The Tadmor and Gur formulation is not recommended for distances less than 500 m. If deposition is included, the results may be invalid, even for receptors beyond 500 m.
2. Except for the Tadmor and Gur set of χ/Q results for less than 500 m, the other parameterizations yield χ/Q results that are essentially indistinguishable in the distances of interest (500 m to about 11 km) at the SRS site.
3. The χ/Q results from the Briggs Open-Country parameterization begin to diverge from the χ/Q results using the various P-G parameterizations at distances of about 10 km.
4. Beyond 10 km, the Briggs Open-Country χ/Q results are conservative and even more so for E and F stability classes (see Figure A-3 of Napier et al., 2011). The Briggs parameterization is universally available with the radiological dispersion toolbox codes and the only available option with the HotSpot code, and,
5. The χ/Q results from P-G parameterizations agree with one another out to the plotted distance of 30 km (see Figure A-3 of Napier et al., 2011).

It is not surprising that the χ/Q results from the P-G parameterizations agree with one another (except for Tadmor and Gur results for less than 500 m) for the entire range of distances given their common origin of the P-G curves and the Project Prairie Grass tracer data. Moreover, the divergence of the Briggs χ/Q results at distances beyond about 10 km should not invalidate its use at these large distances. The divergence seems to simply reflect the empirical foundation of a larger data set that includes data out to 10 km, compared to 1 km for the P-G data set.

Because the Briggs open-country dispersion parameters are partially based on elevated release data acquired at BNL, consideration may be given to using these for atmospheric dispersion modeling of stack releases. The SRS AXAIR code (AXAIR, 1986) uses the Briggs expressions for σ_z, since these expressions were considered more appropriate for stack releases that were common at SRS at the time of its development (Simpkins, 1994; Napier et al., 2011). Another example is the RISKIND code (Yuan, 1993), designed for potential radiological consequences from transport of spent nuclear fuel. It uses the Eimutis and Konicek dispersion parameters if the effective release height is less than or equal to 30 m and the Briggs dispersion parameters for higher elevated releases.

To more accurately predict atmospheric dispersion for specific conditions that differ from those represented by the P-G and Briggs open country parameterizations, adjustment factors have been developed to capture enhanced plume spread acting independently in a single direction, such as horizontally for plume meander and vertically for mechanical turbulence caused by surface roughness. These adjustment factors are discussed in Sections 6.8.1 and 6.8.2. Additionally, wakes caused by aerodynamic effects of the building introduce enhanced dispersion in the horizontal and vertical directions. Building wake dispersion and related modeling approaches are discussed in more detail in Section 6.8.3.

If the nature of radiological and toxic chemical releases makes them neutrally buoyant, as in the release of trace amounts of very fine particulates or of gases that have a molecular weight similar to that of air (28.97 g/mole), plume dispersion approximates a Gaussian distribution in both the crosswind (lateral) and vertical directions.

For continuous releases, the magnitude of the downwind diffusion (σ_x) is negligible in comparison with the speed of the wind. However, if the release is of short duration (a puff) the mean wind speed only acts as a transport agent and the turbulent diffusion in the downwind direction becomes meaningful.

Accordingly, a puff release is described by Gaussian equations in all three dimensions whereas a continuous release is described by Gaussian equations in two dimensions (width and thickness) and a length determined by wind speed and release duration. For a puff release, it is assumed that $\sigma_x=\sigma_y$.

For stability class G, NRC Regulatory Guide 1.145, *Atmospheric Dispersion Models for Potential Accident Consequence Assessments at Nuclear Power Plants,* recommends using a σ_y value that is 2/3 that of stability class F and a σ_z value that is 3/5 that of stability class F. With plume meander and building wake effects this NRC guidance recommends correction factors to σ_y for classes D – G, especially for low wind speeds. For example, for Class G the correction factor varies from a factor of six for wind speeds less than 2 m/s, down to a factor of one (no correction) for wind speeds of 6 m/s and above.

6.5 CHARACTERIZATION OF METEOROLOGICAL AND SITE DATA

The application domain that atmospheric dispersion codes approximate establishes the types of meteorological data needed to drive such codes. The choice of code that the analyst uses to solve a particular application may be limited by the availability and fidelity of meteorological data. This subsection gives a brief discussion of various meteorological data sets often used as input to atmospheric dispersion codes.

DOE-STD-3009-2014, Section 3.2.4.2 provides three options for selecting atmospheric dispersion methodology and the resulting χ/Q and gives the following guidance for development of meteorological data:

> In the case of Option 1, follow the meteorological data guidance within NRC Regulatory Guide 1.23 Revision 1, Meteorological Monitoring Programs for Nuclear Power Plants. For Options 2 and 3, the guidance in both Regulatory Guide 1.23 and in EPA-454/R-99-005, Meteorological Monitoring Guidance for Regulatory Modeling Applications, are acceptable means of generating the meteorological data upon which atmospheric dispersion is to be based. These two guidance documents should be evaluated for their applicability to the site or facility being evaluated. In the development of the meteorological database for Option 3, the impact of local surface roughness on the data may have to be considered.

DOE-STD-3009-2014, Section 3.2.4.2 also provides the following guidance for determination of the Offsite χ/Q, as follows:

> Regarding Option 2, DOE-approved, code-specific guidance for each toolbox code should be consulted. This is especially true with respect to developing χ/Q values using atmospheric dispersion models. Many of these toolbox codes allow for setting a specific parameter within the calculations. These parameter choices may either use the conservative parameters and options established in this section (Option 2) or reflect site-specific conditions to more accurately represent the accident scenario (Option 3). The parameter choices presented for use in Option 2 are given to provide a simple method for determining an appropriate χ/Q value, and the level of overall conservatism established is not reflective of what is required via the other acceptable options.

For codes that do not contain fixed values or calculate the parameters internally, DOE-STD-3009-2014 requires the following parameters be used for ensuring conservative calculation of offsite doses in accordance with Option 2:

- Non-buoyant, ground level, point source release;
- Plume centerline concentrations for calculation of dose consequences;
- Rural dispersion coefficients;
- A deposition velocity of 0.1 cm/sec for unfiltered release of particles (1-10 μm AED), 0.01 cm/sec for filtered particles, or 0 cm/sec for tritium and noble gases;
- A surface roughness of 3 cm;
- A minimum wind speed of 1 m/s;
- Plume meander may be used, consistent with the accident release duration and the appropriate code guidance; and
- Building wake factors should not be credited in the plume dispersion, outside of those already incorporated into plume meander.

The purpose of the required parameters for Option 2 is to produce conservative χ/Q values. Codes that use values more conservative than the required parameter values are acceptable. For example, if a dispersion code uses a minimum wind speed of 0.5 m/s rather than 1.0 m/s, this would result in a χ/Q value that is more conservative than if 1.0 m/s were used. Also, "Codes that do not contain fixed values or calculate the parameters internally" should be interpreted to mean codes that allow for the input of parameters that are less conservative to be set to values provided. Some dispersion codes allow for the adjustment of parameters, such as deposition velocity or surface roughness, to values less than the required parameter values.

The wind speed in meteorological data files is generally assumed to correspond to a reference height of 10 m and represents conditions at a height of 10 m and below. The various toolbox models treat the wind speed variability differently, as follows:

- Meteorological data read into the MACCS2 radiological dispersion software are assumed to correspond to a reference height of 10 m. MACCS2 does not adjust the wind speed used in the Gaussian plume equation for the height of release.[55] Thus, wind speed data in the meteorological data files are input directly into Gaussian plume model equation. The use of the 10-m wind speed is conservative in the calculation of the χ/Q value for an elevated release;

- Meteorological data read into the GENII radiological dispersion software are assumed to correspond to a reference height of 10 m. Wind speed data in the meteorological data files are input directly into the Gaussian plume model equation for release heights of less than 12 m. For releases of higher elevation, the wind profile power law is used to upwardly adjust the wind speed;

- The user specifies the reference height for the meteorological data with HotSpot. With HotSpot designed to read meteorological data files that are formatted for MACCS2, the reference height is 10 m. HotSpot adjusts the wind speed for any release height that differs from the reference height. For release heights of 2 m or less, the wind speed is calculated from the wind profile power law using a 2-m height. The user can disable the wind speed adjustment by specifying a reference height of 2 m for the meteorological data (Homann, 2010). This allows HotSpot to model a ground-level release using the wind speed data directly from the meteorological data files in a way consistent with MACCS2 and GENII (Homann, 2010).

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[55] The algorithm in MACCS2 for determining the plume rise of a buoyant release does make use of wind speed correction with height, but this is the only place where MACCS2 accounts for wind speed variability with height.

6.5.1 PERSISTENCE

The simplest models assume that constant weather conditions prevail during the accident duration, whether unfavorable conditions or typical conditions. DOE-STD-3009-2014, Section 3.2.4.2 states that if representative meteorological data are not available, stability Class F and 1.0 m/s wind speed may be used for unfavorable radiological dispersion consistent with NRC's and DOE's long-standing practice as this approximates the 95th percentile atmospheric dispersion condition. For perspective, Class D stability and 4.5 m/s wind speed are used for "typical" conditions.

The choice of wind speed depends on the guidance document being followed. For sites in valleys where a high frequency of low wind speeds occur (such as Y-12), Class F stability and wind speeds less than 1.0 m/s may possibly apply. For many simple models, a meteorological data couplet of wind speed and stability class and the distance to the receptor are the only inputs that are needed, as the release rate and atmospheric conditions are time-invariant in Gaussian models. [56]

6.5.2 JOINT FREQUENCY DISTRIBUTION (JFD)

The JFD required by many atmospheric dispersion codes is the joint distribution of wind speed according to wind direction and stability class. The JFD is organized into a matrix that gives the percent of the time of each condition for specified numbers of wind speed groups and stability class for each of the 16 wind direction sectors (N, NNE, NE, … NNW).

This distribution is based on an extended period of meteorological observations, five or more years if available, in order to establish temporal representativeness since there are climate variations. DOE-STD-3009-2014, Section 3.2.4.2 requires that "For the calculation of offsite doses, five years of representative, recent meteorological data shall be used as input to the dispersion model", and within the past 10 years is considered to be "recent" as used in this context. The larger number of years smooths out the decadal climatic variations. Temporal representativeness simply means that the data base is sufficiently large to have captured a reasonable number of climatic anomalies such that an additional year of data will not substantively affect radiological and toxic chemical consequence calculations.

The wind speed data are sorted into bins, such as 0 - 1 m/s, 1 - 2 m/s, 2 - 4 m/s, as shown in Table 1 of ANSI/ANS-3.11-2015, *Determining Meteorological Information for Nuclear Facilities*. Since calm wind speeds cannot be used in a Gaussian plume model, the calms are redistributed into the lowest wind speed class based on the frequency of wind directions in the lowest two wind speed classes. The choice of bins may be dictated by the code but for some codes (such as GENII) the user chooses the number of wind speed bins and the ranges of these bins. These would depend upon the wind conditions at the DOE site. The number of frequency bins in this matrix can reach several hundred. For example, if six stability classes (A–F) and six wind speed bins are chosen, the total number of frequencies would be $6 \times 6 \times 16 = 576$. However, not all bins will be populated as stronger winds cannot simultaneously occur with Class A and Class F stability class conditions.

A utility computer program is usually needed to generate a JFD, especially if several years of hourly observations are being used. When a JFD matrix is being generated, the definition of wind direction used in the code should be kept in mind. In meteorology, wind direction has traditionally been defined as the direction from which the wind blows, which is of interest to weather forecasters. However, most

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[56] An exception is that for the MACCS2 code, although a Gaussian model, the release is broken into one-hour segments. Each segment is calculated using the stability class and wind velocity at the time the segment is released.

computer models for atmospheric dispersion and consequence applications, such as those in the DOE Central Registry, use wind direction to mean the direction toward which the wind blows. The downwind (transport) direction is always 180 degrees out of phase with the direction that a meteorologist uses. Thus, the analyst should be aware the wind direction-sector orientation of the particular code being applied.

6.5.3 FULL DATA SET SAMPLING

An alternative to a JFD matrix that is used by MACCS2 and HotSpot is to use the data from all 8760 hours in a year, rather than discrete JFD matrix entries, to achieve the maximum temporal representativeness and therefore highest accuracy in calculating the overall site 95th percentile consequences or the sector-dependent 99.5th percentile consequences.

6.5.4 TREATMENT OF CALM AND VARIABLE WINDS

Industry practice for treatment of calm winds is that wind speeds that are below the threshold wind speed of the mechanical or sonic anemometer are generally set equal to the rated threshold wind speed or wind direction of a mechanical or sonic anemometer, whichever is lower. The threshold wind speed of a mechanical anemometer and wind direction mechanical vane is generally 1.0 mph (0.5 m/s). Sonic anemometers have somewhat lower threshold wind speed and wind direction capabilities and thus can measure even lower wind speeds; inferring wind speed from differences in the speed of sound and generally have a threshold wind speed of 0.6 mph (0.3 m/s).

However, the capability to monitor wind speed to extremely low levels is not the only consideration relative to the treatment of calm wind speeds in plume modeling, as the application domain limitations of the steady-state Gaussian plume model needs to also be taken into account.

- ANSI/ANS-3.11-2015, *Determining Meteorological Information at Nuclear Facilities,* defines a calm as, “any wind speed below the starting threshold of the wind speed or direction sensor; or any wind speed below that which is appropriate for input into plume models, whichever is greater. In the US, a calm wind is defined as any speed less than 1 mph” (0.5 m/s).
- EPA-454/R-99-005, *Meteorological Monitoring Guidance for Regulatory Modeling Applications*, Section 6.2.3 defines calm as “when the wind speed is below the starting threshold of the anemometer or vane, whichever is greater,” but also states that, “…for site-specific monitoring … a calm occurs when the wind speed is below 0.5 m/s”. EPA then recommends “to avoid unrealistically high concentration estimates at low wind speeds (below the values used in validations of these models - about 1 m/s) EPA recommends that wind speeds less than 1 m/s be reset to 1 m/s for use in steady-state dispersion models.”

The *Technical Report for Calculations of Atmospheric Dispersion at Onsite Locations for DOE Facilities* (DOE/ONS, 2015), cautions on the limitations of steady-state Gaussian dispersion modeling, as this type of model has the tendency to overpredict concentrations at the lower end of a range of conservative wind speeds; especially calm wind speeds. This is illustrated in Figure 6-5, which shows the ratios of normalized concentrations (χ/Q) predicted in wakes to observed concentration normalized to actual release rate as a function of wind speed. If the errors in the predicted values were associated with the wake, they would increase with wind speed. The authors observed that the overprediction (ratio >1.0 of the ordinate) is largest and more numerous at very low speeds and decreases with increasing wind speed, which indicates that the problem is underestimation of atmospheric dispersion in low wind speeds by a Gaussian model. The authors concluded that their original premise that the enhanced dispersion was due to building wakes was incorrect. Instead, the apparent enhanced dispersion noted in the vicinity of buildings at low wind speeds in wake dispersion experiments is caused by underestimation of dispersion by the basic dispersion algorithms rather than by increased turbulence in the vicinity of buildings.

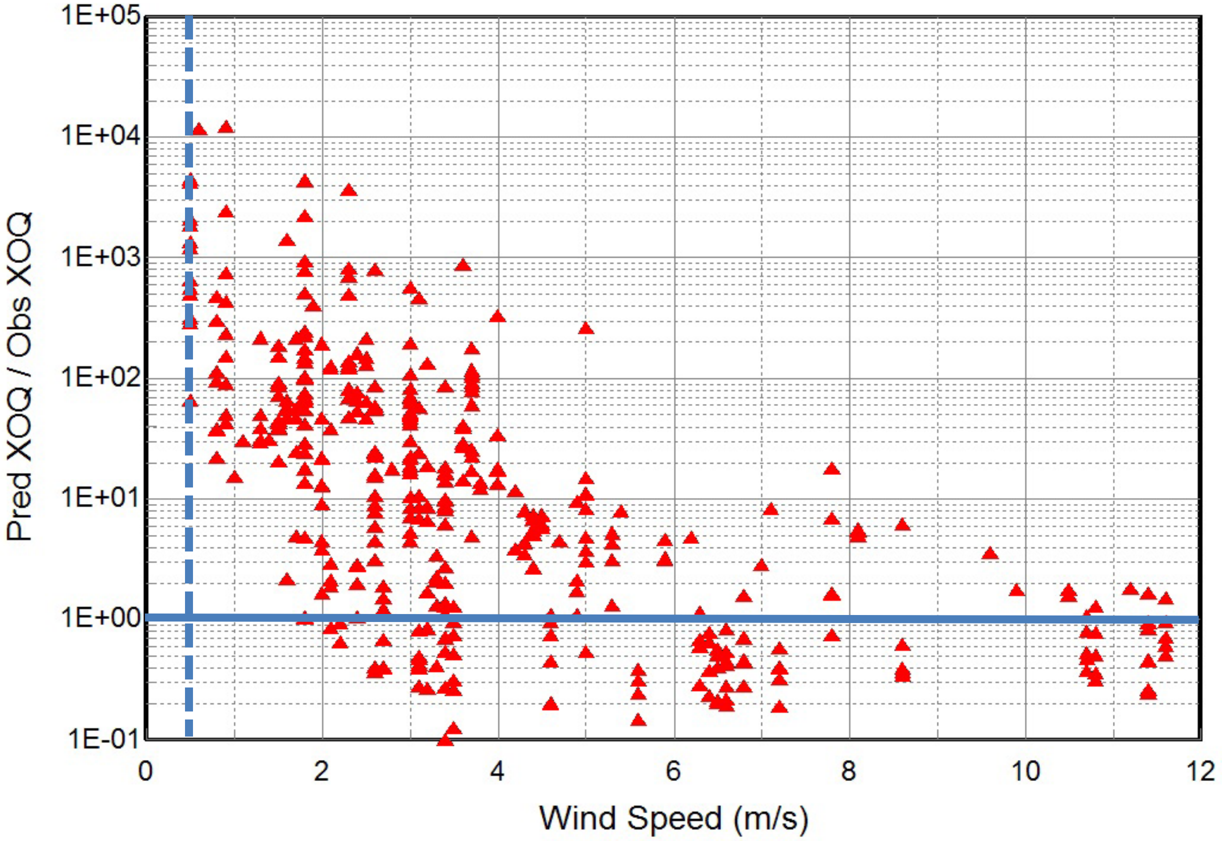

Figure 6-5. Ratios of predicted concentrations in wakes by a model without wake correction to observed concentrations as a function of wind speed (based on McGuire et al., 2007). (Ratios above solid line (Predicted/Observed = 1E+00) are over-predicting the concentration.)

Accordingly, Option 2 of DOE-STD-3009-2014, Section 3.2.4.2, specifies a minimum wind speed of 1.0 m/s (2.2 mph) relative to atmospheric dispersion modeling. This is consistent with generating the site meteorological data using the above EPA recommendation. Setting the calm wind speed to the anemometer threshold is consistent with the NRC Regulatory Guide 1.145 which relies on the NRC Regulatory Guide 1.23 Revision 1. Either method for generating the site meteorological data (EPA-454/R-99-005 or NRC Regulatory Guide 1.23 Revision 1) is acceptable as earlier described.

If a site's conditions have a high incidence of low wind speeds, the site may want to consider other atmospheric dispersion modeling approaches that addresses this condition, or the site should justify that applying Option 2 of DOE-STD-3009-2014 will produce a conservative result when applying the minimum 1.0 m/s (0.5 m/s) wind speed.

Unrealistically high estimates of χ/Q can be calculated under calm wind conditions, a result of the placement of wind speed in the denominator of the Gaussian plume model equation. EPA recommends that wind speeds less than 1.0 m/s be reset to 1.0 m/s for use in steady-state dispersion, and cautions against overly conservative model predictions with wind speeds less than 1.0 m/s (EPA-454/R-99-005).

DOE-STD-3009-2014 requires the use of 1.0 m/s as the minimum wind speed when using one of the Central Registry toolbox codes. MACCS2 substitutes a value of 0.5 m/s for the wind speed whenever it reads a wind speed value of less than 0.5 m/s from a meteorological data file, but this is allowed by DOE-STD-3009-2014 as the 0.5 m/s is a fixed part of the code, and it produces more conservative results than if 1.0 m/s is used. GENII allows the user to set threshold value through the input for the maximum wind speed for calms. Hotspot considers wind speeds down to 0.1 m/s and also considers a G Stability class. However, the analyst should set calm wind speeds to 0.5 m/sec unless there is sufficient justification to reducing it to a lower value.

6.6 METEOROLOGICAL DATA ADEQUACY FOR SAFETY ANALYSIS

The results from atmospheric dispersion codes can be no better than the input data and the conditions under which it is applied. Meteorological data used for consequence assessment needs to meet applicable DOE O 414.1D, Chg.1 quality assurance requirements. The meteorological program manager at the DOE site is responsible for developing quality-assured data. Meteorological data quality assurance programs are based on guidance in DOE-STD-1216-2015 and ANSI/ANS-3.11-2015. Section 5.12 of DOE-STD-1216-2015 states that guidance in quality assurance related to meteorological measurements and meteorological data processing may also be found in ANSI/ANS-3.2-1994 (R1999), *Administrative Controls and Quality Assurance for the Operational Phase of Nuclear Power Plants*. Moreover, Section 7.5 of ANSI/ANS-3.11-2015 also references ANSI/ANS-3.2-1994 (R1999), which presents the general quality assurance criteria for nuclear facilities with respect to meteorological data.

The accuracy of the codes is also limited by the approximations inherent in the models, with results being more reliable nearby the release point than farther away, within the application’s domain. Inaccuracies in the meteorological data tend to amplify uncertainty with increasing transport distance. No matter how effective the meteorological monitoring system is, it is common that yearly data sets may have at least some hours of missing data. Some codes (e.g., MACCS2) require an uninterrupted data set. In order to address this issue, data substitution techniques in ANSI/ANS-3.11-2015 should be employed to complete the data set. For other codes that use JFD data as input, uninterrupted data is not required.

Generally, data need to be input with the full accuracy of the measurements and rounding should be only performed on the final results. Even the most comprehensive atmospheric dispersion codes in use today will likely be uncertain by a factor of two or more, even relatively close to the release point for flat terrain topography; DOE-STD-5506-2007 estimates a factor of four uncertainty. Therefore, one-digit accuracy, or at most two digits, is all that should be reported in the analyst’s results, except perhaps for purposes of comparisons of similar results. Since there are so many uncertainties in the input data streams and within the models, the following phrase gives some perspective: “The mantissa is meaningless, while the exponent is everything.”

The minimal set of meteorological data needed to run an atmospheric dispersion code that requires observational data would be at least one year of wind speed, wind direction, and an indicator of stability class. However, one year of data may not prove to be very temporally representative, as notable climatic anomalies frequently occur on as little as an annual basis (El Niño, La Niña), and decadal climatic anomalies have been noted.

NRC Regulatory Guide 1.194, *Atmospheric Relative Concentrations for Control Room Radiological Habitability Assessments at Nuclear Power Plants*, indicates that the size of the data set used in assessments should be sufficiently large such that it is representative of long-term meteorological trends at the site in question. In this Regulatory Guide, the NRC staff considered 5 years of hourly observations to be representative of long-term trends at most sites. However, the Guide also states "With sufficient justification of its representativeness; however, the minimum meteorological data set is one complete year, including all four seasons, of hourly observations."

A basic rule of thumb is to use at least five years of meteorological data to ensure that temporal representativeness would not be compromised. If a larger data base is available, it should be used, even if the resulting atmospheric dispersion estimates change from prior analyses. Moreover, DOE-STD-3009-2014 Section 3.2.4.2 requires that recent five years of data be used and requires either the directionally independent 95th or directionally dependent 99.5th percentile value. If five years of data are not available, justification for using a shorter period needs to be provided. A reanalysis should be performed every ten years, as the average of meteorological parameters change relatively slowly over time even under climate change conditions.

If onsite meteorological data is unavailable, meteorological data from a nearby weather station can be substituted provided the terrain at that site is similar and the data is spatially representative. Guidance on data substitution is provided in ANSI/ANS-3.11-2015.

6.7 TYPICAL AND UNFAVORABLE DISPERSION CONDITIONS

In calculating plume concentrations, or consequences to the receptor, both "typical" and "unfavorable" dispersion conditions are of special interest in accident analyses for ground-based releases. "Typical" would not be used to establish safety SSCs in a DSA but it is useful for Safety Goal comparison, if over the DOE EG as discussed in Chapter 10, *Hazard Control Selection and Classification*.

> Typical Dispersion Conditions: The median (50th percentile), the mean (average), or the mode (peak) of a distribution could all be considered as representative of "typical." However, the median is the most meaningful for plume dispersion, for several reasons. It is not heavily influenced by outliers (abnormally small or large values), as is the mean. For a bimodal distribution, which is common to dispersion, the mean may fall between the peaks (modes) of the distribution and thus be comparatively infrequent, which could not be considered "typical." The median could also be atypical in this sense but it, at least, has a relevant meaning. In addition, if mode were chosen as "typical", a bimodal distribution could give two valid choices if the peaks are nearly as large.

> Unfavorable Dispersion Conditions: This is normally taken to be the overall site 95th percentile dispersion of the full meteorological data set for at least one year, for which the consequences are smaller 95% of the time and larger 5% of the time. Other dispersion conditions are sometimes used for "unfavorable", such as "worst case", "near-worst case", or specific constant-weather conditions, such as Class F stability and 1.0 m/s wind speed. Near-worst-case conditions, which are most likely G stability class and nearly calm winds are extremely rare and would be overly conservative for most applications. True "worst case" is a single value, that is, the maximum value, obtained only once in the period of interest.

For elevated releases, the above rules of thumb would not apply as they would depend on the release height. Also, the amount of atmospheric dispersion corresponding to 50th or 95th percentile weather depends upon the nature of the release. If the release is a trace constituent, it can be treated with a Gaussian plume or puff model, depending upon the duration of the release. If it is a dense or heavy gas (discussed in Section 9.5.4), it is treated with a heavy-gas model that both limits vertical dispersion due to slumping, while simultaneously entraining ambient air through the sides of the plume. The amount of dispersion for the 50th or 95th percentile conditions would likely be different for a heavy gas model.

For whatever model is used, some rules-of-thumb can be established for non-lofted plumes, and these may be useful for "sanity checks" of results. Such rules-of-thumb at most sites would likely be similar to the following:

95th percentile χ/Q value is about ten times larger than the median χ/Q value for any distance;

50th percentile (median) χ/Q values for ground-level releases are similar to those of Class D and 4.5 m/s wind speed;

95th percentile χ/Q values for ground-level releases are similar to those of stability Class F and 1.0 to 1.5 m/s wind speed; and,

95th percentile χ/Q values at ground level for elevated releases are similar to those of stability Class A and 4.5 m/s wind speed.[57]

For lofted plumes, no such rules-of-thumb are possible as ratios of 95th percentile χ/Q to median, or some constant meteorological condition, χ/Q values vary with distance and the amount of lofting.

High-wind speed scenarios [such as sustained wind speeds of 45 m/s (100 mph)] are also of interest to the analyst. This is about 10 times greater than the wind speed that corresponds to the median χ/Q. High winds are always associated with Stability Class D, which is also the stability class associated with the median weather conditions and represents a well-mixed atmosphere. Because the value of χ/Q varies inversely as the wind speed (see Eq. 6-3), the high-wind speed χ/Q will therefore be about 10% of the median χ/Q. As a rule-of-thumb, for scoping calculations, the analyst can divide the consequences (such as dose) from exposure to radiological or other hazardous materials for median weather conditions by 10 to find the corresponding consequences for high-wind speed scenarios.

Tornados have even greater wind speeds, sometimes exceeding 200 mph (89 m/s) for Enhanced Fujita Scale 5 tornadoes, and can cause a facility to collapse. Moreover, the rapid atmospheric pressure drop can cause other types of releases. This NPH could soon be followed by a lower wind speed that would result in larger dispersion parameters than during the tornado itself. If the tornado causes damage that releases the MAR almost instantaneously, that should be modeled as high-wind dispersion, but slower developing source terms may occur during the subsequent low-wind conditions which should be modeled separately, and the dose consequences summed for the two contributions. Section 6.12.1, *Dispersion Under a High-Wind or Tornado Event,* has a further discussion of high wind or tornado dispersion. In addition, scenarios for environmental restoration projects involving contaminated soil where the source term is based on EPA methods incorporating an assumed wind speed should be modeled with the same wind speed in the dispersion analysis (a sensitivity analysis of wind speed vs. dose consequence may be necessary to determine a conservative analysis to determine the need for safety controls).

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[57] For elevated releases, the worst case stability class is Class A, since σ_z is greatest for that stability class. In addition, fumigation conditions represent a special worst case for elevated releases where the elevated, poorly-dispersed plume is quickly brought down to ground level.

6.8 SPECIAL GAUSSIAN MODELING CONSIDERATIONS[58]

6.8.1 AVERAGING-TIME AND LARGE EDDY PLUME MEANDER

The diffusion magnitude expressions in the previous sections are relevant for short-duration plumes released over relatively smooth terrain. However, plumes tend to meander for two specific reasons: (1) when release duration is longer than some tens of minutes; and (2) under stable light wind conditions when embedded larger eddies can dominate a relatively calm atmosphere. Large eddies, which are present in a stable, stratified atmosphere, tend to become more dominant in this situation, and can augment the magnitude of lateral movement. Therefore, for a receptor that remains in the plume for some time, meandering effectively widens the plume and thus decreases χ/Q. This is accounted for in the Gaussian equation by multiplying the plume width (σ_y) by a plume meander factor.

Two treatments of meander are available as an option in one or more of the toolbox codes, and both involve adjustments to increase the magnitude of σ_y. One approach to plume meander is based on the influence of averaging time and is available as an option in the two radiological consequence toolbox codes, MACCS2 and HotSpot, and one toxic chemical consequence code, EPIcode. Figure 6-6 qualitatively shows how the plume boundaries of the time-averaged plume may differ from those associated from a typical snapshot of the instantaneous plume. The second approach is related to the embedded large-eddy effects that occur under very stable atmospheric conditions.

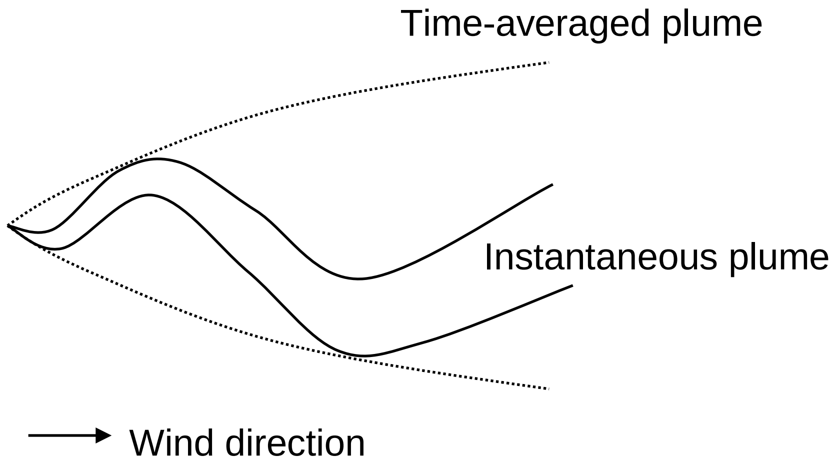

Figure 6-6. Time-Averaging Effect on Plume Boundaries.

The averaging time, also referred to as sampling time, over which the σ_y values were determined from experimental data, establishes the time base, usually on the order of minutes, for the horizontal and vertical diffusion parameters. A longer averaging time than the time base may be applied in the analysis of receptor exposure times for plumes with longer release durations, an option of the HotSpot code. The exposure time is assumed to equal the release duration in these analyses. A longer averaging time leads to greater widening of the plume boundaries. Embedded large eddies also causes movement of the plume centerline with time (the plume swings back and forth), another type of plume meander. The receptor on the time-averaged centerline location is only exposed intermittently to the concentration of the

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[58] Dense gas models are applicable to chemical releases and these types of models are described in Section 9.7.

instantaneous plume centerline due to this movement. As a result, the time-averaged centerline concentration is lower. These effects become even more pronounced with increasing averaging time.

The formulation for the plume meander factor[59] that is applied to σ_y based on the averaging-time concept is given by:

$$\text{Averaging-time plume meander factor} = (\text{release duration} / \text{time base})^n \qquad \textbf{Equation 6-11}$$

The time base and exponent, *n*, are hard wired in EPIcode and HotSpot to values of 10 minutes and 0.2, respectively. MACCS2 and ALOHA allows the user to specify the time base and to input two different values of *n* to correspond to two different time ranges, the exponent is 0.2 for plume duration of one hour or less and 0.25 for a longer duration (DOE, 2004c, *ALOHA Computer Code Application Guidance for Documented Safety Analysis: Final Report*). The averaging-time plume meander factor is never allowed to be less than unity, and the experimental basis is limited to periods of no longer than 100 hours. The release duration can vary from a few minutes for a spill to several hours of a fire. For explosions, deflagrations, or other short-period releases, plume meander should not be applied.

The other type of plume meander is related to embedded large-eddy effects that occur especially under very stable conditions with very light wind speeds and that were observed from tracer studies first performed in the mid-1970s. After careful review of the results of the tracer studies, the NRC developed this plume meander factor and incorporated it in NRC Regulatory Guide 1.145 for atmospheric stability classes D, E, F, and G. The NRC also acknowledged it in several of their atmospheric dispersion models. This Regulatory Guide also recommends not using any meander factor for stability classes A, B, or C at any wind speeds. The NRC method is only applicable to the Pasquill-Gifford horizontal and vertical dispersion curves.

Plume meander is also implemented in several atmospheric dispersion models such as ARCON96, RASCAL, and Version 2.6 of MACCS2 (Napier et al., 2011). ARCON96 (NUREG-6631 Revision 1) and RASCAL increase both the horizontal and vertical diffusion magnitudes; especially under stable light-wind conditions. These two meander factor approaches should not be utilized at the same time.

The large-eddy plume meander factor is applied to augment σ_y and σ_z, but only for distances up to 800 m, where its effects are damped out. Beyond 800 m, σ_y values reflect the augmented spreading up to 800 m plus non-augmented spreading beyond 800 m. The large-eddy plume meander factor ranges between 1 (no meander) and 6. Figure 6-7, taken from NRC Regulatory Guide 1.145 Revision 1, graphically displays the magnitude of the meander factor as a function of downwind distance for stability classes D, E, F and G.

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[59] The plume meander factor is sometimes referred to as the plume expansion factor.

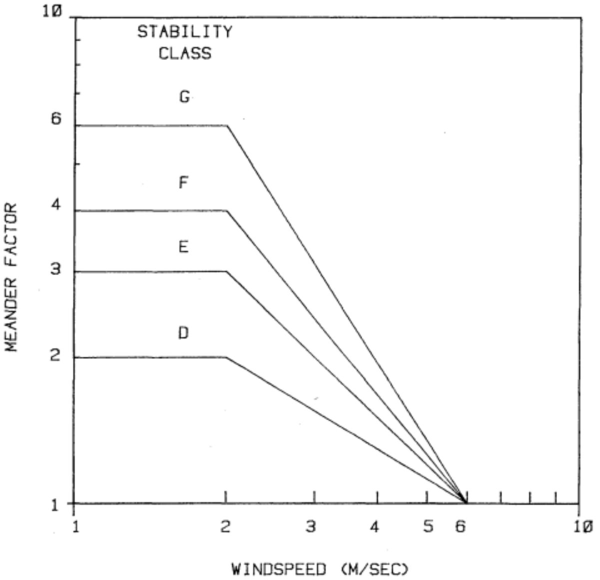

Figure 6-7. Correction factors for σ_y values by stability class (Figure 3, NRC Regulatory Guide 1.145)

The large-eddy plume meander factor actually increases for more stable conditions (from E to G stability class) and increases as wind speeds approach calm under the same stability class.[60] This dependency is exactly opposite to the aerodynamic building wake phenomenon that is very small under these light-wind very stable meteorological conditions, but increases significantly as the wind speeds increase and the stability class becomes neutral or slightly unstable. The faster the winds are that encounter the building, the stronger the flow separation becomes which yields a larger aerodynamic effect on the wind field.

6.8.2 MECHANICAL TURBULENCE DUE TO SURFACE ROUGHNESS

Mechanical turbulence is generated as wind flows over and around irregular obstacles (morphology) on the earth's surface. Such obstacles are both natural (topographic and vegetation) and anthropogenic (buildings and other structures). In general, the rougher the terrain underneath the atmosphere moving above it, the more mechanical turbulence is generated and consequently the better the diffusion. The rougher the surface, the larger the turbulent eddies formed, mainly in the vertical, and thus the greater vertical dispersion, as expressed by an enhancement of σ_z. The increase in σ_z is called the roughness factor and it cannot be less than unity. Because σ_z is increased, the plume-centerline χ/Q is proportionally reduced by the magnitude of the roughness factor.

Mechanical turbulence continually persists once it is generated. The atmospheric mechanical turbulence at a given location reflects the upwind development of the PBL and the contributing influence of upwind surface elements that can be several hundred meters or more away. The surface roughness length (z_0), discussed earlier, is a measure of the amount of mechanical mixing introduced by the surface roughness elements over a region. As an approximation, the roughness length is approximately one-tenth of the actual physical height of the surface roughness elements (Hanna and Britter, 2002). In determining z_0 for

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[60] Meander factor values of one (no widening) are associated with wind speeds of 6 m/s or larger and atmospheric stability classes A, B, and C.

application to plume transport modeling, surface characterization should thus include both upwind, also known as "fetch," and downwind regions with respect to the postulated release location.[61]

McElroy and Pooler first developed "urban" dispersion parameters in *St. Louis Dispersion Study* (1968).[62] As a rough rule of thumb, vertical dispersion is increased by one stability class for urban areas due to the additional mechanical turbulence generated by the buildings (for example, an atmospheric condition resulting in Class F stability in rural environments becomes Class E stability in urban environments). The concrete buildings also reradiate their heat at night resulting in local temperature increases, termed the urban heat island, and cause additional buoyancy turbulence.

The field conditions of the Project Prairie Grass upon which the P-G dispersion parameters were developed are characterized by a surface roughness length of 3 cm (Napier et al., 2011). To more accurately predict dispersion for specific conditions that differ from those represented by the P-G and Briggs open-country horizontal and vertical diffusion parameterizations, adjustment factors have been developed for σ_z to reflect the enhanced mechanical turbulence caused by surface roughness.[63] One commonly used formulation that has been recommended by the American Meteorological Society (AMS) is given below (Hanna et al., 1977).

$$\textit{Surface Roughness Factor} = (z_0/z_{ref})^{n}\ (z_0 \geq z_{ref}) \qquad \textbf{Equation 6-12}$$

where z_{ref} is the reference roughness length associated with the field experiments on which the σ_z curves are based. For a P-G σ_z, the reference surface roughness length is 3 cm[64]. This formulation under-predicts σ_z enhancements observed near rugged terrain (Hanna et al., 1977).

The exponent, *n*, of Eq. 6-12 varies between 0.1 and 0.25, with larger values associated with shorter distances and rougher surfaces (Hanna et al., 1977; Irwin, 1980). Comparing diffusion data for surface roughness lengths of 3 cm and 100 cm for distances up to a few kilometers, in *Atmospheric Dispersion Parameters in Gaussian Plume Modeling. Part II. Possible Requirements for Change in the Turner Workbook Values* (EPA-600/4-76-030b), Pasquill noted a roughness factor of approximately 2, which translates to an exponent value of 0.2. In providing guidance to SRS on dispersion analysis, the PNNL-led review team provided the recommendation that is reflected in Table 6-10 (Napier et al., 2011).

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[61] For example, both the release location and receptor (such as the CW at 100 m) may be in the same open area that may be characterized by a small value for z_o. If this area is relatively small (a few hundred meters in diameter) and is surrounded by a building complex or forest, it may be appropriate to factor in the surface elements in the surrounding region in the determination of z_o. This approach is being used at SRS.

[62] For a detailed description of this study, see Venkatram et al., "The Analysis of Data from an Urban Dispersion Experiment," Atmospheric Environment 38: 3647–3659 (2004).

[63] Note that a surface roughness correction would not be applied with the use of the Briggs urban dispersion parameters because these parameters already reflect the surface roughness effect of large buildings in addition to the urban heat island influence at night. A roughness length of 0.6 cm was reported by Barad (1958), based on the Prairie Grass experiments.

[64] The reference roughness length for the Briggs open country set of dispersion parameters is complicated with the empirical basis that includes data other than that from Project Prairie Grass. Napier (2011) concluded that the P-G value of 3 cm is also applicable to the Briggs open country set of dispersion parameters given that χ/Q results using the Briggs dispersion parameters are essentially indistinguishable to those using P-G dispersion parameters at distances less than 10 km. Based on this reasoning, the 3-cm value for z_{ref} for applications for distances greater than 10 km would reflect a conservative perspective given that the χ/Q results based on the Briggs dispersion parameters are lower than those from the P-G dispersion parameters.

Specifically, a value of 0.2 is recommended for the exponent for distances up to 5 km, and a value of 0.1 for longer distances.

Table 6-10. Surface Roughness Adjustments Recommended PNNL-led Review Team.

Downwind Distance x (km)	**$0.1 < x \leq 5.0$**	**$x > 5.0$**
Roughness Factor Exponent	0.2	0.1
Roughness Factor (for z_o = 3 cm)	1.00	1.00
Roughness Factor (for z_o = 30 cm)	1.58	1.26
Roughness Factor (for z_o = 100 cm)	2.02	1.42

Various methods exist to estimate the surface roughness length. It may be appropriate to assign different values of z_0 for different regions of a site or for different receptor distances (such as the 100 m CW or site boundary distance) for the same postulated release from a given location.[65] It was noted above that the wind speed profile near the earth surface is influenced by roughness effects. This allows z_0 to also be estimated from wind profile observations, if available (Hanna and Britter, 2002).

Table 6-11. General Roughness Lengths for Various Terrain Types.

Terrain Description*	**z_0 (cm)**
Open sea, fetch at least 5 km	0.02
Mud flats, snow; no vegetation, no obstacles	0.5
Open flat terrain; grass, few isolated obstacles	3.0
Low crops; occasional large obstacles, $x/H > 20$	10.0
High crops; scattered obstacles, $15 < x/H < 20$	25.0
Parkland, bushes; numerous obstacles, $x/H \approx 10$	50.0
Regular large obstacle coverage (suburb, forest)	100.0
City center with high-rise and low-rise buildings	≥ 200.0

Note: x/H is ratio of downwind distance to obstacle height

Source: Wieringa, J. "Updating the Davenport Roughness Classification," *Journal of Wind Engineering and Industrial Aerodynamics*," Volume 41, Issue 1-3, October 1992, pp. 357-368.

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[65] One commonly-used method for estimating the surface roughness length is based on matching site observations with guidance tables, shown in Table 6-11. The current DOE Central Registry toolbox codes cannot accommodate more than one roughness factor.

The term “fetch” in Table 6-11 represents the roughness associated with the direction from which the wind is blowing (upwind), as the characteristics of the land covered by the wind in its path to the receptor will determine the ground roughness effects embedded in the air parcel.

An alternative approach is to use the EPA AERSURFACE software, which is based on input of 1992 National Land Cover Data (NLCD92) from the USGS (EPA-454/B-08-001). The NLCD92 data (http://landcover.usgs.gov/natllandcover.php) utilized by AERSURFACE consists of land cover data at spatial resolution of 30 meters, mapped using an Albers Conic Equal Area projection, and based on a 21-category morphology classification scheme, similar to what is shown in Table 6-11. AERSURFACE can be used to determine variations by sector, distance, and season, or an overall composite value.

MACCS2 and ALOHA allow the roughness factor to be entered as a user input that is used to scale σ_z. Historically, Eq. 6-12 has been used, due to its presence in MACCS2 software documentation (DOE, 2004a; NUREG/CR-4691 Vol. 2). None of the other DOE Central Registry radiological consequence codes allow for surface roughness adjustments to σ_z. The meteorological data file for GENII2, however, does include an input value for z_0, but it is not used to calculate a roughness factor. The z_0 value is an essential input for the deposition velocity calculation of GENII2.

Savannah River National Laboratory (SRNL) recently performed a study, *Roughness Lengths for the Savannah River Site* (Weber et al., 2012), where surface roughness was computed from H-Area meteorological tower 15-minute-averaged meteorological data measured at 61 m above the loblolly pine tree canopy using mechanical bivanes. Using the standard deviation of elevation angle and applying a simple formula based on tree canopy height, consistent estimates for roughness around the H-Area tower resulted in a mean value of surface roughness of 1.81 m. Application of this method for the 61-m level at D-Area meteorological tower and N-Area meteorological tower gave mean values of 1.71 m and 1.81 m, respectively. Since roughness results are azimuth dependent, as the fetch is different for each wind direction sector, the results were presented as averages over compass sectors spanning 22.5 degrees azimuth. These calculated values were compared to other methodologies that determine roughness. Additional data was obtained from a sonic anemometer at 61-m on the H-Area tower during a period of a few weeks in 2010 that supported the roughness calculations.

Based on the H-Area tower results, SRNL decided in 2012 to apply a surface roughness of 1.8 m in dispersion modeling applications, as discussed in the Executive Summary of the SRS surface length study (Weber, et al., 2012). This technique can be applied at all DOE sites to determine its site-specific surface roughness.

6.8.3 AERODYNAMIC EFFECTS OF BUILDINGS

The calculation of plume concentrations within the cavity and wake regions of even a simple block-like building is a very complex undertaking and generally requires Computational Fluid Dynamics (CFD) models to account for the all of the eddies generated by mechanical turbulence. A discussion of fluid dynamic principles required to solve this problem is beyond the scope of this Handbook.

Ground-level concentrations at some distance beyond the building, such as beyond five building heights, can be approximated. Another method available is to assign a virtual point source upwind of the building such that when this virtual plume reaches the building, the concentrations at the edges of the building are 10 percent of the centerline concentration.

As discussed earlier, building wake effects are most pronounced under windy conditions, whereas the plume meander effects are most pronounced under light wind conditions.

The Pasquill-Gifford and Briggs open-country dispersion parameters represent short-duration plumes released over relatively smooth and open terrain. When the terrain is marked by natural or anthropogenic obstacles, mechanical turbulence is generated as wind flows over and interacts with these obstacles. Surface roughness length was introduced earlier and formulations were summarized to adjust σ_z for the increased vertical dispersion from this source of mechanical turbulence. These formulations attempt to codify the collective influence of the full spectrum of surface elements that are predominantly along the line of plume transport[66]. As such, the surface roughness length concept is more applicable to long-range dispersion. In the vicinity of the radiological and toxic chemical releases, atmospheric dispersion is more likely to be dominated by the interaction of the plume with the wake and cavity regions of single building or a localized cluster of buildings. Releases from vents and small stacks can be entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs.

The building wake dispersion models that are presented in this section make use of the standard dispersion parameters, σ_y and σ_z, plus application of additional factors to capture increased dispersion from the wake effects. In implementing these models, the analysts should generally make use of σ_y and σ_z values that are free from any other adjustments such as for plume meander or surface roughness effects.[67] The building wake dispersion models presented in this section are applicable to releases that are modeled as ground-level and non-buoyant and are based on the treatment of the atmosphere as an incompressible fluid, for mathematical simplicity.

Figure 6-8 depicts the cavity and wake zones[68] behind a sharp-edged building (Hosker, 1981).[69] The aerodynamic effect of this building exerts two influences on the release. The first influence is the entrainment of flow in the vicinity of the building into the cavity region behind the building. The second influence is the enhancement of lateral and vertical dispersion associated with the cavity and wake regions.

The calculation of plume concentrations within the cavity and wake regions of even a simple block-like building is very complex and beyond the capability of most models, perhaps with the exception of CFDs. However, the ground-level concentrations at some distance beyond the building, such as beyond five building heights, can be approximated. Several methods have been proposed. In one, Eq. 6-5 is modified to account for the cross-sectional building area, A:

$$\frac{\chi(x,y=0,z=0,h=0)}{Q} = \frac{1}{\pi(u\sigma_y\sigma_z + cA)}$$ **Equation 6-13**

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[66] The contributing influence of surface elements that are several hundred meters upwind of the release may be important for receptors that are a short distance away.

[67] The use of σ_z values that are adjusted for surface roughness for example, could involve the double-counting, to some extent, of the building's impact on diffusion. The analyst will need to technically justify any use of σ_y and σ_z values that already incorporate other adjustments in its atmospheric dispersion modeling protocol.

[68] The term wake is occasionally used in the published literature in reference to the cavity and wake zones, collectively.

[69] See also Hunt, J. C. R. et al., "Kinematical studies of the flows around free or surface mounted obstacles: (cont.)

where *c* is the building shape factor, usually taken to be 0.5, and *A* is the smallest cross-sectional area of the building between the source and receptor. Another method is to assign a virtual point source upwind of the building such that when this virtual plume reaches the building, the concentrations at the edges of the building are 10% of the centerline concentration. This corresponds to σ_y = width/4.3 and σ_z = height/2.15, a commonly applied option used with MACCS2. The distance to this virtual point source can then be back-calculated, using the existing wind speed and atmospheric stability class.

Both HotSpot and EPIcode codes allow for the specification of a vertical area source that can represent the initial dispersion (σ_{y0}, σ_{z0}) associated with cavity releases. The user inputs a horizontal dimension (L_H) and vertical dimension (L_V) to define the area source. From these input values, values of σ_{y0} and σ_{z0} are calculated, a virtual source location, upwind of the actual source is determined, and adjusted dispersion parameters calculated as discussed above for MACCS2.

The GENII2 software has two model options for building wake dispersion that are documented in the software design documents (*GENII Version 2 Software Design Document*, Napier et al., 2009).

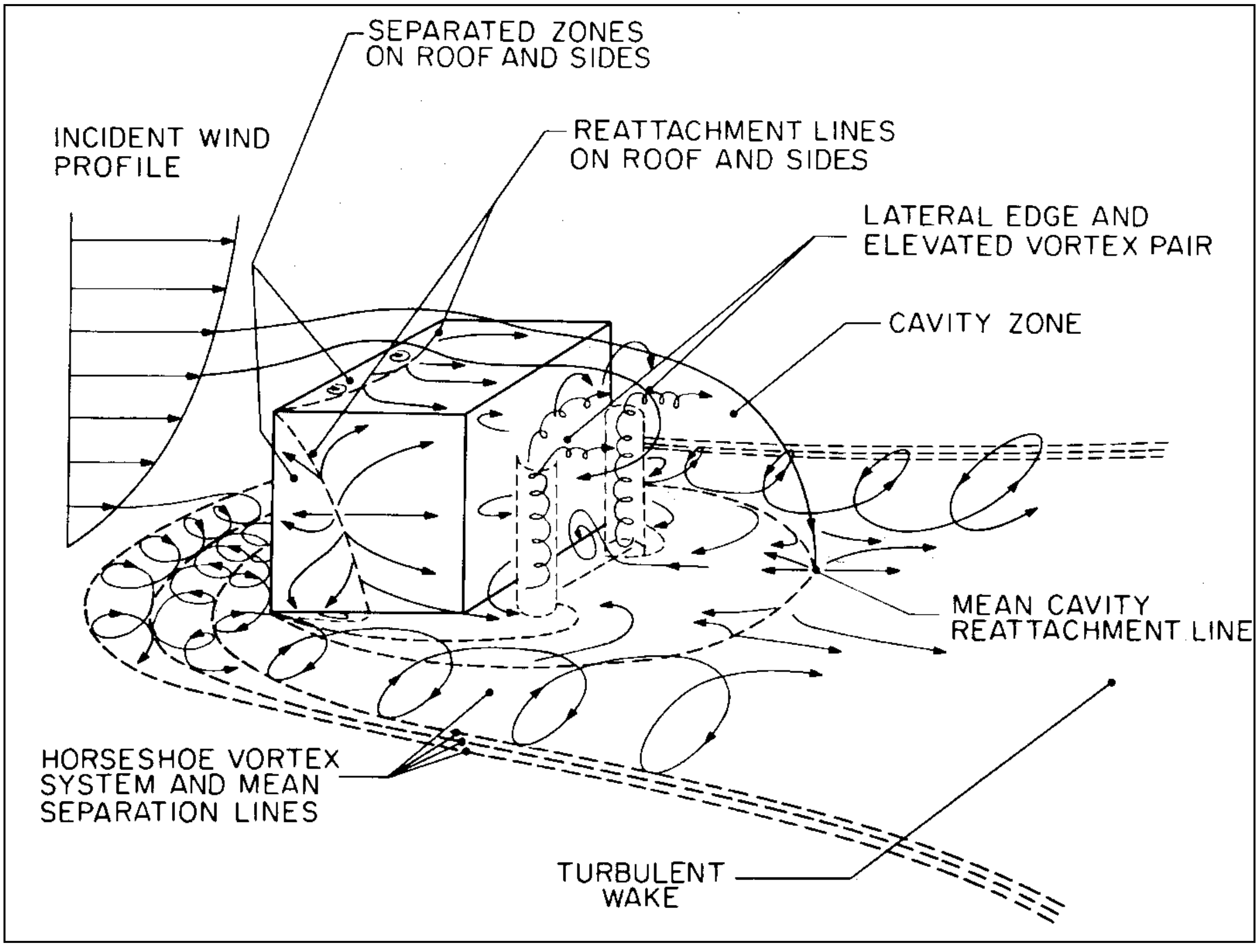

Figure 6-8. Schematic of Turbulent Air Flow around a Sharp-Edged Building.

(cont.) applying topology to flow visualization," J. Fluid Mech. 86, Part I, pp 179-200, 1978; Woo, H.G.C. et al., "Wind Tunnel Measurements in the Wakes of Structures," NASA CR-2806, NASA/Marshall Space Flight Center, Al, 1977.

6.8.4 PLUME MODIFICATIONS THROUGH DECAY, DAUGHTER IN-GROWTH, AND DEPOSITION PROCESSES

Atmospheric dilution and diffusion dominate the redistribution processes but they are not the only processes that affect the concentration distribution of a radioactive or toxic chemical material in a plume. With respect to radioactive materials, the concentration of a radioisotope of interest can decrease with time through a radioactive decay process, or can increase through the decay and in-growth of another daughter isotope.

Mass transfer processes in the atmosphere remove gases and particulates from the plume and can also reinsert particulates back into the atmosphere. The primary removal processes are dry deposition from gravitational settling and fallout, and wet deposition or precipitation scavenging from rain, snow, or hail. Reinsertion of deposited material back into the atmosphere to be transported to a new location is termed resuspension. These mass transfer processes are important in determining the ultimate fate of small respirable particulates, as well as ingestible particulates from radioactive compounds and chemically toxic materials.

The parameter Q represents the rate of release of material into the atmosphere. In the following discussion, the meaning of this parameter is extended to include other processes that change the radionuclide abundances and quantities of the material. These include decay and in-growth, removal of the material by dry and wet deposition processes, and resuspension of removed material. It may be noted that in some atmospheric dispersion models, the quantity χ/Q refers to only the atmospheric dispersion processes discussed earlier. Other models include the other processes discussed below. In NRC Regulatory Guide 1.111, *Methods for Estimating Atmospheric Transport and Dispersion of Gaseous Effluents in Routine Releases from Light-Water-Cooled Reactors*, NRC introduces the term depletedχ/Q, which is the concentration in the plume after dry deposition processes have removed, or depleted, some the material. NRC Regulatory Guide 1.111 also introduces the term D/Q, which is dry deposition. Accordingly, when using atmospheric dispersion models, note which definition is being used for χ/Q.

In-growth and decay of radioactive materials immediately occurs following their release into the atmosphere, regardless of the location of the material, whether within the plume, in materials that have fallen to the ground, or in materials that have been resuspended into the air. Decay refers to the loss of a given isotope through radioactive disintegration over time. In-growth refers to the build-up of one isotope by the decay of another, that is, it is the daughter product of the decay of this other isotope, termed the parent. The abundance of an isotope at any given time is a function of its decay rate as well as that of the parent isotope, if any, and the time since release.

For the initial atmospheric plume, not the resuspended plume, the time, t, is the transport time, that is, the distance (x) traveled divided by the average transport wind speed (u). For material deposited on the ground or for a resuspended plume, the time will be longer. The concentration of isotope, I, can be adjusted by multiplying the χ/Q by $A_i(t)/A_i(0)$ to account for the decay and in-growth of isotope i.[70] This is not of concern for long-lived, slowly decaying isotopes, such as Pu-239, but can be important for shorter-lived fission products from a criticality accident or from a reactor.

The rate of dry deposition is usually expressed in terms of a deposition “velocity” (V_d), a term having the units of velocity that expresses the rate of mass-transfer from the plume to the ground at the atmosphere-

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[70] See Chapter 8 and Equation 8-4 for further discussion.

ground surface interface. The deposition "velocity" is defined as a deposition flux, ω_d (Bq m^{-2} s^{-1}) divided by the near surface air concentration, χ (Bq m^{-3}):

$$V_d = \omega_d(x, y) / \chi(x, y, 0) \qquad \textbf{Equation 6-14}$$

The amount of material deposited on the ground at any particular location is the product of the deposition flux, ω_d, and the release duration. The dry deposition velocity is essentially a proportionality factor, and although it has the same units as a velocity, it is not a true velocity. With respect to Equation 6-14, the dry deposition velocity is evaluated at ground level. However, some codes apply a slightly higher elevation (e.g., GENII2; at height of one meter). A variety of mechanisms contribute to dry deposition. Gravitational settling is the dominant contributor for particles with diameters greater than or equal to 10 microns Activity Median Aerodynamic Diameter (AMAD).[71] For smaller-sized particles in the respirable range (<10 microns) other processes dominate, including turbulent diffusion, surface impaction, and Brownian diffusion. Values of V_d are a function of numerous meteorological variables (wind speed, atmospheric stability), impingement environment (terrain, land-use type, vegetation), and the particle size distribution and density of the particles. Generally, values for dry deposition velocity increase with increasing wind speeds, atmospheres that are more unstable, larger particle sizes, and terrain with higher surface roughness values. From various field experiments conducted over many years, dry deposition velocities are found to vary widely by several orders of magnitude, from 0.001 cm/s to 180 cm/s for particulates and from 0.002 cm/s to 26 cm/s for gases. Regardless of how V_d is determined, there are large uncertainties associated with it and there is currently no single accepted theoretical description of dry deposition that covers all common natural environments. However, parameterizations exist for many conditions of interest and are reasonably accurate for the conditions from which they were developed. Early dry deposition models are described in "*A Model for Predicting Dry Deposition of Particles and Gases to Environmental Surfaces*" (Sehmel and Hodgson, 1978), which were developed from wind tunnel experiments. The results of this model are consistent with a wide-range of historical deposition velocity measurements but did not take into account the effects of atmospheric stability or surface roughness from different land-use categories that were outside the scope of the aforementioned wind tunnel experiments. The default deposition velocity values originally recommended in the DOE Guidance Report for MACCS2 (DOE, 2004a) were based on the Sehmel and Hodgson model.

The current generation of atmospheric transport and diffusion models estimate the deposition velocity by analogy to electrical systems, where the deposition velocity is formulated as the inverse of the sum of resistances. GENII2 incorporates resistance-based deposition models. In these models the deposition velocity is calculated in time and 3-dimensional space because its value is dependent on time-varying atmospheric conditions and 3-dimensional variable surface characteristics.

A 2010 paper entitled "Development and Validation of a Size-resolved Particle Dry Deposition Scheme for Application in Aerosol Transport Models" presents more recent research in dry deposition modeling (original source: Petroff, A. and Zhang, L., 2010, Geosci. Model Dev., 3, 753-769, doi:10.5194/gmd-3-753-2010, as cited in Sugiyama et al., 2014). The research is constructed on the premise that while no single theoretical description of deposition processes exists that is valid for all land use types, deposition properties should be possible to parameterize over a wide range of natural environments based on available deposition velocity measurements. This model provides one of the most complete theoretical descriptions of deposition available and has been parameterized to match a large number of experimental data sets covering multiple surface types and land-use characteristics. This model has not yet been

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[71] Activity Median Aerodynamic Diameter is the diameter of the particle for which half the activity is associated with particles larger than and half the activity associated with particles smaller than this size particle.

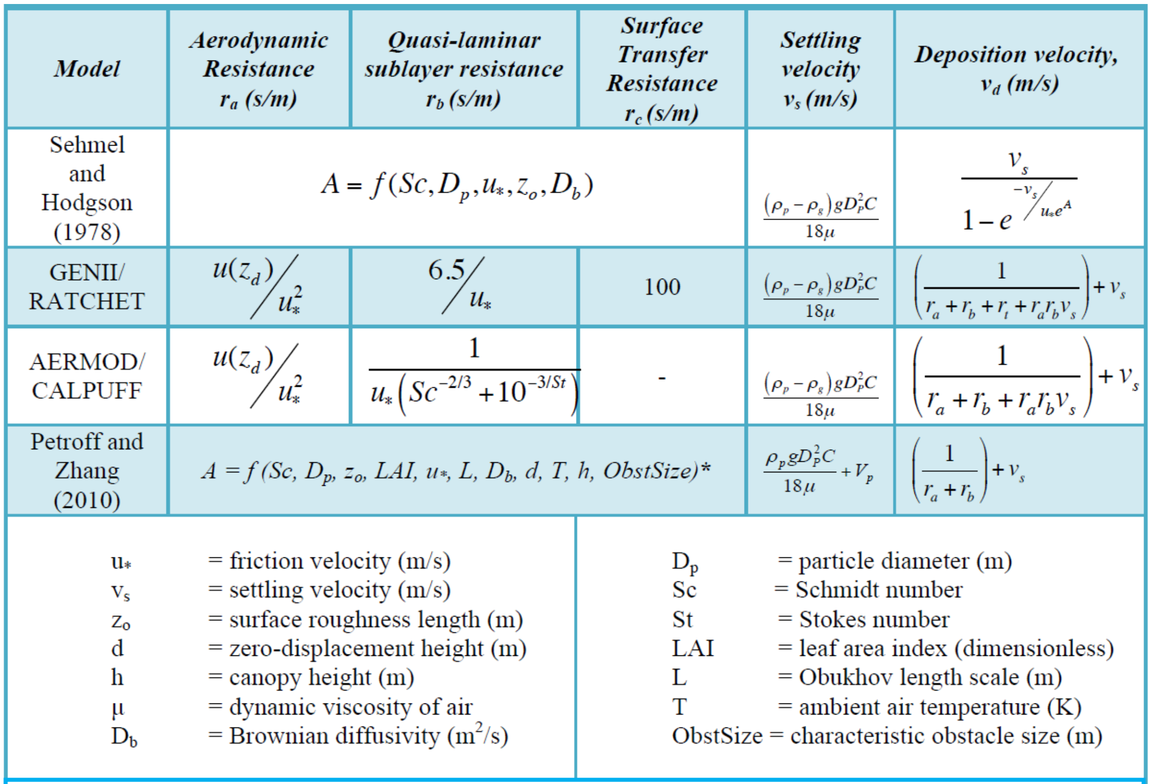
incorporated into any widely-used atmospheric dispersion models as it requires micrometeorological inputs that are not available from routine weather observations. However, it is used in one of the in-house atmospheric models at the National Atmospheric Release Advisory Center (NARAC). These models are summarized in Table 6-12.

The DOE Safety Software Central Registry includes atmospheric transport and diffusion models that either internally calculate deposition velocity using a formulation of a dry deposition model or that require the user to specify an appropriate value. For models like GENII2 that include a dry deposition model within the code, appropriate site-specific parameters (particle size distributions, particle density) should be specified that are representative of site-specific conditions. The analyst should follow the accompanying DOE guidance document for inputting site-specific parameters and follow the requirements in DOE-STD-3009-2014 for radiological consequences modeling.

Other atmospheric dispersion models, and DOE toolbox codes such as MACCS2 and HotSpot, require that deposition velocity be specified by the user. Guidance for specifying an appropriate value is contained within the software user’s manual or within the accompanying DOE Guidance Documents (DOE, 2004a; 2004b; 2004c). For a more conservative simplistic analysis, it is recommended that a default deposition velocity value be specified. The latest guidance from DOE contained in DOE-STD-3009-2014 specifies a deposition velocity of 0.1 cm/s for unfiltered release of particles (1-10 µm AED), 0.01 cm/s for filtered particles, and 0 cm/s for tritium and noble gases. Although using 0.1 cm/s or using 0 cm/s will produce virtually the same results for close-in distances, a non-zero value acknowledges that particulate deposition is occurring. For DOE reservations with distant site boundaries, a 0.1 cm/s dry deposition velocity may significantly lower the dose at those distances. Also, note that the deposition velocity depends on particle size. For the 0.3-µm particle, the recommended deposition velocity is 0.01 cm/s (DOE HSS Safety Bulletin 2011-02).

When a more site-specific value is desired to refine the analysis, the analyst may calculate a site-specific value using an external dry deposition model (e.g. GENII2, CALPUFF, Petroff and Zhang), and then use the calculated value as an input parameter to the code. Site-specific values are desirable when the default value produces overly-conservative estimates of exposures. External models should be evaluated for appropriateness for the situation being modeled. External models can be used in one of two ways: 1) executing the model after applying appropriate SQA; or, 2) performing a hand calculation or spreadsheet using the deposition velocity model formulation. The specific model formulation can be obtained from the model’s software design document or from the original published literature. The analyst should also follow the guidance specified in DOE-STD-3009-2014 for using site-specific methods and the atmospheric dispersion modeling protocol in Section 6.11.

Table 6-12. Summary of Deposition Velocity Models of Interest (This table was reproduced from Sugiyama et al., 2014).



Model	***Aerodynamic Resistance r_a (s/m)***	***Quasi-laminar sublayer resistance r_b (s/m)***	***Surface Transfer Resistance r_c (s/m)***	***Settling velocity v_s (m/s)***	***Deposition velocity, v_d (m/s)***
Sehmel and Hodgson (1978)	$A = f(Sc, D_p, u_*, z_o, D_b)$			$\frac{(\rho_p - \rho_g) g D_P^2 C}{18\mu}$	$\frac{v_s}{1 - e^{-v_s / u_* e^A}}$
GENII/ RATCHET	$u(z_d) / u_*^2$	$6.5 / u_*$	100	$\frac{(\rho_p - \rho_g) g D_P^2 C}{18\mu}$	$\left(\frac{1}{r_a + r_b + r_t + r_a r_b v_s}\right) + v_s$
AERMOD/ CALPUFF	$u(z_d) / u_*^2$	$\frac{1}{u_*\left(Sc^{-2/3} + 10^{-3/St}\right)}$	-	$\frac{(\rho_p - \rho_g) g D_P^2 C}{18\mu}$	$\left(\frac{1}{r_a + r_b + r_a r_b v_s}\right) + v_s$
Petroff and Zhang (2010)	$A = f(Sc, D_p, z_o, LAI, u_*, L, D_b, d, T, h, ObstSize)$*			$\frac{\rho_p g D_P^2 C}{18\mu} + V_p$	$\left(\frac{1}{r_a + r_b}\right) + v_s$

u_* = friction velocity (m/s)
v_s = settling velocity (m/s)
z_o = surface roughness length (m)
d = zero-displacement height (m)
h = canopy height (m)
μ = dynamic viscosity of air
D_b = Brownian diffusivity (m^2/s)

D_p = particle diameter (m)
Sc = Schmidt number
St = Stokes number
LAI = leaf area index (dimensionless)
L = Obukhov length scale (m)
T = ambient air temperature (K)
ObstSize = characteristic obstacle size (m)

*The Petroff and Zhang model uses a complex formulation that depends upon the dominant land-use category, the Monin-Obukhov length, the surface friction velocity, the air temperature and the particle size distribution as inputs.

Per DOE-STD-3009-2014, wet deposition is not evaluated in DOE hazard and accident analyses, however, this topic is addressed here for completeness to include a discussion of this phenomenology. Wet deposition, or precipitation scavenging, is more difficult to parameterize than dry deposition, as it depends upon cloud physics parameters that vary in time and space that are usually unavailable to the analyst. Each type of precipitation (rain, snow, or hail), passing through the plume collects particulates by accretion and scavenges soluble gases. The rate of depletion by wet deposition, dQ/dt, is proportional to the amount of material in the plume (Q). Thus, the change of material in the plume (dQ/dt), can be represented in Equation 6-15.

$$dQ / dt = -\Lambda Q \qquad \textbf{Equation 6-15}$$

where Λ represents the washout coefficient (s^{-1}). The solution to Eq. 6-15 over a time interval Δt gives

$$Q / Q_0 = \exp(-\Lambda \Delta t) \qquad \textbf{Equation 6-16}$$

Q_0 represents the amount of material entering this interval and Q represents the amount leaving. The value of Δt depends on the transport wind speed and the distance interval being evaluated. As with dry deposition, Eq. 6-16 would be an adjustment factor to apply to χ/Q for wet deposition occurring in the distance interval Δx during time interval Δt.

The washout coefficient, Λ, is a function of the precipitation rate, the type of precipitation (rain, snow, hail), and the type of material being scavenged (particulate or gas). For particulates in rain, the washout coefficient can be approximated by a power law of the rainfall rate in Equation 6-17:

$$\Lambda = a\, I^{\,b} \qquad \textbf{Equation 6-17}$$

where I is the precipitation rate (mm/hr) and a and b are dimensionless empirical coefficients that depend upon the particle size distribution. For example, in the MACCS code (NUREG/CR-4691), the values used are $a = 9.5\times10^{-5}$ and $b = 0.8$. For gases, the washout coefficient depends upon the solubility of the effluent as well as the precipitation rate. Families of empirical curves have been developed for various rainfall rates to estimate the washout coefficient. This procedure is made more complex by the spatial variability of the rainfall. Frequently, rainfall rates vary significantly within a rainfall event, and different washout coefficients may need to be applied to various segments of the plume as it travels to the receptor. This is virtually impossible to do with a steady-state Gaussian model and would need to be addressed by 3-dimensional Lagrangian mass-consistent codes, which are briefly discussed in Section 9.7. The use of a Doppler radar system to provide spatial representations of precipitation rates can assist this calculation.

An accurate estimation of washout is needed in the near-field for elevated releases because of the efficiency of this removal process for both particulates and gases. As an example, during an unscheduled release from the Ginna Nuclear Plant in 1980, the *maximum* ground-surface concentrations of ^{131}I were measured just beyond the containment building in the snow. In addition, larger doses from the Fukushima Dai-Ichi release in 2011 were the result of wet deposition that occurred days after the release. Although accurate estimations of washout are needed, most computer models treat it in only a cursory manner, if at all.

Plume depletion accounts for the material removed by either or both of the deposition processes, and accordingly reduces, or depletes, the χ/Q value. Depletion of the plume by either dry or wet deposition processes also results in soil contamination. Contaminated soil can be subsequently resuspended as a new source term should the soil be dry coupled with windy atmospheric conditions. Resuspension is generally higher in urban regions due to increased anthropogenic activities.

Although resuspension processes can contribute to exposure to individuals, the acute effect is small and therefore DOE-STD-3009-2014 does not require its inclusion in a DSA analysis.

6.8.5 PRINCIPLES GOVERNING PLUME RISE AND DOWNWASH

Two physical processes can each propel a neutrally-buoyant plume vertically upward to a level higher than that of its initial release, an effect called plume rise. The first process is termed momentum plume rise, in which the vertical efflux velocity of the radiological or toxic chemical release propels the plume upward, further above its elevated emission point. The second process is termed buoyancy plume rise, which occurs if the temperature of the plume is warmer than that of the ambient air.

Accounting for stack-tip downwash of the plume is essential in either process. Downwash can occur under high wind-speed conditions, and it can also occur if the release is from a vent or small stack into the wake and cavity behind the building. A brief discussion follows on both of these plume rise processes that can be integrated into an atmospheric dispersion model to account for these effects. Most atmospheric dispersion models calculate both momentum rise and buoyancy rise and consider that the dominant one is the one giving the greater plume rise.

6.8.5.1 MOMENTUM PLUME RISE

The calculation of momentum plume rise requires knowledge of the vertical efflux speed and the horizontal wind speed at the point of release, and the diameter of the stack from which the effluent is released[72]; the smaller the stack diameter the greater the efflux speed for a given mass flux. As the plume is transported downwind and away from its source of momentum, the upward momentum is gradually dissipated and ultimately the wind bends the plume over into the horizontal plane. The amount of momentum plume rise is a function of the ratio of the vertical efflux speed to the wind speed. Any additional plume rise only occurs due to plume buoyancy effects.

For radioactive effluents that are released from free standing stacks whose design meet the EPA Good Engineering Practice (GEP) stack height criteria, the entire effluent escapes the influence of the facility structures. GEP stack height is defined as 1.5 times the height of the nearest facility structure plus either the height or width of that structure, whichever is larger.[73]

For releases from structures that meet GEP stack height criteria, and under neutral or unstable stability conditions (stability classes A – D), plume rise can be calculated from:

$$\Delta h = 1.44\, d\, (v_e / u)^{2/3}\, (x / d)^{1/3} - C \qquad \textbf{Equation 6-18}$$

where Δh is the amount of plume rise (m) above the release level, v_e is the efflux speed (m/s), u is the horizontal wind speed (m/s), x is the downwind distance (m), and d is the diameter of the stack (m). This equation shows the relationship between the two competing parameters, v_e, and u. C is the downwash correction factor and is set to zero if $v_e/u \geq 1.5$, or:

$$C = 3\, (1.5 - v_e / u)\, d \qquad \textbf{Equation 6-19}$$

if $0 < v_e/u < 1.5$. Under stable atmospheric conditions (E – G stability classes), the following two empirical equations are evaluated, and the smaller value is applied:

$$\Delta h = 4\, (F_m / S)^{1/4} \qquad \textbf{Equation 6-20}$$

and

$$\Delta h = 1.5\, S^{-1/6}\, (F_m / u)^{1/3} \qquad \textbf{Equation 6-21}$$

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[72] Momentum plume rise equations do not apply to stacks that direct the plume horizontally or downward (“J” stacks).

[73] Note that 1.5 times height of building plus height of building equals 2.5 times height of building, which matches the NRC guidance. If the building is squat (wider than tall) “1.5 times height plus width” will exceed the “2.5 times height” rule.

where F_m is the momentum flux

$$F_m = v_e^2\ (0.5\ d)^2 \qquad \textbf{Equation 6-22}$$

S is the stability parameter

$$S = (g\ /\ T)\ (d\Theta/dz) \qquad \textbf{Equation 6-23}$$

g is the acceleration of gravity (m/s^2), T is the ambient temperature (K), and $d\Theta/dz$ is the potential temperature lapse rate (K/m), which is the sum of the actual temperature lapse rate and the adiabatic lapse rate.

For plume rise from non-GEP stacks or building vents, empirical relationships from field studies were developed at the Millstone Nuclear Power Plant in 1978. The central result of this study is that there are two forces acting on the plume. The efflux velocity (v_e), which can be visualized as an escape velocity, and wind speed (u), which can be visualized as a capture velocity. Accordingly, the v_e/u ratio is the driving parameter. When $v_e/u > 5$, the vertically-directed momentum flux, which affects escape from the building, dominates the horizontally-directed wind speed, which affects capture in the building wake, and the release is treated as elevated. This means that although the release emanated from a short stack or a vent, it still will fully escape the aerodynamic effects of nearby buildings due to the high momentum flux coupled with low wind speed. The GEP stack height equations apply in this case. On the other end of the spectrum, when $v_e/u < 1$, the release is effectively ground-level and no plume rise occurs. Two intermediate cases were also developed from the field study. These are the partially entrained and the partially elevated cases and are expressed in terms of an entrainment coefficient, E_t, which is the fraction of the plume entrained into the wake and cavity behind the building. The remainder escapes entrainment.

Partially Entrained: For cases where $1.5 < v_e/u < 5$, a portion of the plume is entrained and the remainder of the plume remains elevated. An entrainment coefficient can be calculated for this case as follows:

$$E_t = 0.30 - 0.06\ v_e\ /\ u \qquad \textbf{Equation 6-24}$$

Partially Elevated: For cases where $1 \leq v_e/u \leq 1.5$, an entrainment coefficient can be calculated for this case as follows:

$$E_t = 2.58 - 1.58\ v_e\ /\ u \qquad \textbf{Equation 6-25}$$

In both of these cases, the elevated portion of the plume is subject to plume rise, while the entrained portion of the plume is down-washed to ground level.

6.8.5.2 BUOYANCY PLUME RISE

The calculation of buoyancy plume rise requires knowledge of the effluent temperature or the energy released in a fire or other energetic event and the ambient temperature at the point of release.[74] If the plume temperature is higher, positive (upward) buoyancy occurs, while for a relatively cold plume, negative buoyancy occurs. The stability class of the atmosphere also affects the buoyancy rise, at least initially. Unlike momentum rise, which may take only 30 to 40 seconds, buoyancy rise may continue for

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[74] For indoor fires assume no plume rise, to be conservative. The plume will cool and plate out as it exits the facility, and as there is no way to accurately estimate the extent of cooling, assume there is no plume rise. An indoor air temperature may be used if there is a need to quantify the exit temperature.

many minutes due to its slower upward speed compared to momentum rise. The buoyancy rise can be calculated in two parts. The first is the initial rise and is dependent on the stability class. The second is the gradual rise and is independent of stability class. The larger of the two is then chosen as representative.

The initial plume rise is independent of distance downwind, but is dependent on stability class. For classes A – D, and buoyancy fluxes less than 55 m^4/s^3, the plume rise is given by (Briggs, 1975)

$$\Delta h = 21.425\, F_b^{\,3/4}\, u^{-1} \qquad \textbf{Equation 6-26}$$

where F_b is the buoyancy flux. For fluxes greater than 55 m^4/s^3, the plume rise is given by

$$\Delta h = 38.71\, F^{\,3/5}\, u^{-1} \qquad \textbf{Equation 6-27}$$

For classes E – G, the plume rise is given by

$$\Delta h = 2.6\, [F_b / (u\, S)]^{1/3} \qquad \textbf{Equation 6-28}$$

except for calm conditions, for which it is appropriate to use

$$\Delta h = 4\, F_b^{1/4}\, S^{-3/8} \qquad \textbf{Equation 6-29}$$

The gradual plume rise, which is independent of stability class, can be calculated from the empirical relation

$$\Delta h = 1.6\, F_b^{1/3}\, x^{2/3}\, u^{-1} \qquad \textbf{Equation 6-30}$$

The buoyancy flux depends upon whether the release is from a stack or from a fire. For a stack release, the buoyancy flux is

$$F_b = g\, v_e\, d^2\, \Delta T / (4\, T_s) \qquad \textbf{Equation 6-31}$$

Where, ΔT is the stack gas temperature (T_s) minus ambient temperature. For a fire it is given by

$$F_b = 8.79 \times 10^{-6}\, \Omega \qquad \textbf{Equation 6-32}$$

where Ω is the rate of release of sensible heat (watts)[75]. Eq. 6-29 would let the plume rise indefinitely, so it is necessary to cap the plume rise. Several methods of capping the buoyancy rise have been used. One way of doing this is to terminate the use of Eq. 6-27 when one of the following three conditions occurs: (1) when Δh reaches $300\, F_b/u^3$ (Briggs, 1975); (2) when the plume centerline has reached the height of the top of the mixed layer; or (3), when one hour has elapsed since the plume release began.

6.8.6 PLUME IMPACTION

DOE sites that are located in mountainous terrain may need to address plume impaction of elevated releases, especially if a large rise in the topography is nearby (see Figure 6-1). With respect to this type of morphology, the analyst should screen any elevated releases that may have the potential for impaction

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[75] The total energy released in a fire can be partitioned into various forms, such as sensible heat, radiant heat, and latent heat. Sensible heat gives rise to changes in temperature and density and thus it determines the buoyancy flux.

using the EPA code CTSCREEN. This code is a Gaussian plume dispersion model designed as a screening technique for plume impaction assessments in complex terrain. CTSCREEN is also a screening version of the CTDMPLUS model. This code and its user guide can be accessed at https://www.epa.gov/scram/air-quality-dispersion-modeling-screening-models.

6.9 DOE CENTRAL REGISTRY OF RADIOLOGICAL DISPERSION AND CONSEQUENCE ANALYSIS CODES

Since 2004, a collection of computer codes, including those for performing atmospheric dispersion and radiological or toxic chemical consequence analyses, have been designated as Toolbox codes in the DOE Safety Software Central Registry (CR) and managed by the DOE Office of Quality Assurance & Nuclear Safety Management Programs (AU-32). While these models have widespread use and have accumulated considerable levels of analyst understanding, they still warrant careful consideration in the preparation of inputs and assumptions to ensure that the resulting radiological and toxic chemical consequence outputs are technically defensible and consistent with expectations of the analysis, and that resulting safety control sets are adequate, robust and implementable. Accordingly, every Toolbox model needs to be independently evaluated according to the SQA principles in DOE O 414.1D*, Quality Assurance*, and additional useful guidance in DOE G 414.1-4, *Safety Software Guide for use with 10 CFR 830 Subpart A, Quality Assurance Requirements* (2010). Modeling techniques inherent in the toolbox software and guidance for their use, including input requirements, are discussed below. Note that model evaluation is not one of the 10 work activities to be considered per DOE O 414.1D, Attachment 4 nor is this topic discussed in DOE G 414.1-4A.

Of the eight toolbox codes that comprise the DOE Safety Software Central Registry (CR), three are applicable to radiological dispersion and consequence analysis applications (GENII, MACCS2, and HotSpot) and two are applicable to toxic chemical dispersion and consequence analysis applications (ALOHA and EPIcode). The other toolbox codes address fires (CFAST), in-facility transport (MELCOR) and biological uptake (IMBA). The three radiological dispersion computer models are listed in Table 6-13 along with their respective developing organization, toolbox version, the year designated for the DOE Safety Software Central Registry, and current version supported by their developer. Additional information on the DOE Safety Software Central Registry and individual atmospheric dispersion and consequence analysis computer models is available through the website http://energy.gov/ehss/safety-software-quality-assurance-central-registry.

Inclusion of a code into the DOE Safety Software CR provides DOE users the assurance that the SQA level is adequate for safety analysis applications along with implementation of applicable site-specific SQA requirements per the site’s quality assurance program. These requirements might include site acceptance testing, user training, configuration control, and error reporting. In the case of a specific DOE Safety Software CR computer code, the gap analysis against SQA standards and requirements and the code guidance development process are specific to the version at the time the computer software was designated for the Central Registry. If a later version of the computer code is being considered for use, the DOE contractor is responsible for determining that the quality assurance level of that code version meets applicable DOE requirements.

Table 6-13. Computer Models in DOE Safety Software Central Registry for Radiological Consequence Analysis.
(Content shown is current as of publication date)

Computer Code	Lead /Developing Organization	Version/ Year Designated for the Toolbox	Current Version Supported by the Developer
GENII	Bruce Napier / Pacific Northwest National Laboratory	V1.485 / 2004 V2.10.1 / 2013	V2.10.1
HotSpot	Steve Homann / Lawrence Livermore National Laboratory	V2.07.1 / 2010	V3.01
MACCS2	Nate Bixler / Sandia National Laboratory	V1.13.1 / 2004	WinMACCS V3.7; MACCS2 V2.6.0

The codes in the CR were developed outside of DOE and in other Federal agencies (NOAA, NRC, or EPA)]. Access to the toolbox codes or their use is subject to agreements, conditions, and restrictions established by the code owners or Federal Agencies. The CR is currently managed by AU-32 within EHSS and the focus of AU-32 is to work with the code developers/owners to have the Toolbox codes updated (closing the gaps) and maintained following SQA provisions of applicable national consensus standards such as ANSI/ASME NQA-1-2008 which is the preferred standard cited in DOE O 414.1D for safety software.

In the preface to the DOE Central Registry, DOE states that the Chief Health, Safety and Security Officer (DOE/HS-1, which is currently the AU-1 organization) is responsible for managing the Safety Software Central Registry. However, the toolbox code owners are responsible for ensuring that the codes are maintained in accordance with established DOE O 414.1D requirements. and DOE G 414.1-4A provides additional SQA guidance.

As stated on the DOE/AU website, use of the CR toolbox codes is not mandatory. Of the three options given in DOE-STD-3009-2014, Section 3.2.4.2 for radiological dispersion analysis, only Option 2 requires the use of a toolbox code. However, using the toolbox codes offers a number of advantages to DOE and its contractors, which include:

- The evaluation performed provides valuable information on the code regarding application of SQA requirements;
- The evaluation generally extends beyond the DOE safety software quality assurance criteria to the review of the code’s capability to properly perform safety basis calculations;
- The DOE-specific guidance documents identify limitations and vulnerabilities not readily found in other code documentation;
- Due to the established pedigree, quality assurance assessments of the toolbox code by the users (DOE personnel and site contractors) may be reduced in scope; and
- Increase of user base and experience across the DOE complex.

ALOHA, EPIcode, GENII, MELCOR, CFAST, and MACCS2 were the original six computer codes designated for the DOE Central Registry in 2003, and each code’s SQA, gap analysis, and code usage guidance documents were published in 2004. The gap analyses for these six codes were completed before issuance of DOE O 414.1C, *Quality Assurance*, and the safety software guidance, DOE G 414.1-4[76]. The two documents provided a framework for the evolving DOE requirements for safety software. With the release of DOE O 414.1C and DOE G 414.1-4, and subsequently DOE O 414.1D the safety software requirements were more clearly identified (Attachment 4 to the respective Orders) and guidance for meeting the requirements provided.

HotSpot V2.07.1 was added to the CR in 2010 after a detailed SQA evaluation that determined that the adequacy of the HotSpot SQA program and associated documentation, with some modifications (gaps), that met the safety SQA requirements of the DOE O 414.1D. With the available SQA documentation, the necessity of a separate guidance document was not established. HotSpot has been recently upgraded to Version 3.01 and further revision to the code is underway following which the code developer intends to request a subsequent SQA evaluation by DOE/AU-33.

More detailed discussions of the capabilities of MACCS2, GENII, and HotSpot are given below. These cover available toolbox atmospheric transport and diffusion models for radiological analysis. The toolbox models for toxic chemical consequence analysis, ALOHA and EPIcode, are addressed in Section 9.7. Additional supported radiological consequence codes (e.g. RASCAL, NARAC, RSAC-8, HYRAD, ARCON96), which have had some use at various DOE sites, should be evaluated on a case-by-case basis as to their applicability to the safety analysis that is undertaken. Should the analyst select any of these other codes, an atmospheric dispersion modeling protocol (see Section 6.11) needs to be developed and approved by the DOE site office.

The three radiological toolbox codes listed in Table 6-13 are briefly discussed below. The toolbox version of these codes is available through the Radiation Safety Information Computational Center. Table 6-14 summarizes important features of the toolbox software and serves as a roadmap to the guidance given in this Handbook with respect to radiological consequence analysis.

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[76] DOE O 414.1C, and its supporting Safety Software Guide, were issued 6-17-05.

Table 6-14. Summary Guidance on the Use of Computer Models in DOE Central Registry for Radiological Dispersion Analysis.

Model Feature	GENII	HotSpot	MACCS2	Guidance
Prescriptive Meteorology Capability	Not readily available as an option	User-defined wind speed and stability class can be input via one of the meteorological input modes	User-defined wind speed and stability class can be input via one of the meteorological input modes	Generally has been used for modeling dispersion for a high wind event. Another example is that stability class F and 1.0 m/s wind speed may be used when site-specific hourly meteorological data are not available.
Plume Transport with Hourly Meteorological Data	One continuous plume generated for each hour based on constant wind direction, wind speed and stability class	One continuous plume generated for each hour based on constant wind direction, wind speed and stability class	For each source term, one continuous plume generated for each hour with constant wind direction, but wind speed and stability class changing after each hour of transport; up to 4 plumes can be used to transport and disperse 4 distinct source terms	The GENII2, HotSpot and MACCS2 approaches are compliant with DOE-STD-3009-2014.
Years of Meteorological Data	Up to ten years in single code execution	Up to five years in single code execution	One year per code execution – mean value of 95th or 99.5th percentile χ/Q from all executions typically determined	Five years is recommended (DOE-STD-3009-2014, Section 3.2.4.2).
Percentile Output for a Given Distance Based on Statistical Sampling of Meteorological Data	95th percentile for each wind direction sector, considering only plumes traveling in the given sector	95th percentile from overall cumulative probability distribution from all directions combined	95th and 99.5th percentile from overall cumulative probability distribution from all directions combined	The approach of HotSpot/MACCS2 is conservative and accepted by DOE-STD-3009-2014 even though not fully compliant with NRC Regulatory Guide 1.145. Determining the maximum sector result from GENII2 is a conservative approach with respect to DOE-STD-3009-2014.

Model Feature	**GENII**	**HotSpot**	**MACCS2**	**Guidance**
Wind Speed Profile	i) Reference height for meteorological data is an input value in first line of meteorological input data file ii) Wind speed is adjusted for release heights that differ from reference height iii) Release heights less than 12 m are modeled using 10-m wind speed iv) Surface wind speed is used together with roughness length (z_0) input in meteorological data file for determining friction velocity (u_*)	i) Default reference height for meteorological data is 10 m, but the user may change it. ii) Wind speed is adjusted for release heights that differ from reference height.	i) Reference height for meteorological data is always 10 m ii) Wind speed is not adjusted for release heights that differ from reference height	The 10-m wind speed is recommended for ground level releases. For elevated releases above 10 m, adjustment of the wind speed is standard practice (HotSpot, GENII2); no adjustment is conservative (MACCS2).
Treatment of Calm Wind Speeds	User specifies minimum wind speed value (any wind speed values in meteorological data file less than minimum value is reset to minimum value)	Software resets any wind speed values in meteorological data file less than 0.1 m/s to 0.1 m/s	Software resets any wind speed values in meteorological data file less than 0.5 m/s to 0.5 m/s	Specifying a minimum wind speed of 1.0 m/s is recommended (DOE-STD-3009-2014, Section 3.2.4.2).
Dispersion Parameter Sets	• Eimutis and Konicek (NRC) • Pasquill-Gifford (EPA) • Briggs Open Country • Briggs Urban	• Briggs Open Country • Briggs Urban	• Tadmor-Gur • Briggs Open Country • Eimutis and Konicek (NRC) • Briggs Urban	Briggs Urban set not recommended. Tadmor-Gur not recommended for distances less than 500 m. The toolbox version of MACCS2 has a lookup table error which may limit which dispersion parameters can be used. See Section 6.4.2.

Model Feature	GENII	HotSpot	MACCS2	Guidance
G Stability Class	i) Modeled explicitly with Eimutis and Konicek (NRC) set of dispersion parameters ii) Modeled as F stability class for other sets of dispersion parameters	i) Vertical dispersion modeled as F stability class ii) Modeling of horizontal dispersion specified by user to be equivalent modeled as any stability class in range of A through F	Modeled as F stability class	Modeling G stability class as F stability class is recommended. Experiments have shown that plume meander under class G yields dispersion conditions that are no more conservative than under Class F.
Adjustment of horizontal dispersion parameter (σ_y) for plume meander	No adjustment currently modeled	Averaging time method	i) Averaging time method ii) NRC method	The averaging time method is recommended; no adjustment is conservative.
Adjustment of vertical dispersion parameter (σ_z) for surface roughness (z_o) effects	No adjustment (User enters z_o value in meteorological data file that is used to define the wind speed profile and calculate the deposition velocity)	No adjustment	User enters roughness adjustment factor	Equation 6-12 or either Equation 6-13 or 6-14 is recommended together with one of the methods discussed to determine z_o; no adjustment is conservative for ground-level non-buoyant releases.
Adjustment of initial values (at source) for σ_y and σ_z for building wake effects	User inputs building dimensions and software determines initial σ_y and σ_z values	User inputs building dimensions and software determines initial σ_y and σ_z values	User inputs initial values for σ_y and σ_z	Increased dispersion from building wake effects should only be used for ground-level releases. No other adjustments should be made to the dispersion parameters for plume meander or surface roughness effects. Ignoring building wake dispersion is generally more conservative. Option 2 in DOE-STD-3009-2014 does not allow for crediting of building wake factors.

Model Feature	GENII	HotSpot	MACCS2	Guidance
Effective Stack Height	User enters effective release height	User enters effective release height	User enters effective release height	The use of plume rise equations in Appendix E is recommended to determine effective release height taking into account stack-tip downwash and aerodynamic entrainment effects of buildings. Assuming ground release is generally more conservative.
Plume Buoyancy	Plume rise model from stack available as an option. Not recommended for fire-release modeling.	• Stack plume rise model • Pool-fire plume rise model (open field)	Plume rise model from stack available as an option.	The three models employ similar models for plume rise from a stack as long as the stack meets GEP criteria. The HotSpot pool fire model is only applicable with an open field release. When using MACCS2 to model fires, the guidance of this Handbook should be followed, including inputting the height of the tallest co-located structure to account for building entrainment that can inhibit plume rise. Ignoring buoyant plume rise is conservative.
Deposition Velocity for Respirable Source Term	Software determines value for each meteorological sample using other input data and algorithms in the model	User enters value	User enters value single value	The GENII2 deposition velocity model is approved for safety analysis. When GENII2 is not used for the dispersion and consequence analysis, the 95th percentile deposition velocity determined from the GENII2 output is recommended as input to either the MACCS2 or HotSpot software. Alternatively, the default value of 0.1 cm/s for an unfiltered release may be used.
Resuspension	Option available to user	Option available to user	Option available to user	Resuspension does not need to be modeled per DOE-STD-3009-2014 since that this atmospheric redistribution mechanism develops slowly; including this dose pathway is conservative.

Model Feature	**GENII**	**HotSpot**	**MACCS2**	**Guidance**
Radioactive Decay During Plume Transport	Option available to user	Option not available to user	Option available to user	Decay of radioactive isotopes in the plume is a function of the travel time and the half-life of each specific radionuclide that is present in the plume. In practice, this effect is appreciable with radioisotopes of half-life on the same order or shorter than the time to reach the receptor under consideration. For non-reactor facilities, inadvertent criticality event would be the primary accident type for which this factor is important.
Grid Spacing	User selection	User selection	User selection	Grid spacing can have an impact on the radiological dose calculations.
Mixing Height Treatment	Variable depending on data input	Seasonal, user input	Seasonal, user input	Mixing height represents the lid on vertical dispersion. Once the plume reaches the mixing lid, it reflects back to the ground.

6.9.1 MACCS2

The MELCOR Accident Consequence Code System (MACCS) code,[77] and its successor, MACCS2,[78] are based on a straight-line Gaussian plume model. MACCS was developed originally for the NRC, whereas MACCS2, an enhanced version, was developed to address DOE applications.

MACCS2 V 1.13.1 is a DOE toolbox code, and because it is a comprehensive and flexible code it is one of the most widely used codes in the DOE/NNSA complex. The MACCS2 package includes three primary enhancements: (1) a more flexible emergency response model; (2) an expanded library of radionuclides; and (3) a semi-dynamic food-chain uptake model. The new code features allow detailed evaluations of potential consequences to workers at nearby facilities on large DOE reservations and allow the user to assess the potential impacts of over 800 radionuclides that could not be considered with the earlier MACCS code.

MACCS2 requires significant user experience to set up input files which include:

- Range intervals;
- Population distribution;
- Weather scenario;[79]
- Release height, number, and duration of plumes;
- Radionuclides released;[80]
- Organ doses and health risks;
- Dose conversion factors;
- Evacuation timing and routes;
- Costs of decontamination and interdiction;
- Sensible heat;
- Radiation shielding parameters; and
- Deposition and resuspension.

WinMACCS V 3.10, a new version of MACCS2 with a Windows-based user interface, has been released, but has not yet (as of Handbook publication) been approved as a toolbox code (McFadden et al., 2007).

MACCS2 has also been successfully used in modeling the atmospheric dispersion and consequences of a plume of Pu-239 particulates resulting from an HE detonation, although it was not originally designed for that purpose.

DOE Safety Advisory 2009-05, *Errors in MACCS2 χ/Q Calculations*, describes a problem at large distances (greater than 2 km) with the lookup table with MACCS2 versions 1.13.1 and 2.4 (DOE Safety Advisory 2009-05; Napier et al., 2011) and it details an approach for avoiding the error. When using this approach, the results should be verified to ensure the error was adequately addressed. PNNL evaluated the Safety Advisory approach and found it to be insufficient at addressing the problem (Napier et al., 2011). This error has been fixed with MACCS2 Version 2.6. The PNNL team recommends the use of

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[77] NUREG/CR-4691; NUREG/CR-6059.

[78] NUREG/CR-6613; NUREG/CR-6547.

[79] Constant weather, various variable-weather scenarios (such as using one year of hourly averages of wind speed and direction, stability class, precipitation), and type of weather sampling.

[80] Over 800 can be specified in MACCS2, an increase of over 500 from MACCS.

the power law approach (Tadmor and Gur dispersion parameters) that avoids this potential error when using MACCS2 for distances greater than 500 m (Napier et al., 2011).

The toolbox version of the code (MACCS2 V1.13.1) is not strictly compliant with DOE-STD-3009-94 CN3, Appendix A calculation requirements for determination of the overall site 95th percentile χ/Q. However, its results can be viewed as providing a reasonable approximation to this level of consequence, and can be used for the Option 2 χ/Q method from DOE-STD-3009-2014, Section 3.2.4.2. Historically, MACCS2 has been used to calculate the offsite 95th percentile χ/Q for DOE facilities despite the fact that the methodology used does not take into account variations in site boundary distances. As stated in DOE-EH-4.2.1.4:

> MACCS2 and MACCS do not comply fully with … [NRC Regulatory Guide 1.145 Position 3] methodology for determination of direction-independent 95th percentile dose to the offsite individual. It may be used to conservatively evaluate the 95th percentile direction-independent dose to receptors equidistant to the source.
>
> Given site-specific data, the 95th percentile consequence is determined from the distribution of meteorologically-based doses calculated for a postulated release to downwind receptors at the site boundary that would result in a dose that is exceeded 5% of the time. DOE-STD-3009 allows for variations in distance to the site boundary as a function of distance to be taken into consideration. Assuming the minimum distance to the site boundary applies in all directions is a conservative implementation that is easily supported by MACCS2 and that essentially makes the calculations sector independent.

6.9.2 GENII

The Hanford Environmental Radiation Dosimetry Software System, GENeration II (GENII), is also based on a straight-line Gaussian plume model. GENII V1.485 (Napier et al., 1988), which is a DOS-based toolbox code, is available from the Radiation Safety Information Computational Center as package CCC-601. A newer, Windows-based version, GENII V 2.10.1, with a user-friendly interface (FRAMES) has been evaluated and approved as a toolbox code.

The GENII code has been thoroughly documented and was developed under a stringent quality assurance program based on ANSI/ASME NQA-1-2008. It has been used in consequence calculations by safety analysts for many years.

GENII is a comprehensive and flexible code with a strong emphasis on environmental dispersion processes beyond those of atmospheric dispersion (aquatic dispersion, groundwater transport). (See Chapter 7.) To quote from the APAC Working Group 5 report (APAC/TEEL-5, 1998):

> GENII is a radiological assessment computer code system that estimates individual and collective doses to humans from the environmental transport of radionuclides in the atmospheric, surface water, and other environmental media, such as biotic transport and manual redistribution to the surface from buried waste. GENII is used for a variety of radiological assessments including 1) acute atmospheric releases, 2) chronic atmospheric releases, and 3) residual soil contamination.

GENII V 2.10.1 has extensive libraries of isotopes and associated dose conversion factors. It calculates doses from inhalation, ingestion, and external radiation (cloudshine and groundshine).

The required meteorological data to drive the code consists of JFDs of wind speed and stability class for each of the 16 wind directions, usually taken to be 22.5-degree azimuth compass directions, with the first one centered on north. The toolbox version of the code (GENII V 1.485) is not strictly compliant with DOE-STD-3009-94, CN3 Appendix A calculation requirements for determination of the overall site 95th percentile dose. However, its results can be viewed as providing a reasonable approximation to this level of consequence. Users should also recognize that the older version uses atmospheric dispersion models that do not account for plume depletion from wet and dry deposition phenomena or resuspension.

The GENII code also allows the user to specify radionuclide concentrations in the environmental media, as may be produced from another code or previous analysis. In this mode, GENII will calculate the corresponding radiological doses from various pathways.

6.9.3 HOTSPOT

The HotSpot Health Physics Codes, or HotSpot program, provides a first-order approximation of the radiation effects associated with the atmospheric release of radioactive materials. The toolbox version of this code is Version 2.07.1 (Homann, 2010) and, as with the other two radiological consequence codes, is based on the Gaussian plume model. The user inputs a 95 percent meteorological condition[81] and selects various source term options and dose output options. The software is also used for safety analysis of facilities handling radioactive material. HotSpot atmospheric dispersion model codes are a first-order approximation of the radiation effects associated with the short-term (less than a few hours) atmospheric release of radioactive materials.

As is true for MACCS2, HotSpot is not strictly compliant with DOE-STD-3009-2014, and for the same reasons. HotSpot Version 3.0.1, has been released, but has not yet been approved as a toolbox code.

6.10 ATMOSPHERIC DISPERSION OPTIONS IN DOE-STD-3009-2014

Three options are given in DOE-STD-3009-2014 to evaluate atmospheric dispersion and the resulting χ/Q:

- Option 1: Follow a process based on NRC Regulatory Guide 1.145*;*
- Option 2: Use a DOE-approved toolbox code and apply the conservative parameters; or
- Option 3: Use site-specific methods and parameters as defined in a site/facility specific DOE-approved modeling protocol.

All three options evaluate the χ/Q at the MOI using either a 95th percentile for a “directionally independent” method or a 99.5th percentile for a “directionally dependent” method. NRC Regulatory Guide 1.145 defines how to derive the “95th percentile directionally independent” and the “99.5th percentile directionally dependent” χ/Q values. For each of these, the minimum distances to the site boundary in 45° azimuth-wide sectors centered on 16 directions (N, NNE, …) is to be derived and the χ/Q value for each hour during the year is to be calculated. The term “directionally independent” as used in

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[81] Hotspot Version 2.07.1 and Version 3.01 can also work with hourly observations.

DOE STD-3009-2014 means that the determination of the overall site 95th percentile χ/Q is calculated by creating a cumulative probability distribution for all sectors combined based on all the meteorological annual data and using the actual site boundary distance for each sector, and choosing the 95th percentile value. The "99.5th percentile directionally dependent" value is found by creating a cumulative probability distribution for each sector using the actual site boundary distances, determining the 99.5th percentile value for each, and choosing the maximum value.

The value of χ/Q using Option 1 can be accomplished manually using a spreadsheet. Option 3 allows the use of software generated at the site if it follows a DOE site-approved atmospheric dispersion modeling protocol. For Option 2, one of the toolbox codes is to be used. It should be noted that the often-used MACCS2 software does not fully comply with NRC Regulatory Guide 1.145, as explained above, yet is accepted by DOE as the 95th percentile value for the closest point on the site boundary is conservative. POSTMAX V2.0 (Sartor, 2009), software developed at LANL, can be used to generate the 95th percentile value of χ/Q from the MACCS2 output that is compliant with NRC Regulatory Guide 1.145. POSTMAX2 has been subjected to SQA at LANL (Letellier and Ashbaugh, 2001) but it is not one of the toolbox codes, so therefore anyone using POSTMAX2 for a DSA will need to do their own SQA.

6.11 ATMOSPHERIC DISPERSION MODELING PROTOCOL

The following 15-step modeling protocol provides additional dispersion analysis guidance beyond that of Section A.7 of DOE-STD-3009-2014 and is applicable to both radiological and toxic chemical releases. This modeling protocol guidance addresses evaluation of the MOI receptor, as appropriate, for submittal to the DOE Safety Basis Approval Authority (SBAA) for approval prior to its application. Guidance for implementing the recommendations below can be found elsewhere in this chapter and in Chapter 8 regarding radiological dose estimation, or in Chapter 9 regarding toxic chemical consequences.

The 50-mile population dose calculation is included for situations where accidents cannot be prevented or mitigated to less than the 25-rem EG and a comparison to DOE Policy 420.1, *Department of Energy Nuclear Safety Policy*, may be required; or if necessary, for evaluation of beyond DBA/EBA accidents (Section 3.1) to provide a risk perspective of any "cliff edge" effects or insights for emergency planning.

The 100 m CW is not included in this modeling protocol since guidance has already been established in OE-3:2015-02, *Atmospheric Dispersion Parameter (χ/Q) for Calculation of Co-located Worker Dose*. Section 6.13 provides specific guidance for the CW χ/Q. Assumptions and inputs for the CW evaluation that are different from the MOI dispersion analysis are documented in the DSA Chapter 3 hazard evaluation methodology, or alternately, in the accident analysis methodology. The 15-step modeling protocol worksheet looks like this:

1. Identify dispersion model and version number chosen and the basis for its selection:
    a. Identify dispersion model and version number chosen, and indicate whether it is an approved version of a toolbox code available through the DOE CR.
    b. Describe the appropriateness of the modeling technique relative to the site-specific and facility-specific application and the basis for its selection.
    c. State whether the default values recommended in the DOE guidance document for the DOE Central Registry toolbox code will be used, or technically justify the use of alternate values.
    d. If a DOE CR toolbox code is not used, describe the SQA assessment has been performed, or will be performed on the selected code.

   Note 1: Safety SQA requirements in DOE O 414.1D need to be met prior to using any code that is not in the DOE CR toolbox.

   e. In lieu of selecting a DOE CR toolbox code or other industry-accepted code, the proposed dispersion analysis may be performed within a spreadsheet, if it is documented as an engineering calculation that complies with applicable site SQA requirements.

      Note 2: DOE sites may choose any modeling approach it deems applicable to facility-specific phenomenology and site-specific atmospheric dispersion, as long as it is approved by the DOE SBAA prior to its application for the DSA accident analysis. The SBAA is expected to rely on subject matter experts experienced in dispersion analysis and/or an expert review panel for evaluating the selected modeling approach.

2. Specify the receptors to be evaluated:
   a. MOI
   b. Other sensitive receptors
   c. 50-mile population (when needed)

3. Describe site- and facility-specific elements:

   a. *Release height*: Indicate the height of the release above plant grade and determine whether it is sufficiently high to escape the aerodynamic effect of nearby buildings to become elevated.

      Note 3: If the release height is less than 2.5 times higher than nearby adjacent buildings, the release height should be set to zero (i.e., ground-level release).

      Note 4: If release is from a stack 2.5 (or more) times higher than nearby adjacent buildings, but the stack is not seismically-qualified, it should be treated as a ground-level release.

   b. *Terrain profile to determine potential interactions (plume impaction)*: If the release height is determined to be ground-level then terrain effects do not affect the analysis unless it is a dense gas release that may be gravity-fed into a nearby depression. For elevated releases, impaction of the plume on a downwind hill or mountain should be incorporated into the analysis. If a non-toolbox code has been selected to model the impact of terrain effects on atmospheric dispersion, describe the site's unique terrain profile.

   c. *Surface roughness data source (population, terrain)*: Identify the surface roughness or terrain type (i.e., urban, rural) applicable to the analysis for the site morphology and indicate how this affects the horizontal and vertical turbulence parameters. Provide a technical basis for the establishment of site roughness parameters inclusive of tree types, density, configuration, topography, building locations and types, and local land use.

      Note 5: Surface roughness considers both upwind (i.e., fetch) and downwind characteristics of the release point, and the value used for the MOI could be different from that for a 50-mile population dose calculation.

   d. *Population distribution within 50-mile radius*: For population dose calculations, determine the population in each of the annular sectors, the census year represented, and whether day-night population distributions are to be applied and the justification for their application.

      Note 6: Population doses are included in this Handbook since it may be of interest for special risk assessments to compare to the DOE Safety Goal in DOE P 420.1, Department of Energy Nuclear Safety Policy, and could be used to provide perspective should a facility have mitigated doses to the MOI that exceed the 25 rem EG.

   e. *Site map with locations of receptors of interest*: Develop a map of the DOE site with DOE-controlled property line and MOI site distances for the 16 sectors, in conformance with NRC Regulatory Guide 1.145, and other relevant boundaries, inclusive of the Perimeter Intrusion and Detection Alarm System or other security physical control boundaries.

   f. *Location of release points*: Develop a map that shows the location of all release points that are being analyzed, or describe whether the release is not associated with fixed locations (e.g., a release in a large outdoor waste staging area).

   g. *Mixing Layer Height*: Select the appropriate mixing layer height and justify its selection.

4. Describe release characteristics:

   a. *Initial plume dimensions*: Should the release become entrained in the wake and cavity of a nearby building, describe the method to calculate the initial horizontal and vertical plume dimensions, if treated as a virtual point source.

   b. *Positive and negative buoyancy*: If plume buoyancy occurs due to sensible heat of the release, or its density, as in a hydrogen release, indicate its applicability to the analysis and the analytical technique to be employed to account for it. For heavy gas (dense gas) releases, determine if the release quantity, boiling of a cryogenic liquid, and/or density of the release, represented by the Bulk Richardson Number, would subject it to dense gas dispersion conditions and describe the analytical technique to be employed to account for it. See footnote 55 with respect to indoor fires.

   c. *Elevated or ground-level release*: Based on the presence of a nearby or adjacent building, determine whether the release is elevated or down-washed to ground level. For elevated releases of gamma-emitting radionuclides, additional cloud shine dose calculations using an appropriate finite plume model may be necessary. Describe the finite plume model to be used.

   d. *Aerodynamic influence of nearby buildings*: Establish the appropriate code to account for the aerodynamic effect of the buildings on the release.

   e. *Energetic releases*: Identify the code to be used for each energetic release situation and the justification for its use. Releases from fires can be modeled with MACCS2 and Hotspot. For other energetic releases (e.g., detonations, deflagrations, delayed ignition, BLEVEs), codes other than MACCS2 or HotSpot that are better suited to assess release dynamics for energetic events may be employed if an effective release height calculation cannot be justified for input to an appropriate Gaussian model.

      Note 7: ALOHA V 5.4.6 is a toolbox code that is designed to address detonations, delayed ignition, radiant heat from a fire, and a BLEVE.

5. Describe source term phenomenology and characterization, as applicable to any particular accident scenarios:

   a. *Particulate and Pressurized Liquid Releases: Five-Factor Formula (MAR, DR, ARF, RF, LPF)*: Include a discussion whether the unmitigated and mitigated source terms, as determined by the DOE-HDBK-3010-94 methodology, warrant any special considerations for input to the dispersion analysis, or state why there are none.

      Describe if the source term has any special physical release properties that may influence dispersion or consequence estimates. Indicate whether it will be modeled other than as a point source, not already addressed in the considerations above, or whether it will be modeled considering momentum from the discharge velocity, or as a buoyant release due to elevated discharge temperature of the release, fire, or explosion.

If credited in the mitigated analysis, identify LPF from building configurations and presence or absence of HEPA filters.

b. *Particulate and Pressurized Liquid Releases: Particle-Size Distribution*: Since particle size distribution spectra are very important for establishing RF, ARF, and deposition velocity, establish the applicable particle size distribution from DOE-HDBK-3010-94, supplemented by representative studies and experiments. If the particle size distribution is unknown, assume a conservative distribution from available data to bound the calculation.

c. *Pressurized and non-Pressurized Gaseous Releases: Release Period and Release Rate*: Determine gaseous release as a function of time for pressurized gaseous releases.

   If gaseous release is constant and continuous establish a constant release rate as input to a peer-reviewed Gaussian plume model.

   If release is for a brief period (i.e., less than a minute), establish a release quantity as input to a peer-reviewed Gaussian puff model.

d. *Pressurized Liquid and Gaseous Releases: Density with respect to ambient atmosphere*: Select appropriate code to address whether positive buoyancy or negative buoyancy is applicable.

   Note 8: HPAC SCIPUFF has been used to address positively buoyant gases (e.g., hydrogen) and ALOHA, DEGADIS, SLAB and HPAC have been used to address negatively-buoyant gases (e.g., chlorine).

e. *Gaseous Releases: Reactivity on release to the atmosphere*: Effects of atmospheric chemistry should to be considered on releases that may undergo chemical transformation during transport to the MOI and population (e.g., uranium hexafluoride and anhydrous ammonia).

f. *Gaseous Releases: Fire scenario chemical transformation*: Oxidation of radionuclides or toxic chemicals in fires result in new substances, depending on temperature and availability of oxygen. Peer-reviewed literature should be consulted in the determination of the new substances to be evaluated.

   Note 9: Seek assistance from a process chemical engineer or chemist to determine the new substances and their quantities to be evaluated.

g. *Pressurized Gaseous Releases*: Identify the size of the orifice and whether choked flow is applicable. Due to the nature of this type of release, it is non-linear and the release rate decreases with time.

   Note 10: Consult technical literature for release rate characterization and if flow is choked by speed of sound limitation.

h. *Pressurized Liquid and Non-Pressurized Liquid Releases*: Determine the evaporation rate of the puddle using appropriate mass balance methodology. Unless release is confined in an impoundment basin, an unconfined puddle depth should be justified based on the surface type, or a depth of 1 cm may be assumed consistent with 40 CFR 68, *Chemical Accident Prevention Provisions,* guidance for a worst case spill (EPA-550-B-99-005).

   Note 11: ALOHA V 5.4.6 has a useful mass-balance algorithm, or manual calculation methods presented in Appendix B can be applied.

i. *Pressurized Liquid Release*: Depending on the substance and the pressure and temperature that it is stored, the release will be in two phases. Immediate flashing results in a gaseous puff and a puddle. The puff should be evaluated with a Gaussian puff model and the subsequent puddle evaporation by a Gaussian plume model.

   Note 12: HPAC and ALOHA Version 5.4.6 contain useful algorithms to determine flash-aerosol-puddle quantities. Manual calculation methods presented in Section 4.3 of this Handbook can also be applied.

j. *Sensible Heat from Fire*: Determine impacts of sensible heat from fire in terms of radiant heat impacts on human skin exposure and on facility integrity.

   Note 13: ALOHA V 5.4.6 contains useful algorithms to determine radiant heat impacts of sensible heat.

k. *Deflagration*: Determine energetic release propagation rate. If slower than the speed of sound, a deflagration fireball results. Select the appropriate peer-reviewed code to establish impacts to workers, public, the environment, and SSC integrity.

   Note 14: NASA fireball code (Dobranich et al., 1997) addresses this phenomenology and the analyst may wish to consult this report for guidance.

l. *Detonation*: Determine energetic release propagation rate. If faster than the speed of sound, a detonation occurs. Select the appropriate peer-reviewed code to establish impacts to workers, public, the environment, and SSC integrity.

   Note 15: ALOHA V 5.4.6 contains useful algorithms to determine overpressures from detonations.

m. *Detonation (delayed ignition)*: Delayed ignition detonations may occur hours after release and depend on the mechanical turbulence generated by obstacles (trees, buildings) in its transport path.

   Note 16: ALOHA V 5.4.6 contains useful algorithms to determine overpressures from delayed ignition detonations.

n. *BLEVE*: Determine whether a fire of a tanker or container can result in a BLEVE.

   Note 17: ALOHA V 5.4.6 contains useful algorithms to determine overpressures from a BLEVE.

6. Describe meteorological data sources and assure its fidelity:

   a. *Onsite instrumented meteorological tower*: Indicate whether an onsite source of representative meteorological data is available and if so, indicate locations of meteorological towers on site map with release locations. The meteorological program should monitor wind speed, wind direction, and an indicator of atmospheric stability (e.g., temperature difference, sigma theta, sigma phi).

   b. *Heights of measurement*: Identify the heights of measurement for each of the meteorological parameters that will be used in the analysis. Ideally, wind speed and wind direction data are measured at the standard 10-meter height. If wind speed is measured at a non-standard height, wind speed power law height adjustments should be considered. The temperature difference minimum height should be at least 35 meters if the delta T method is used to determine stability class.

   c. *Certification of data quality*: Indicate whether the onsite meteorological data has been quality assured under the guidance of Section 7.4 of ANSI/ANS-3.11-2015. Provide a certification from the site meteorological program manager, or other organization accountable for the effective operation of the meteorological program.

  d. *Pre-processing and averaging methodology*: Demonstrate that the raw meteorological data have been appropriately pre-processed and averaged to be applicable to the assessment.

  e. *Missing data handling techniques*: Since all meteorological data bases have some gaps due to calibrations and instrument malfunctions and missing data needs to be addressed, demonstrate that the data base has appropriate missing data handling as part of its quality assurance program.

  f. *Offsite representative meteorological source (e.g., National Weather Service)*: If quality-assured onsite meteorological data are not available, determine a surrogate data source nearby the site and demonstrate that it is spatially representative.

7. Describe meteorological data application to dispersion assessment:

   a. *Applicable meteorological parameters*: State which meteorological parameters will be used in the dispersion assessment.

   b. *Calm wind speed threshold and handling methodology*: Calm wind speed handling methodology is very important to consequence assessments since very light wind speeds are part of the 95% and 99.5% meteorology. Demonstrate that calm wind speeds are appropriately handled in the data base and are tied to the threshold wind speed limitations of the mechanical or sonic anemometry.

   c. *Turbulence typing methodology*: Choose the technique to type turbulence and demonstrate that the methodology selected is representative of the site's roughness and other site-specific and facility-specific characteristics.

   d. *Incorporation of surface roughness in turbulence typing*: Since surface roughness affects mechanical turbulence generation, the horizontal and vertical dispersion parameters should reflect this. Demonstrate whether the site should be characterized as a rural or urban site by profiling the site's roughness. Rough rural sites can be described using rural dispersion parameters with an applicable roughness correction but should never be classified as urban.

   e. *Wind speed power law height adjustments*: If wind speed and wind direction measurements are at any height except the standard of 10 meters, appropriate wind speed height adjustment techniques (e.g., power law) should be invoked. Power law exponents are a function of atmospheric stability class. Indicate which power law methodology is employed and justify why it is applicable to the site.

8. Select meteorological data period:

   a. *1-5 years*: At least 5 years of recent meteorological data are needed to demonstrate temporal representativeness. Depending on completeness of the data record, consecutive years of recent meteorological data are preferred (EPA, 2000). Identify the years of data that will be evaluated, and explain any anomalies, such as years being excluded if not able to be certified. If data base is shorter than 5 years, a representativeness demonstration is required to determine any uncertainties.

   b. *More than 5 years*: If meteorological data are available in this temporal range, use as much as are available. The larger the data base, the less likely a climatological "Black swan" is missed in the statistics.

9. Select appropriate atmospheric dispersion parameters:

   Demonstrate that the dispersion parameters are applicable to site characteristics. The dispersion parameters can be taken from the following menu:

   a. Pasquill-Turner-Gifford (rural terrain, hand scaling)
   b. Briggs urban and rural
   c. McElroy-Pooler (urban terrain)
   d. Eimutis and Konicek curve fitting of the Pasquill-Turner-Gifford data

   Note 18: Eimutis and Konicek are used in MACCS2. However, the analyst should be aware of the table lookup error in the toolbox version of the MACCS2 code.

   e. Tadmor and Gur curve fitting of the Pasquill-Turner-Gifford curves

   Note 19: Tadmor and Gur are used in MACCS2, but are not recommended for the MOI within 500 m of the release.

   f. Other dispersion parameters resulting from special site atmospheric tracer studies and/or other peer-reviewed evaluations.

10. Select plume averaging time, if different from release duration, and demonstrate its applicability to selected horizontal and vertical dispersion parameters.

    a. If time-based meander factors are used, ensure that the time basis is consistent with the technical basis of the selected dispersion parameters (e.g., 3 minutes for P-G-T).

11. Describe release duration and exposure period:

    a. Demonstrate that the selected release duration range is applicable to the assessment.
    b. Use a peer-reviewed dispersion model appropriate for the scenario in question. For Gaussian models, use a *plume* code for releases longer than one minute, and for a period shorter than one minute, use a puff code or turn off any time-based meander corrections in a plume code. For energetic releases, use an appropriate codes other than MACCS2 or HotSpot that are better suited to assess release dynamics for energetic events, or justify use of an effective release height input to an appropriate Gaussian model.

12. Describe aerodynamic building effects:

    a. *NRC Regulatory Guide 1.145 technique*: Demonstrate that this conservative plume downwash into the lee-side cavity is applicable to the assessment.
    b. *Other peer-reviewed technique*: Identify other peer-reviewed techniques, such as discussed in Section 6.8.3 of this Handbook, and demonstrate that this other technique is applicable to the assessment.

13. Describe dry deposition and plume depletion:

    a. *Dry deposition technique*: Indicate whether the dispersion assessment will include dry deposition and provide justification for the site-specific methodology employed. Refer to LLNL-TR-654366, *Deposition Velocity Methods for DOE Site Safety Analysis* and “Detailed Technical Basis for Default Dry Deposition Values” in the DOE/HSS Safety Bulletin No. 2011-02 for guidance.

Note 20: For tritium dispersion modeling, an appropriate deposition velocity is 0 cm/sec. Deviation from this deposition velocity value needs to be justified.

  b. *Plume depletion technique*: Indicate whether the dispersion assessment will include plume depletion and provide justification for the site-specific methodology employed.

14. Describe *χ/Q* statistics and determine applicability to the assessment.
    a. *Direction-Independent (overall site) 95-percentile*: Usual choice for conservative evaluations of the cumulative distribution of the annual meteorological data for all 16 sectors accounting for the distance to site boundary in each sector.
    b. *Direction-Dependent 99.5-percentile*: Acceptable alternative to the direction-independent 95th percentile for conservative evaluations based on the maximum sector cumulative distribution determined using actual site boundary distances for each sector.
    c. *Other percentile*: Demonstrate applicability to the dispersion assessment of any other percentile than those above for use in realistic analysis of Beyond Design/Evaluation Basis Accidents, if that option will be used.
15. Provide a summary of the basis for the conclusion that the selection of the parameters and input values, as identified above, will provide an overall radiological dose or chemical exposure consequence that is bounding and conservative. Include a list of conservatisms below.

Note 21: Peer-reviewed models used in this protocol need to meet the SQA criteria in DOE O 414.1D and DOE G 414.1-4A.

6.12 NON-GAUSSIAN DISPERSION MODELING

6.12.1 DISPERSION UNDER EXTREME WIND OR TORNADO EVENT

Dispersion under extreme (high) wind or tornado event conditions warrants additional considerations with respect to consequence analysis. The analysis performed for an extreme-wind/tornado event condition; severe enough to challenge SSC integrity, should initially address the effect of the event, including its incidence and return period, causing the release. Site-specific data may be used to characterize the extreme meteorological conditions, using a Probabilistic Wind Hazard Analysis (PWHA). Guidance for developing a PWHA is identified in ANSI/ANS-2.3-2011 (R2016), DOE-STD-1020-2016, *Natural Phenomena Hazards Design and Evaluation Criteria for Department of Energy Facilities*, and DOE-HDBK-1220-2017, *Natural Phenomena Hazards Analysis and Design Handbook for DOE Facilities*. If the analysis determines releases are likely to occur after the initial storm impact, the assessment should incorporate the appropriate meteorological conditions.

Once the SSC failure is established, consequences from the unmitigated release through the breached barrier in a less-turbulent atmosphere following the event should be evaluated at locations that include the maximum exposure point and other locations of interest. The simultaneous assumption of an extreme wind or tornado accident scenario with minimal dispersion lends high confidence as to the conservatism of the final result.

Section B.3 of NRSD-2015-TD1 (2015) refers to a 1996 study by Weber and Hunter, *Estimating Dispersion from a Tornado Vortex and Mesocyclone (U)*, that provides a peer-reviewed technique to determine downwind concentrations from releases caused by extreme winds or tornado that removed a primary confinement barrier. In the specific scenario studied, the tornado damages the structure and draws the released substance into its vortex. This scenario is comparable to an accident characterized by an instantaneous release and a short exposure time. The study is illustrative of the considerations for the conditions resulting from a tornado that would first be assessed and calculated at the maximum exposure point. A second and longer-term phase would also be included to account for a secondary release, potentially without crediting the presence of a structure. The two receptors may be at different distances from the source of release.

Weber and Hunter (1996) indicated that atmospheric transport and diffusion of a release from the facility into the environment during a tornado can be modeled with a DBA dilution factor (Ψ/Q), designated for a specific class tornado and applied for the distance from the facility to the receptor. The Ψ/Q parameter (units of s/m^3) represents the time-integrated ground-level centerline air concentration normalized by the mass released, and is analogous to the χ/Q value that is calculated from the Gaussian plume equation for neutrally buoyant releases. The Fujita scale (F1 to F5) is commonly used to categorize tornadoes. For most DSAs, the tornado is assumed to be either F2 or F3. Figure 6-9 shows Ψ/Q values as a function of downwind distance for different mean translational speeds of an F2 tornado.

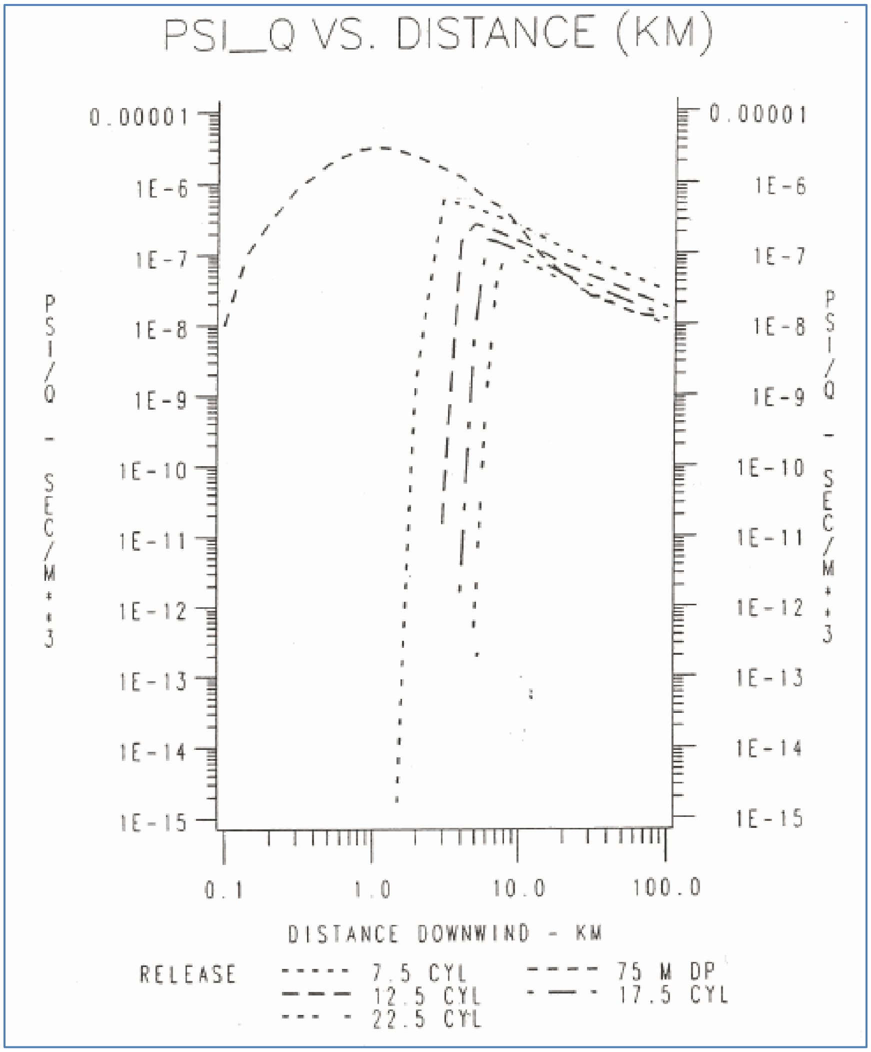

Figure 6-9. Maximum time-integrated ground-level centerline air concentration (s/m^3) versus downwind distance (km) for different mean translational speeds from 7.5 m/s to 22.5 m/s.[82]

The consequence analysis should select a maximum Ψ/Q for the assumed translational speed. For example, a translational speed of 7.5 m/s leads to a maximum air concentration at approximately three kilometers downwind. The product of the maximum Ψ/Q value and the release rate yields the ground level air concentration at the maximum exposure point and locations of interest.

6.12.2 FINITE PLUME EXTERNAL DOSE MODELING

Chapter 8 addresses radiological dose consequences, primarily from the inhalation pathway. However, depending on the mix of radionuclides, it is possible that inhalation doses may not be controlling, especially if an elevated radionuclide release has a higher proportion of strong gamma-emitting isotopes (such as Co-60, Xe-133, Cs-137). In this particular circumstance, the semi-infinite plume Gaussian model may not be sufficient for establishing radiological consequences and a finite plume external dose model may need to be applied. For an elevated plume, the concentration at the ground level and concomitant inhalation dose is zero, whereas, the dose from the gamma radiation of the overhead plume can be much greater than zero.

There are several codes available to calculate gamma shine doses, including *External Dose Conversion Factors From Finite Airborne Radioactive Plumes* (Momeni, 2001) and *Monte Carlo N-Particle Transport Code System* (MCNP, 1998), the latter a Monte Carlo transport code. With respect to the finite-cloud sector-average model (Hamawi, 1976), the long-term gamma-ray dose in the atmosphere from a sector-averaged plume may be expressed as a product of several factors multiplied by a sum of two attenuation integrals.

Since INL operates a reactor capable of releasing gamma-emitting fission products, it has included a finite plume model within its radiological consequence code, *RSAC-6 Radiological Safety Analysis Computer Program* (Schrader and Wenzel, 2001). The latest version of this code is RSAC-8. Although ORNL operates a high-flux irradiation reactor, it does not employ a finite plume code in its suite of dispersion models.

6.12.3 PLUMES FROM ENERGETIC EVENTS[83]

In the initial phase of an energetic event in air, a volume of gas is created that is hot and of high pressure. Because the gas is hot, it rises through its own buoyancy and by the overpressure of the event (see Section 4.3.1). This gas expands rapidly until it equilibrates with the atmospheric pressure. These initial processes determine the plume's initial dimensions and height. After it reaches equilibrium with the ambient atmosphere, conventional atmospheric diffusion processes act on this plume, carrying it downwind as it continues to expand through turbulent diffusion.

HotSpot V 2.07.01 (Homann, 2010), includes atmospheric dispersion models for a nuclear explosion, non-nuclear plutonium explosion, non-nuclear uranium explosion, fire, and tritium release. These models estimate the short-range (<10 km) downwind radiological impact following the release of radioactive

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[82] Downdraft speed is 10 m/s and height of the cylindrical mesocyclone is 3500 m (from Weber and Hunter, 1996). (fn. 82 cont.) CYL refers to the modeled cylindrical shape of the tornado and M DP refers to the results of another tornado modeling study, for comparison.)

[83] See Section 9.5 for additional discussion.

material resulting from a short-term release (<few hours), explosive release, or fuel fire event. The nuclear explosion program estimates the effects of a surface-burst nuclear weapon, which includes prompt effects (neutron and gamma, blast, and thermal).

Virtual source terms are used to model the initial atmospheric distribution of source material following an explosion and fire. The release is partitioned into 5 segments at varying heights up to the cloud top with upward virtual source terms as shown in Section 9 (*HotSpot Algorithms*) of the HotSpot V 2.07.1 User's Manual, reproduced in Figure 6-10. The cloud radius is equal to 0.2 cloud top.

The non-respirable release component is the fraction of the total quantity of material involved, available for dispersion into the atmosphere, which has a separate non-respirable deposition velocity default value of 8 cm/sec, and is used to determine ground shine, submersion, and plume depletion.

The non-respirable release component is the fraction of the total quantity of material involved, available for dispersion into the atmosphere, which has a separate non-respirable deposition velocity default value of 8 cm/sec, and is used to determine ground shine, submersion, and plume depletion.

Another code has been developed expressly for this purpose, the Explosive Release Atmospheric Dispersion (ERAD) code from SNL (Boughton and DeLaurentis, 1992). This code is a three-dimensional numerical simulation of particle dispersion in the atmosphere and includes cloud dynamics, buoyancy effects, and turbulent diffusion. It was designed to run on a small field-deployable computer. The details of this model are beyond the scope of this guidebook, but to summarize, it treats particle dispersion as a stochastic process that can be simulated with a Lagrangian Monte Carlo method. Comparisons with field tracer data (Roller Coaster) show reasonably good agreement between the model predictions and measurements.

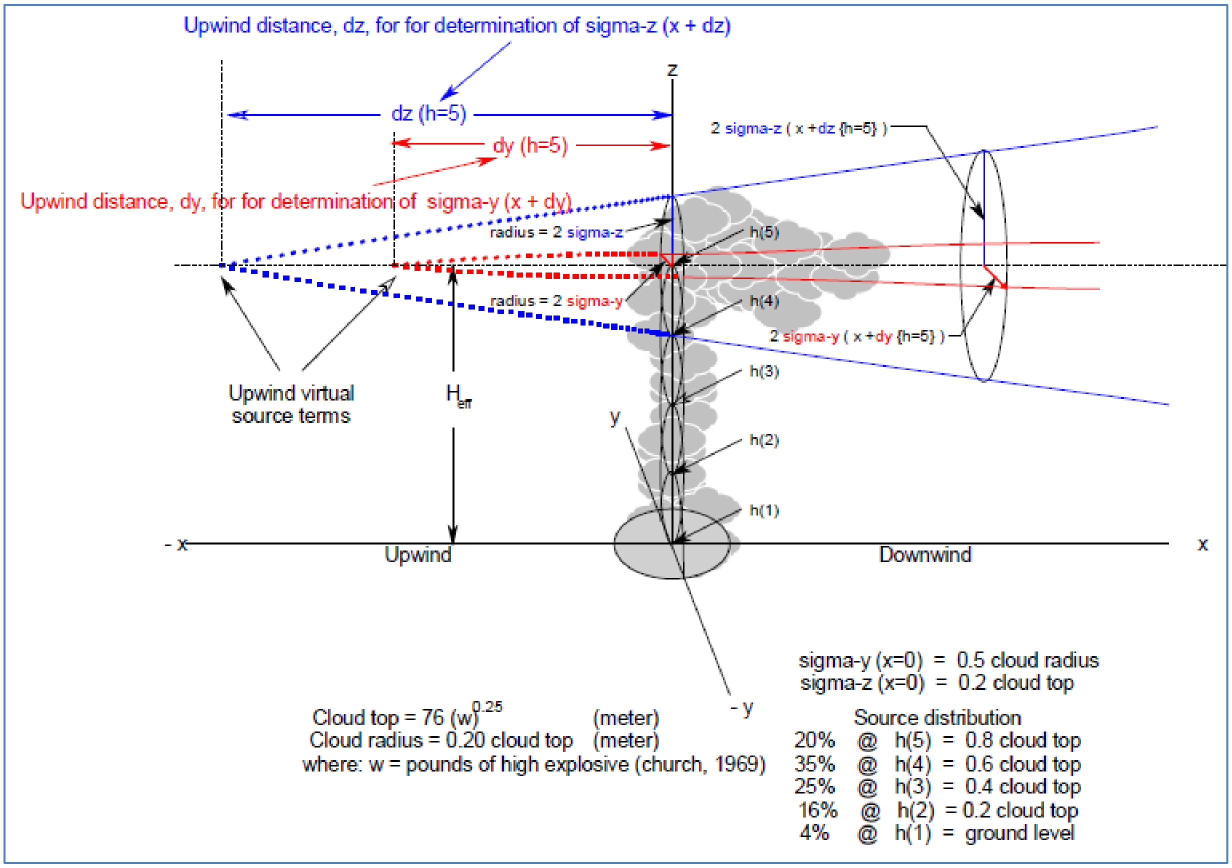

Figure 6-10. Virtual Source Terms used in HotSpot for Explosion or Fire.

ERAD is difficult to use, in that the required array of three-dimensional meteorological data cannot be easily obtained for code input, and the final consequence statistics cannot be easily derived. An alternative method was therefore derived that makes use of a dispersion and consequence code that is commonly used at DOE sites, namely, MACCS2 (see below). In this method, *Plutonium Explosive Dispersal Modeling Using the MACCS2 Computer Code* (Steele, 1998), equations are derived that give the cloud top height and the cloud radius as a function of time and amount of explosive used. Because the plume asymptotically approaches the “final” height and size, the expressions are evaluated at three minutes following the detonation, as the height and size are nearly the same then as their asymptotic values. This leads to two simple expressions. The cloud top height (*CTH*) is given by

$$CTH\ (m) = 75\ w^{1/4} \qquad \textbf{Equation 6-33}$$

where *w* is the weight of the explosive in pounds of TNT equivalent. The cloud radius (R) is

$$R\ (m) = 16\ w^{1/4} \qquad \textbf{Equation 6-34}$$

These expressions are found to match observations surprisingly well. For use in MACCS2, the initial height of the plume is set to *CTH* – *R*, and the initial cloud size is set to $\sigma_y = \sigma_z = R$. The resulting plume concentrations are found to match observations about as well as ERAD did. Note that the above discussion does not apply to indoor explosions.

6.13 CO-LOCATED WORKER DISPERSION FACTOR

As mentioned in, Section 6.2, *Key Receptors*, the CW is a hypothetical individual located at a distance of 100 meters from a facility (building perimeter) or estimated release point. Unmitigated CW dose calculations are used to evaluate whether SS controls are needed for protection of onsite workers. DOE-STD-3009-2014, Section 3.2.4.2 requires that:

> A χ/Q value of 3.5 x 10^{-3} sec/m^3 shall be used for ground-level release evaluation at the 100 meter receptor location unless an alternate onsite χ/Q value is justified. This value may not be appropriate for certain unique situations such as operations not conducted within a physical structure. When an alternate value is used, the DSA shall provide a technical basis supporting the need for the alternate value and the value selected.

The threshold for designation of SS controls is a 100 rem dose and the χ/Q value of 3.5 x10^{-3} s/m^3 is part of the unmitigated dose calculation for the 100-m CW receptor. New nuclear facilities or major modifications to existing facilities apply the χ/Q value specified in the Standard; however, there may be a limited number of situations where this value is not appropriate for the release conditions, and an alternate value may be more appropriate. NSRD-2015-TD01 and OE-3 were issued in 2015 to establish the regulatory basis of this χ/Q value. A discussion of this technical report and OE-3 follows.

6.13.1 TECHNICAL REPORT FOR CW X/Q VALUE

NSRD-2015-TD01 assesses the “default χ/Q value” and its technical and regulatory bases (DOE/ONS, 2015). The purpose of the technical report is to explore the sensitivities of the radiological χ/Q value, previously stated is conservative. The χ/Q value in Appendix A to DOE-STD-1189-2008 was based on NUREG-1140, *A Regulatory Analysis on Emergency Preparedness for Fuel Cycle and Other Radioactive Material Licensees*, that applied Gaussian plume dispersion methodology for a 95% conservative meteorological condition with a building size of 10 m × 36 m, and included other commonly utilized conservative assumptions (e.g., centerline concentrations).

Although the default χ/Q value was based on a number of conservative assumptions, the technical report determined that atmospheric dispersion calculations were most sensitive to variations in initial plume dimensions that were driven by the aerodynamic effects of the physical structure at the point of release. The technical report analyzed sensitivity studies using the radiological consequence codes MACCS2 and ARCON96 (NRC Regulatory Guide 1.194, *Atmospheric Relative Concentrations for Control Room Radiological Habitability Assessments at Nuclear Power Plants*), and the toxic chemical codes ALOHA and EPICode, to conclude that the default χ/Q value represents a conservative estimate of atmospheric dispersion for calculating both radiological and toxic chemical exposure of the CW, where the release is subject to aerodynamic effects from a facility building with a nominal cross-sectional area of 10 m × 36 m. However, the technical report also acknowledged that for uncommon situations where there is a radiological or toxic chemical release from a facility smaller than that assumed in the analysis (e.g., tank farm piping), where the enhanced turbulence from the aerodynamic effects of the facility on the wind field would be smaller, the default χ/Q value may not provide as conservative an estimate of atmospheric dispersion; specifically when benchmarking against Gaussian plume models such as MACCS2.

6.13.2 ALTERNATE X/Q VALUE JUSTIFICATION

DOE-STD-3009-2014, Section 3.2.4.2, allows the application of an alternate χ/Q value as long as the need for this alternate value is justified and its technical basis is documented in the DSA. Although limited, there are situations that may warrant the use of an alternate χ/Q value. As the Technical Report demonstrates, inherent to the default χ/Q value is the assumption that the release is from a nuclear facility with a building size of at least 10 m × 36 m. However, if the building size is smaller than 10 m × 36 m, or if there is no building structure at all, the default χ/Q value may no longer be as conservative and an alternate technique is justified.

Moreover, there may still be a need for using an alternate χ/Q value when the release is from a sufficiently large building. This situation may arise when updating a DSA that was based on DOE-STD-3009-94, CN3 or DOE-STD-3009-2014. DOE sites that already have existing CW values calculated in their DSA should consider the need for updating their analysis to the specified value in DOE-STD-3009-2014 and the impact that it has on control selection. If the updated analysis establishes that no change to SS designation occurs, or no new SSCs or SACs are identified, then the DSA justification documents the selected χ/Q value, and provides a rational that use of the alternate χ/Q value would not impact safety control selection.

When an alternate χ/Q value is used in situations where the default χ/Q value may not be appropriate, the DSA justification should be commensurate with the method of calculating the alternate χ/Q value. The following two subsections discuss hand-calculation and computer code methodologies for calculating a χ/Q value where the default value is demonstrated to not be appropriate.

6.13.2.1 HAND CALCULATIONS FOR A X/Q VALUE WHERE THE DEFAULT VALUE IS NOT APPROPRIATE

Attachment E of NSRD-2015-TD01 provides a simple approach for determining a χ/Q value in situations where the default χ/Q value is demonstrated to not be appropriate for a conservative unmitigated analysis. The approach applies the Gaussian plume equation methodology, basing the initial plume dimensions, σ_{yi} and σ_{zi}, on the actual building width and actual building height that the release emanates from, as shown in Eq. 6-35.

$$\boldsymbol{\frac{x}{Q}(x = 100, y = 0, z = 0, H = O) = \frac{1}{\pi\, U\left(\sigma_{yi}+\sigma_{y_{100}}\right)\left(\sigma_{zi}+\sigma_{z_{100}}\right)}} \qquad \textbf{Equation 6-35}$$

Where:

U = Wind speed diluting the plume (m/sec);
σ_{y100} = Standard deviation of concentration in the horizontal direction from 100 m of plume travel (m);
σ_{z100} = Standard deviation of concentration in the vertical direction from 100 m of plume travel (m);
σ_{yi} = Standard deviation of concentration in the horizontal direction based on the aerodynamic effects of the building width (m); and,
σ_{zi} = Standard deviation of concentration in the vertical direction based on the aerodynamic effects of the building height (m).

The initial plume dimensions can be calculated from Eq. 6-36.

$$\sigma_{yi} = W/4.3 \quad \text{and } \sigma_{zi} = H/2.15 \qquad \textbf{Equation 6-36}$$

Where:

W = shortest building width (m); and,
H = minimum building height (m).

The intent of this approach is to address the potential issue concerning releases emanating from locations that either do not have a physical structure or where the building is smaller than 10 m × 36 m. For releases from locations without any physical structure, Eq. 6-36 simply reverts to the ground-level release equation (Eq. 6-5) for a plume that has traveled 100 m with no horizontal and vertical plume expansion to account for the aerodynamic effects of a facility on the wind field. This simple hand calculation or spreadsheet calculation can be quickly executed without employing an atmospheric dispersion computer code, which is consistent with the original intent of establishing a default χ/Q value. Examples of how to use the equation are provided in Attachment E of NSRD-2015-TD01 for different structure dimensions and when no structure is nearby. Case 2 from Table E-1 of the technical report is replicated below for releases from locations without any physical structure assuming that the 95 percent meteorology is Stability Class F and 1 m/s wind speed.

NSRD-2015-TD01 Table E-1 Case 2: For stability class F at a distance of 100 m, the Eimutis-Konicek[84] curve fit algorithms give the following standard deviation of concentration in the horizontal and vertical directions without a building present.

$$\sigma_y = 0.0722 \times 100^{0.9031} = 4.62 \text{ m}$$

$$\sigma_z = 0.086 \times 100^{0.74} - 0.35 = 2.25 \text{ m}$$

$$\chi/Q = 1 / [\pi \times 1 \text{ m/s} \times 4.62 \text{ m} \times 2.25 \text{ m}] = 3.1 \text{ x } 10^{-2} \text{ s/m}^3$$

The above χ/Q value can be adjusted by for plume meander[85] due to longer release duration. The standard deviation of concentration in the horizontal direction (σ_y) is adjusted by the plume meander factor (e.g., for a two-hour plume duration and a 3-minute time base) the plume meander factor would be (120 min/3 min) $^{0.25}$ = 2.515, yielding σ_y = 11.62 m, and χ/Q = 1.2Ex10^{-2} s/m^3.

DOE-STD-3009-2014, Section 3.2.4.2 requires that the "DSA shall provide a technical basis supporting the need for the alternate value and the value selected." The DSA justification should explain the rationale why the default χ/Q value is not representative for the particular situation, or other rationale for not adopting the default value, and document how the σ_{yi} and σ_{zi} were calculated from structure dimensions that affect the wind field and the resultant χ/Q value used. If a release is affected by a nearby larger structure, the larger structure width and height should be used in the χ/Q calculation.

6.13.2.2 COMPUTER CODE MODELING FOR A X/Q VALUE WHERE THE DEFAULT VALUE IS NOT APPROPRIATE

The following guidance is provided for a conservative unmitigated analysis when site-specific modeling is performed to estimate CW consequences at 100 m. Use of any alternate dispersion methodologies or

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[84] Eimutis-Konicek curve fit algorithms were selected since the Tadmor-Gur curve fit algorithms should not be used for distances within 500 m.

[85] Other computer codes evaluate plume meander differently, for example, the ARCON96 plume meander is independent of release duration and represents meander caused by larger eddies that are present in the atmosphere under stable light wind conditions.

attributes discussed below needs to have a valid technical basis and should be discussed with and approved by the DOE SBAA. The process is similar to that of documenting the proposed methodology and input assumptions in a atmospheric dispersion modeling protocol, described in Section 6.11, *Atmospheric Dispersion Modeling Protocol*. If an MOI modeling protocol is being developed, it can be extended to include the CW for cases in which the default value is not appropriate.

Dispersion modeling inputs for unmitigated consequences for the 100 m CW is expected to generally be the same as for the offsite atmospheric dispersion and consequence analysis if using the same computer code, unless unique to the CW evaluation. Dispersion attributes for the CW unmitigated analysis are as follows, and where noted, may apply to the toxic chemical dispersion analysis.

1. Use a DOE Toolbox Code and input values consistent with its guidance document such as the DOE-EH-4.2.1-MACCS2-Code Guidance, *MACCS2 Computer Code Application Guidance for Documented Safety Analysis*.

   Note 1: Other site-specific developed computer codes or industry-recognized computer codes can be considered if they have undergone appropriate validation and verification in accordance with DOE O 414.1D SQA requirements and appropriate technical justification provided.

2. Worst case meteorological assumptions (i.e., overall site 95th percentile or sector-dependent 99.5th percentile) can be based on local site meteorological data per Section 6.10 of DOE-STD-3009-2014, for radiological and toxic chemical releases.

3. Surface roughness of 3 cm (rural) is assumed for radiological and toxic chemical releases, unless an alternate site-specific value can be technically justified by peer-reviewed studies per guidance in Section 6.8.2, Mechanical Turbulence Due to Surface Roughness.

4. Aerodynamic effects of the facility on the wind field cannot be credited unless shown to yield more conservative or bounding results.

5. Dry deposition velocities are selected consistent with the default values provided in Section 6.8.4, Plume Depletion through Decay, Daughter In-Growth, and Deposition Processes, unless a site-specific value can be technically justified by peer-reviewed studies.

6. Plume buoyancy may be included when modeling outdoor fires or for fires venting through a large breach in the facility provided that it is not credited in a non-conservative manner.

7. Dispersion parameters are applicable to site characteristics.

   Note 2: Tadmor-Gur dispersion parameters are not recommended for close-in distances, under 500 meters.

8. Release duration and plume meander are consistent with the MOI atmospheric dispersion analysis unless there is a valid reason to adopt other assumptions unique for the CW atmospheric dispersion analysis.

7 AQUATIC DISPERSION AND GROUNDWATER TRANSPORT

7.1 OVERVIEW

Although a less frequent consequence of a radiological accident, a discharge of a liquid radionuclide effluent is considered in hazard evaluation or accident analysis for DOE facilities for unique situations. Slowly developing dose pathways from accidental releases are generally not analyzed in DSAs due to the relatively long time for potential liquid releases from facilities to reach dose receptors, and the ability of programmatic controls to mitigate any release or ingestion prior to a prolonged exposure period needed to significantly contribute to the overall DBA consequence. At least one DOE site historically evaluated water pathway release events, but only in the context of BDBAs. DOE-STD-3009-2014, Section 3.2.4.2 provides the following discussions regarding liquid releases to water pathways:

> For some types of facilities such as liquid processing with the potential for significant spills to the environment outside the facility, the surface and groundwater pathways may be more important, and accident releases usually would be expected to develop more slowly than airborne releases. More time would also be available for implementing preventive and mitigative measures.
>
> However, quick-release accidents involving other pathways, such as a major tank rupture that could release large amounts of radioactive liquid effluents to water pathways, should be considered.[86]

This chapter addresses potential dose consequences via surface water pathways at significant uptake locations, that is, maximum exposure locations that could affect the unmitigated dose estimates to the CW and the MOI. Moreover, the dose contribution from water pathways may be important to the overall 50-yr Total Effective Dose (TED), including the airborne pathway, for the selection of SS or SC controls and derivation of TSRs. The event may also warrant discussion in DSA Section 3.3.2.6, Environmental Protection, as described in DOE-STD-3009-2014, Section 4, to ensure that the facility design and operational features are available to reduce the potential for large liquid effluent releases to the environment.

Liquid effluent releases to surface water bodies can occur from accidents involving liquid process lines, waste tanks, cooling or evaporation systems, and primary-to-secondary leakage paths, as well as from other off-normal conditions. Such releases to surface bodies generally require relatively long periods of time (e.g., hours to days) before the general public could be impacted. However, the availability of longer response times enables the execution of various administrative controls, such as protective actions (i.e., evacuation and sheltering) and food and water interdiction countermeasures.

Dose consequences from liquid effluent releases are dependent on the volume of release, the duration of the release, the soil characteristics in the area around the point of discharge and the configuration of drainage and containment networks that redirect effluents away from the release location. Examples of natural and anthropogenic drainage networks include discharge canals, sewers, viaducts, creeks, rivers, and lakes.

For the purposes of DSA preparation, industry- accepted models, summarized in two NRC guidance documents, should be consulted when relevant accident scenarios result in discharges to streams, rivers, lakes, or oceans that require subsequent analysis.

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[86] See also Appendix A.3 of DOE-STD-3009-94 CN3)

7.2 NRC REGULATORY GUIDANCE ON AQUATIC DISPERSION AND DOSE CALCULATION

The following applicable NRC regulatory guides, both issued in 1977, should be consulted:

- Regulatory Guide 1.109, *Calculation of Annual Doses to Man from Routine Releases of Reactor Effluents for the Purpose of Evaluating Compliance with 10 CFR Part 50 Appendix I*; and
- Regulatory Guide 1.113, *Estimating Aquatic Dispersion of Effluents from Accidental and Routine Reactor Releases for the Purpose of Implementing Appendix I.*

Regulatory Guide 1.109 describes basic features of the dosimetric calculation models and suggests parameters for the estimation of radiation doses to man from effluent releases.

With respect to Regulatory Guide 1.113, this guidance:

- Describes the basic features of aquatic dispersion models and suggests methods of determining values of model parameters for the estimation of aquatic dispersion of both routine and accidental releases of liquid effluents;
- Describes general approaches for analysis of normal and accident releases into various types of surface water bodies;
- Provides guidance on the use of calculation models and specification of accompanying parametric values to perform aquatic dispersion of routine or accidental releases of radioactive material to a surface body of water. Groundwater pathway models are not addressed;
- Provides additional guidance on selection of model types rather than to specify models; Accordingly, the use of models other than those described Regulatory Guide 1.113 is acceptable; and
- Indicates that in situ tracer studies can provide accurate site-specific predictions as an alternative to modeling.[87]

7.3 DOCUMENTED SAFETY ANALYSIS APPROACH

Each liquid effluent release assessment should be evaluated applying a graded approach as described in DOE-STD-3009, such as being commensurate to the hazard category of the facility, remaining operational time of the facility, magnitude of potential consequences, and the complexity of the aqueous pathways for exposure and environmental contamination. Methods for this evaluation are addressed in the remainder of this chapter.

In addition, regarding evaluation of environmental protection in the DSA, the primary focus of the DSA hazard evaluation or accident analysis should be on process design, SSCs, and engineered operational controls which would preclude any potential for a large liquid effluent release to the environment. If precluding large liquid effluent releases is not feasible, a secondary approach would be to impose engineering controls to limit the magnitude of the loss of process liquids. These controls include sewer networks to conduct liquids to a collection system (e.g., settlement basin and weir), or a berm or containment basin (e.g., dike) to limit the extent of the release within the facility or site control. Should additional preventive or mitigative controls be required, the results of the dose contribution from the

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[87] Although specific surface-water models are considered in Regulatory Guide 1.113, representative of models found in the published literature at the time, the stated purpose is to use them as a framework for discussing the specific classes of models that they exemplify.

water pathway may provide insights on the effectiveness of these controls.

7.4 LIQUID EFFLUENT RELEASE KEY RECEPTORS

The dose contribution from the water pathway may or may not be significant compared to the airborne pathway dose contribution. Normally, the CW is evaluated at 100 m from the release, and the MOI is evaluated at the site boundary. However, the aqueous release pathway may result in a higher dose at locations beyond these distances. Therefore, the analysis should consider these farther onsite and offsite locations if it could affect the overall unmitigated maximum dose estimates for the CW and MOI. The CW and MOI are assumed to be located at the point of maximum concentration of the dispersed effluent stream at an uncontrolled onsite or offsite location, respectively.

Regulatory Guide 1.113 specifies that the location of surface water users and the types of water uses, out to a distance of 50 miles from the site, should be established to identify other important receptors for dose pathway analyses.

7.5 LIQUID EFFLUENT RELEASE REDISTRIBUTION MECHANISMS AND UPTAKE

Regulatory Guide 1.113 provides guidance on initial mixing, far-field mixing, deposition, and resuspension in sediments, as well as uptake mechanisms with respect to aquatic dispersion models. The following provides a brief summary of each physical mechanism.

7.5.1 INITIAL MIXING

The major factors in the initial mixing phase are momentum and buoyancy of the liquid effluent, the outfall location and configuration, and receiving water characteristics; principally the current and depth.

7.5.2 FAR-FIELD MIXING

The initial mixing will result in a homogeneous plume of radionuclides which ultimately yield to generally slower far-field aquatic transport and diffusion processes. In the far-field mixing region, much longer distances and time frames result in an appreciable reduction of the concentration of the radionuclide plume, as clean water further dilutes it.

The longer time frames associated with the aquatic dispersion process indicates that radiochemical physical transformations and radioactive decay and daughter ingrowth could be important factors in the dose calculation. Moreover, the size of the receiving water body and its overall transport behavior (e.g., current velocity) needs to also be considered.

Each principal water body has its own unique transport characteristics due to different boundary conditions and flow rates. The following describe such differences on the aquatic dispersion process:

- Rivers: Advective and turbulent flows throughout with variable boundaries.
- Estuaries: Established transitional zone between distinctly different water bodies, marked by oscillating tidal flow and weak net transport.
- Small lakes and reservoirs: Strong boundary limitations and weak transport.
- Oceans and large lakes: Large overall extent and appreciable advection of pollutants.

Depending on the analysis, the complexity of models for estimating the radionuclide concentration at some point in the far-field may range from simple dilution factor considerations, to solving the advection and dispersion equations in one-, two-, or three-dimensional spaces. The latter case is particularly true for river system discharges. The selection of the aquatic dispersion model should be based on the complexity of the system and the requirements of the analysis.

During surface water release events, some constituents may be present as volatilizing liquids or in a dissolved gas form. These contaminants can be released from the liquid-air interface as pressure changes are encountered. Equation 7-1 provides a simple approach to calculate the time-varying release rate, assuming that the radionuclide is uniformly mixed over the vertical water column.

$$[dC/dt]_e = K(C - C_s) \qquad \textbf{Equation 7-1}$$

Where,

$[dC/dt]_e$ = Time-varying release rate (Ci/s)

K = Depth average loss coefficient (s^{-1})

C = Vertically uniform gas concentration of the contaminant, with typical units for a radionuclide gas contaminant of activity per unit volume (Ci/m^3)

C_s = Saturation value (Ci/m^3)

Note that the saturation value is usually set equal to zero.

As noted in Section 3.3.6 of NUREG/CR-3332, *Radiological Assessment: A Textbook on Environmental Dose Analysis*, K is related to the actual surface transfer coefficient, $K_{L,}$ by

$$K = K_L/H \qquad \textbf{Equation 7-2}$$

where,

K_L = Surface transfer coefficient (m/s)

H = Water column height (m)

The water column height is the height of a conceptual “stack” of the water body layers receiving the radionuclide or chemical pollutant. The water column extends from the surface to the bottom of the water body of interest and includes all layers. Values of K_L are usually determined from experimentation or from the literature.

7.5.3 DEPOSITION AND RESUSPENSION IN SEDIMENTS

As contaminants are transported in the surface water body, adsorption processes may remove material from the aqueous phase and incorporate material onto sediments. This is similar to the atmospheric process of deposition. Both suspended and bed sediments may adsorb contaminants, although suspended sediments are usually more effective on a per unit weight basis. The process is reversible and while the initial reduction of contaminants from a water body can be pronounced, over longer periods of time these contaminants can be resuspended.

Examples of long-lived radionuclides that have been retained in sediments after chronic or acute release near DOE nuclear facilities have been Cs-137 and various Pu species. A counterexample is tritium, which due to the ubiquity of water and hydrogen in the environment, shows little to no evidence of preferential localization in sediments.

The extent to which a radiological species can be adsorbed is referred to as the equilibrium distribution coefficient, or K_d. The equilibrium distribution coefficient is a function of the state of the radionuclide and its concentration, the sediment characteristics, and the nature of the water body. K_d values are derived from field data and experimentation, and are defined as the amount of contaminant sorbed on sediment/amount of radionuclide left in solution.

7.5.4 UPTAKE MECHANISMS

The aquatic dispersion model can also be linked to dose through human uptake mechanisms, where the most important pathway is water ingestion. Moreover, additional uptake mechanisms may be of importance. This includes direct food ingestion from marine foodstuffs, or indirect food ingestion through use of contaminated irrigation water sources. External exposure is also of importance in some situations, including aquatic recreation or shoreline exposure. The need to evaluate these other pathways should be discussed with the DOE Safety Basis Approval Authority.

7.6 AQUATIC DISPERSION MODELS AND COMPARISONS

7.6.1 CLASSES OF AQUATIC DISPERSION MODELS

There are 14 classes of aquatic dispersion models that have been developed for application to surface water bodies. These are addressed in Regulatory Guide 1.113 and the model characteristics and surface water body applications are listed in Table 7-1.

Table 7-1. Aquatic Dispersion Model Classes.

Class of Aquatic Dispersion Model	Aquatic Dispersion Model Characteristics	Surface Water Body Applications
Stream tube model	Steady-state, two-dimensional, analytical solution	Non-tidal rivers
Transient release model	Transient, two-dimensional, numerical quadrature solution	Non-tidal rivers
Gaussian diffusion model	Steady-state, three-dimensional, analytical solution	Open coastal waters
Transient source model	Transient, two-dimensional, numerical quadrature solution	Open coastal waters
Numerical model	Transient, two-dimensional, numerical solution of conservation equations of mass and momentum	Open coastal waters
Tidally-averaged analytical model	Steady-state, one-dimensional, analytical solution	Estuaries
Tidally-averaged, short-duration analytical model	Transient, one-dimensional, analytical or numerical quadrature solution	Estuaries
Tidally-averaged numerical model	Transient, one-dimensional, numerical solution of constituent transport equation	Estuaries
Intra-tidal numerical model	Transient, one-dimensional, numerical solution of conservation equations of mass, momentum, and constituent concentration	Estuaries
Completely-mixed model	Transient, homogeneous, analytical solution	Lakes, reservoirs, and cooling ponds
Plug-flow model	Steady-state, homogeneous, analytical solution	Lakes, reservoirs, and cooling ponds
Partially-mixed model	Steady-state, homogeneous, analytical solution	Lakes, reservoirs, and cooling ponds
Stratified reservoir lumped parameter model	Steady-state, homogeneous (within stratified layer), analytical solution	Lakes, reservoirs, and cooling ponds
Numerical stratified reservoir models	Transient, one- or two- dimensional, numerical solution of conservation equations of mass, momentum, and constituent concentration	Lakes, reservoirs, and cooling ponds

7.6.2 AQUATIC DISPERSION MODEL ATTRIBUTES AND CHARACTERISTICS

For a release from a large body of water such as a river, aquatic dispersion models have been developed that account for advection and dispersion effects. These models should take into account the required complexity necessary to account for change in concentrations. In many situations, a two-dimensional model is sufficient.

Table 7-2 provides the analyst with the major attributes and characteristics to consider in the selection of an aquatic dispersion model for DSA preparation with respect to release type, dimensional dependence, contaminant transport, time dependence, solution technique and dose pathways. Overkill occurs when the analyst uses a more sophisticated model than is warranted and NCRP Report No. 76, *Radiological Assessment: Predicting the Transport, Bioaccumulation, and Uptake by Man of Radionuclides Released to the Environment*, warns against common misuses of aquatic dispersion models.

Table 7-2. Attributes and Characteristics of Aquatic Dispersion Models.

Attribute	Characteristics
Release Type	Acute; Chronic
Dimensional Dependence	One-dimensional; Two-dimensional; Three-dimensional
Contaminant Transport	Solute; Particulate
Time Dependence	Steady-state; Dynamic
Solution Technique	Finite Element; Finite Difference
Dose Pathways	Water Ingestion; Food Ingestion and Longer-Term Food Chain; Submersion; External Shine, Shoreline Exposure

7.6.3 COMPARISON OF AQUATIC DISPERSION MODELS

Several aquatic dispersion models are available and five (5) of these codes are briefly summarized. More in-depth information may be located in the referenced model descriptions. A brief comparison of the release types, regulatory use, model types, and output of these 5 aquatic dispersion models is presented in Table 7-3.

7.6.3.1 LADTAP2

NUREG/CR-4013, *LADTAP II: Technical Reference and User Guide*, (LADTAP2) analyzes environmental doses following routine surface water releases of radiological liquid effluents from nuclear facilities. LADTAP2 provides a hydrological and exposure pathway and examines doses to individuals, population groups, and biota via ingestion and external exposures. Calculated population doses provide information for National Environmental Policy Act (NEPA) evaluations and for determining compliance with Appendix I of 10 CFR 50, *Domestic Licensing of Production and Utilization Facilities*.

LADTAP2 selects one of four hydrological models to represent mixing in the effluent impoundment system and receiving surface waters. The four model types are: (1) direct release to the receiving water; (2) plug-flow; (3) partially-mixed; and (4) completely-mixed. All but the direct release model account for radiological decay and daughter ingrowth during transit through the impoundment system. Optional models are available to estimate aquatic dispersion in non-tidal rivers and near shore lake environments.

The exposure pathway model estimates exposure of selected groups at various water usage locations in the environment. Water concentrations at usage locations are related to impoundment system effluent concentrations by a dilution factor and the transit time that allows for radioactive decay during transport. Consequence calculations examine all potential pathways: ingestion of aquatic foodstuffs, irrigated terrestrial food crops, drinking water (freshwater sites only), boating and swimming.

7.6.3.2 STREAM2

STREAM2 (Chen, 1998) is an aqueous release emergency response code which analyzes the transport of pollutants from a release point to various points downstream on the Savannah River. This model is conservative and assumes a constant river flow, no transport losses, and uniform mixing in stream cross-sectional areas.

User input includes the time, date, type, location, calculation units, amount, and duration of the release. Input data are used to calculate the pollutant concentrations and transport time at downstream locations, which may be displayed in graphical and tabular form.

7.6.3.3 GENII 2.10.1

GENII Version 2.10.1 analyzes environmental contamination resulting from both far- and near-field scenarios. Annual, committed, and accumulated doses following acute and chronic releases can be calculated. Surface water transport is modeled using the same LADTAP2 mathematical models.

7.6.3.4 RIVER-RAD

RIVER-RAD uses a compartmental linear transfer technique to model radionuclide transport as a series of transfers between compartments, including the water and sediment sub-compartments. Radionuclide transfer pathways include upward volatilization from the water compartment, movement of radionuclides with the river flow rate, deposition (settling) and resuspension.

7.6.3.5 DISPERS

DISPERS (NUREG-0868) is a collection of mathematical models used for computing the dispersion and fate of routinely or accidentally released radionuclides in surface water and groundwater. Five programs, all of which are straightforward dispersion simulations, are included. These are SSTUBE, TUBE, RIVLAK, GROUND, and GRDFLX (see NUREG-0868).

Table 7-3. Comparison of Aquatic Dispersion Models.

Parameter	Aquatic Dispersion Model				
	LADTAP2	**STREAM2**	**GENII 2.10.1**	**RIVER-RAD**	**DISPERS**
Release types	Routine	Acute	Routine and acute	Routine and acute	Routine and acute
Regulatory use	NEPA and 10 CFR 50 Appendix I	Emergency response	Consequence assessment	Dispersion calculations	Dispersion calculations
Model and/or calculation types	Direct release; Plug-flow; Partially and Completely mixed	One-dimensional; WASP5 calculations	LADTAP2 models	Compartmental linear transfer model	Two- and three-dimensional models
Output	Dose and Concentration	Concentration	Dose and Concentration	Concentration	Concentration

7.7 GROUNDWATER TRANSPORT

7.7.1 OVERVIEW

Although radiological and chemical species release to the groundwater can be a concern for operating nuclear facilities, the principal facilities for which groundwater release is a likely pathway are mining and milling operations, and long-term waste disposal areas. Estimates of flow and transport in groundwater are important in assessing the performance of a disposal system because they are probable pathways between hazardous waste and the environment.

The concepts, models, and data development methods used in these models are outside the scope of the guidance given here, and can be found elsewhere.[88] The relative unimportance is due to the relatively small likelihood of acute release conditions needing to be addressed in the groundwater for most DOE facilities. Additionally, airborne and surface water pathways will tend to dominate the acute phase of accident consideration. However, the ultimate fate of the released contaminants for EIS and other types of safety analysis may need to address the groundwater pathway. The analyst seeking to apply a groundwater model as a tool to assist facility safety analysis should consult other compendia listing more detailed subject information.

7.7.2 GROUNDWATER FLOW AND CONTAMINANT TRANSPORT

Two behaviors need to be captured to model contaminant transport in groundwater media. The first is movement of the carrier fluid and the second is the mass transport of the dissolved contaminants.

In modeling contaminant releases to the groundwater, radionuclide travel may be in the unsaturated zone above the water table or in the zone of saturation. While flow is for the most part downward in the

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[88] This material is excerpted from NUREG/CR-3332.

unsaturated region, flow is predominantly lateral in the saturated zone.

Flow can be governed by many anisotropies in the saturated region depending on the media and layers of sedimentation. From Chapter 4 of NUREG/CR-3332, and under the assumption of a homogeneous isotropic medium, the major flow direction can be assumed to follow Darcy's law where the flow volume per unit area (V_x) is shown in Equation 7-3:

$$V_x = -K \, dH/dx$$ **Equation 7-3**

Where,

K = Hydraulic conductivity, dependent on fluid and medium properties, which for an isotropic homogeneous saturated medium, determines rate at which water moves through a porous medium for a given hydraulic gradient (cm/s)

H = Total head, which is pressure head + elevation head (cm)

dH/dx = Hydraulic gradient in the direction of flow (cm)

This relationship assumes the gradient is constant over the increment. The actual velocity of a contaminant would be larger than the flow volume per unit area since water is moving through pore spaces.

It should be noted that the actual velocity of a contaminant would be larger than the flow volume per unit area since water is moving through pore spaces. The pore or seepage velocity U may be approximated by the effective porosity, as shown in Equation 7-4:

$$U = V_x / n_e$$ **Equation 7-4**

Where,

V_x = Volumetric flow rate per unit area in direction x (cm/s)

n_e = Effective porosity, open volume for flow per unit total volume of the medium of interest (dimensionless)

Chapter 4 of NUREG/CR-3332 provides additional information.

7.7.3 TRITIUM IN SEDIMENTS

Examples of radionuclides that have been retained in sediments after chronic or acute release near nuclear facilities have been cesium and plutonium species. Recent work has shown that even tritium, in the form of organically bound tritium (OBT), can be retained in sediments near sources of OBT discharge (Morris, 2006).

7.7.4 GROUNDWATER TRANSPORT MODEL CONSIDERATIONS

Recommendations for the use of groundwater models is given by the National Council on Radiation Protection and Measurements (NCRP), which is an advisory body whose recommendations on radiation protection matters provide the scientific basis for U.S. standards (NCRP Report No. 76). The report summarizes both surface water and groundwater transport and dispersion models and provides general guidance on their use.

As the simplest and most conservative approach, the safety analyst can assume that no dispersion occurs as the contaminants are transported in the medium of interest, and that the transport velocity is constant.

More complex treatments consider that net convection in one dimension and dispersion in all three dimensions. Furthermore, the dispersion or velocity of transport can vary both spatially and temporally. As the modeling complexity grows, there is a commensurate difficulty in preparing input data and identifying the appropriate sources of information.

The transport of contaminants through the ground can be estimated using tracers, groundwater dating, or mathematical modeling. Mathematical modeling involves solving equations of mass transport for the water and for dissolved constituents such as radionuclides.

In applications involving high-level waste repositories, an additional equation for heat transport is required, but models for applications of this type are outside the scope of the Handbook. Results are obtained from the transport equations through simplifying approximations that allow analytical closed-form solutions or through numerical methods.

Numerical solutions generally employ one of following three solution techniques: finite differences, finite elements, or network analysis. Numerical methods generally require an extensive input data set. The availability of this data needs to be considered by the analyst as the lack of required data may make sophisticated numerical modeling impractical.

8 RADIOLOGICAL CONSEQUENCE ASSESSMENT

This chapter provides guidance to the safety analyst regarding evaluation of radiological doses and health risks. It discusses the different types of radiation and the effects these radiation types can have on the human body, its organs, and its tissues. The factors that are considered in estimating the dose a receptor may receive following the atmospheric release of radioactive material are covered in detail. Finally, the health risks associated with radiological doses and the standards for radiation protection, in terms of dose or air concentration, are discussed.

8.1 FUNDAMENTALS

Radiological doses arise from exposure to plumes of radioactive material, including deposition from plumes, and from exposure to prompt (direct) radiation from a criticality accident. The general modes of exposure include:

- Inhalation of radioactive material (particulates and gases) while immersed in a plume;
- Inhalation of particulates from deposited material that have been resuspended by traffic and/or by wind;
- Ingestion of food products through meat, vegetable and fish pathways and ingestion of water contaminated by deposition from the plume;
- Gamma radiation from the plume (cloudshine);
- Gamma radiation from particulates deposited on the ground from deposition (groundshine);
- Skin contamination from deposition;
- Prompt (direct) radiation from a criticality accident; and
- Direct radiation from a loss-of-shielding accident.

As described in Section 3.2.4.2 of DOE-STD-3009-2014, radiological consequences for the DSA accident analysis are presented as a TED based on integrated committed dose to all target organs, accounting for direct exposures, as well as a 50-yr dose commitment. The dose pathways to be considered are inhalation, direct shine, and ground shine. DOE-STD-3009-2014 also states that direct shine and ground shine from gamma emitters only need to be evaluated if they cause an upward change in the qualitative consequence level (see Table 2-8, Consequence Thresholds). DOE-STD-3009-2014 specifies that ingestion (except when the water pathway could significantly contribute to the overall radiological consequences), resuspension, and skin contamination need not be included in a DSA. Accordingly, slowly-developing dose pathways, such as ingestion of contaminated food, water supply contamination, or particle resuspension, are not included. However, quick-release accidents involving other pathways, such as a major tank rupture that could release large amounts of radioactive liquids to water pathways, should be considered (See Chapter 7). In this case, potential uptake locations should be the evaluation points for radiological dose consequences.

In the case of a criticality accident, doses arise from both the plume of fission products that may be released and from the prompt radiation. Prompt radiation from a criticality accident is of concern primarily for facility workers located near the accident site since effects from criticality accidents are generally confined to the near-field. Depending on the size and duration of the criticality accident, and evaluation of shielding provided by the structure, the prompt radiation dose contribution may also be important for the evaluation of consequences to 100 m co-located worker. The distance of concern for prompt radiation depends primarily upon the number of fissions in the first spike and the amount and type of shielding (such as concrete walls) between the worker and the site of the criticality accident. (See Appendix B of this Handbook for additional information on criticality.)

On the other hand, for actinide exposure, inhalation of Pu-238, Pu-239, and Pu-240 particulates is the primary radiological concern as the body does not have effective excretory mechanisms to remove it. According to NUREG-1140, for actinide releases, cloudshine, groundshine, skin contamination, and ingestion doses are insignificant in comparison, with the exception of the release of significant gamma emitters where cloudshine doses would become meaningful. Radiological dose from inhalation of enriched uranium particulates is of lesser concern, although may still have significant consequences warranting the need to consider SS controls. Inhalation of depleted uranium particulates is trivial by comparison, and for depleted and natural uranium, chemical toxicity is normally of greater concern than its radioactivity. See Section 9.4.4 for the toxicity associated with uranium compounds. Skin absorption of tritium is a special case and should not be ignored.

8.1.1 TYPES OF RADIATION

Four types of radiation are important to consider in DSAs: alpha (α), beta (β), gamma (γ), and neutron. α, β, and γ radiations are emitted from atomic nuclei during radioactive disintegration, or decay, of the nucleus. Alpha particles are energetic helium nuclei, consisting of two protons and two neutrons, with a charge of +2[89]. Beta particles are energetic electrons, with a charge of -1e, or positrons, with a charge of +1e; they have a mass about 0.01 percent that of the alpha particle. Gamma radiation consists of electromagnetic waves or photons, and have energy similar to that of x-rays. Being photons, gamma rays have neither charge nor mass. Gamma radiation accompanies alpha and beta radiation when an atomic nucleus disintegrates. Neutron radiation is emitted when a nucleus fissions, or breaks into fragments, such as during a criticality event.[90] Neutron radiation consists of energetic neutrons, particles with zero charge and mass similar to that of protons, that is, about 25 percent of the mass of alpha particles.

When any or all of these radiations strike an organ or tissue of the body, they can deposit some or all of their energy, causing cell damage. The manner of energy deposition varies with the type of radiation. Some types of radiation, principally alpha and beta, deposit their energy primarily through the production of ionization. When they strike an atom, they strip off an electron, thus ionizing the atom. The two charged particles formed, the electron and the ion, are referred to as an ion-pair. The electron that is stripped off the atom may be sufficiently energetic that it can cause further ionization. The amount of ionization created depends upon the mass, charge, and energy of the particle. Particulate radiation (α, β, neutron) can also deposit its energy through the dissociation of molecules and through elastic scattering, which causes heating.

Alpha-decay energy is on the order of several million electron volts (MeV)[91]. For example, plutonium, uranium, and americium isotopes all emit alpha particles with energies on the order of 5 MeV. Because an alpha particle is doubly charged and massive, it can ionize many atoms before exhaustion. For example, an alpha particle traveling through air will create on the order of 50,000 ion pairs for each

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[89] The basic unit of charge is that of the electron, but with a reversal of sign. The charge of an electron is -1.60E-19 coulomb.

[90] Neutrons can also be produced through (α, n) reactions, in which an alpha particle strikes the nucleus of an atom, causing the emission of a neutron. This is generally not important for dose calculations as the additional dose from the neutron radiation is balanced by the decreased dose from the lost alpha particle.

[91] An electron volt (eV) is the kinetic energy of an electron after being accelerated through an electric potential difference of 1 V. It is equal to 1.60E-19 Joules.

centimeter it travels. Because it creates so much ionization, it deposits its energy quickly, and penetrates only a short distance into a tissue.

Beta-decay energy is on the order of tens of keV to a few MeV. For example, the beta-decay energy of Pu-241 is 21 keV. During beta decay, the emitted electron, or positron, is accompanied by an anti-neutrino or neutrino, with which it shares the energy. The beta-decay energy is the sum of the energies of the electron and neutrino. Thus, for Pu-241, the maximum energy the electron can have is 21 keV; normally, it will have only a fraction of this. Because the beta particle is singly charged and not very massive, it cannot create nearly as much ionization as an alpha particle. A beta particle traveling through air will create on the order of 100 ion pairs for each centimeter it travels. In addition to causing ionization, beta particles also can be scattered elastically by atomic electrons. Because a beta particle does not lose its energy as rapidly as does an alpha particle, and because of elastic scattering, it can penetrate more deeply into tissue. However, it travels an irregular path in tissue because of elastic scattering. This gives rise to the emission of electromagnetic radiation called *bremsstrahlung* (German for “braking radiation”), which in turn can deposit its energy in the surrounding tissue.

The energy of a gamma ray is on the order of tens of keV to a few MeV. For example, the energy of one of the several possible gamma rays that accompanies the alpha decay of Pu-239 is 52 keV. A gamma photon will create only about one ion-pair per centimeter in air. A gamma photon can also lose its energy through Compton scattering from electrons and even from interactions with the nucleus of an atom; although the latter are minor in comparison with photoionization and Compton scattering. Gamma radiation is capable of penetrating deeply into a person’s body.

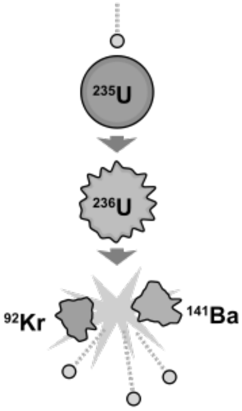
8.1.2 NUCLEAR FISSION

Nuclear fission yields two large fission fragments (nuclei of other isotopes), multiple neutrons, and other radiation (alpha particles, beta particles, or gamma rays). Fission fragments are highly radioactive. To reach a stable configuration, these fission products may continue emitting radiation for wide-ranging time periods; from milliseconds to many years.

The energy of a fission neutron is on the order of a few keV to about 10 MeV. Because the neutron has no charge, it will not create many ion-pairs. It loses it energy primarily through elastic scattering. However, it can also cause nuclear transformations, especially when it has slowed, through elastic scattering, and become a “thermal” neutron. These nuclear transformations can lead to the emission of other radiations, such as α and γ. Neutron absorption through nuclear transformation is primarily by hydrogen and nitrogen in the human body. Elastic scattering of neutrons is primarily by the hydrogen in the body. Like gamma radiation, neutron radiation is very penetrating.

Neutrons resulting from fission are categorized as either prompt or delayed. Prompt neutrons are emitted virtually simultaneously with fission (< 1E-14 second); whereas delayed neutrons may not be emitted for many seconds after fission. Prompt neutrons are “born” fast and are of high energy in the 1-20 MeV range, while delayed neutrons are born with an average energy of less than 0.5 MeV.

As an example, in the sketch to the right, a ^{235}U nucleus absorbs a neutron, becomes unstable, and fissions into two radioactive isotopes; ^{92}Kr and ^{141}Ba, while also releasing three neutrons and multiple gamma rays (not shown).



8.1.3 RADIOACTIVITY

Radioactive decay is the spontaneous disintegration of a radioisotope accompanied by emission of ionizing radiation (α, β, and/or γ). It is the process by which a nucleus of an unstable atom reaches a more stable configuration by the release of energy or mass. The activity of a radioisotope is measured in units of rate of decay, commonly called disintegrations per second (dps). The SI unit is the Becquerel (Bq), defined as one dps. The historical, and still commonly used, unit of activity is the curie (Ci), which is equal to 3.7E+10 dps. Thus, 1 Ci = 3.7E+10 Bq. Lower radioisotope activities are measured in disintegrations per minute (dpm).

Specific activity is the activity per unit mass, and is measured in units such as Bq/kg or Ci/g. The specific activity of Ra-226 was originally defined as 1 Ci/g. The specific activity of a mixture of radionuclides is the sum, over all the radionuclides in the mixture, of the products of specific activities and mass fractions.

The activity of a sample of any given radionuclide decreases exponentially with time, providing it is not being created by the decay of another radionuclide. If N is the number of atoms of a specific type of radionuclide in a sample of material, the change in this number, dN, in a small interval of time, dt, is proportional to N and to dt. This is written

$$dN = -\lambda N\, dt \qquad \textbf{Equation 8-1}$$

where the negative sign is needed to show that N decreases with increasing time. The constant of proportionality, λ, is called the decay (or transformation) constant and is measured in inverse time units, such as s^{-1}. The disintegration rate, or activity (A), is given by

$$A = -dN/dt = \lambda N \qquad \textbf{Equation 8-2}$$

The solution to equation (8-1) is

$$N = N_0\, e^{-\lambda t} \qquad \textbf{Equation 8-3}$$

where N_0 is the number of atoms at time $t = 0$. Thus, equation (8-2) can be written

$$A = A_0\, e^{-\lambda t} \qquad \textbf{Equation 8-4}$$

where $A_0 = \lambda N_0$ is the activity at time $t = 0$.

Because the decay is exponential, the time interval to decrease the number of atoms in a sample by a given factor is a constant. For example, the time to decrease by a factor of two, called the half-life ($t_{½}$), is obtained by inverting equation (8-3):

$$t_{½} = -\,(1/\lambda)\ln(½\, N_0/N_0) = (1/\lambda)\ln(2) = 0.693/\lambda. \qquad \textbf{Equation 8-5}$$

The half-life of Pu-239, for example, is 2.44E+04 yr, while that of U-235 is 7.1E+08 yr. The specific activity of U-235 is therefore about 30,000 times smaller than that of Pu-239, which is the main reason it does not present as great a radiological hazard as Pu-239 for a given amount of material as it is producing fewer decays, and therefore less energy, per unit time.

Instruments that measure the amount of radioactivity in a material usually present their results in terms of counts per minute (cpm). These are then converted to disintegrations per minutes (dpm) by knowing the efficiency of the counter and geometry of the measurement. In the case of surface contamination, the measurements are expressed in terms of activity per unit of area, such as cpm/100 cm^2, which are then converted to dpm/100 cm^2. To derive the amount of material involved, the dpm is divided by 60 to get dps, or Bq. This activity can then be converted to the number of atoms of the radionuclide present by dividing by the decay constant, or the number of grams present by dividing by the specific activity.

8.2 EFFECTS OF RADIATION ON THE BODY

Radiation damages the body as it deposits its energy, primarily through ionization, in organs and tissues. Because alpha radiation can be stopped by the body's outermost layer of dead skin cells, it poses no external hazard to the body; rather, its primary hazard is through inhalation and ingestion. Beta radiation can barely penetrate the skin to cause some damage; and it can also damage the eye. Like alpha radiation, its damage comes principally from inhalation and it also comes from ingestion. Gamma radiation and neutrons, on the other hand, can penetrate the body directly from external sources; material that emits gamma radiation and neutrons can, of course, be inhaled or ingested, but this is not the normal mode of exposure. Skin contamination from fallout from the plume causes tissue damage principally from β radiation.

Both short-term (acute) and long-term (chronic) exposures are important. External radiation from cloudshine, groundshine, skin contamination, or prompt radiation gives a short-term or even instantaneous dose, whereas internal radiation from inhalation and ingestion gives a long-term committed dose. A long-term dose can also arise from continual exposure to external radiation, as in a work place. If a radioactive particle is inhaled or ingested, it will cause damage as long as it remains in the body, because it contains many radioactive atoms that continue to disintegrate. An organ or tissue irradiated for an extended time (chronic exposure) may develop cancer or suffer other deleterious effects.

8.2.1 DOSE EVALUATIONS

The effects of exposure to ionizing radiation were originally defined in terms of the amount of ionization in air produced by gamma radiation and x-rays. The unit used was the Roentgen (R), now defined as the ratio $\Delta Q/\Delta m$, where ΔQ is the sum of all charges of one sign produced in air when all the electrons liberated by photons in a mass Δm of air are completely stopped in air. It is equal to 2.58×10^{-4} coulombs produced in 1 kg of air. This is equivalent to 1.61×10^{15} ion-pairs produced per kilogram of air, or an energy deposition of 87.3 ergs/g of air (Turner 1986). Absorption of 1 R of radiation in tissue corresponds to about 95 ergs/g of tissue; this unit is called the rep (roentgen-equivalent, physical). The rep is no longer used.

Today, dose is expressed as an absorbed dose, that is, the amount of energy deposited in matter, or as an equivalent dose, a measure of damage done in tissue. The traditional unit of absorbed dose is the rad (radiation absorbed dose) and is defined as 100 ergs absorbed in 1 g of material. The newer standard international unit is the gray (Gy), which is defined as 1 J absorbed in 1 kg of material. Thus, 1 Gy = 100 rad. This equality applies to any type of radiation absorbed in any type of material.

The dose of most interest in accident analysis is the equivalent dose, as this is a measure of the biological damage. The amount of damage depends upon the type of radiation, as well as the amount of energy absorbed. The equivalent dose H_T to a particular tissue T is equal to the absorbed dose D_T in that tissue times a radiation-weighting factor w_R.

$$H_T = w_R\, D_T$$ **Equation 8-6**

where w_R is a measure of the amount of damage done by the radiation. If more than one type of radiation impacts the tissue, H_T is calculated by summing over all radiation types. Table 8-1 gives the radiation weighting factors from 10 CFR Part 20, *Standards for Protection Against Radiation,* for the four radiation types considered here. This table can also be located in ICRP-60.

Table 8-1. Radiation Weighting Factors.

Type, Energy Range		Radiation Weighting Factor, w_R
Alpha	any energy	20
Beta	any energy	1
Gamma	any energy	1
Neutrons	< 10 keV	5
	10 keV to 100 keV	10
	>100 keV to 2 MeV	20
	>2 MeV to 20 MeV	10
	> 20 MeV	5

The traditional unit for equivalent dose is the rem (roentgen-equivalent man). The newer international unit is the sievert (Sv). The relation between them is the same as between gray and rad (1 Sv = 100 rem). Sometimes the unit centisieverts (cSv) is used in place of rem.

Example: Assume a medical x ray gives the lungs an absorbed dose of 1 rad (0.01 Gy). The equivalent dose would be 1 rem (0.01 Sv), as x-rays are similar to gamma rays and have a radiation weighting factor of one. On the other hand, if the absorbed dose of 1 rad to the lungs were from inhalation of plutonium, an alpha emitter, the equivalent dose would be 20 rem (0.2 Sv), as the radiation weighting factor for alpha radiation is 20.

The radiation-weighting factor is related to the stopping power of the material, expressed as Linear Energy Transfer (LET):

$$LET = dE/dx$$ **Equation 8-7**

where dE is the average energy locally imparted to the medium by a charged particle traversing the distance dx. Alpha and beta particles have high and low LET, respectively. Gamma radiation, although not a charged particle, is considered equivalent to low LET radiation. Neutrons have a moderate to high LET, depending upon their kinetic energy.

The definition of equivalent dose does not differentiate between short-term and long-term dose, or between external and internal exposure. A related term is committed equivalent dose, which is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults (such as workers) or 70 years for children (as in the general population); it does not include external exposures. The committed equivalent dose is thus a subset of the equivalent dose. This has led to some confusion as some have incorrectly used equivalent dose exclusively for external radiation, apparently as a counterpoint to committed equivalent dose, which is used exclusively for internal radiation.

Doses are also calculated for the body as a whole. This is done by summing over all organs the product of an organ weighting factor and the equivalent dose for that organ. This sum is called the effective dose, formerly called the effective dose equivalent (EDE), a term still used. The organ weighting factors represent the fraction of the total health risk resulting from uniform whole body irradiation that could be attributed to that particular tissue or organ; these factors are between zero and one; their sum over all organs and tissues is one. The weighting factors (also called tissue weighting factor) for the various organs are shown in Table 8-2, as taken from ICRP-60, *Recommendations of the International Commission of Radiological Protection*; for comparison, ICRP-26, *Recommendations of the ICRP*, values are also shown, as they may still be used for existing safety analyses in nonreactor nuclear facility DSAs.

Table 8-2. Organ Weighting Factors.

Organ	**Organ Weighting Factor**	
	ICRP-26	**ICRP-60**
Bladder	–	0.05
Bone Marrow (red)	0.12	0.12
Bone Surface (skeleton)	0.03	0.01
Breast	0.15	0.05
Colon	–	0.12
Esophagus	–	0.05
Gonads	0.25	0.20
Liver	–	0.05
Lung	0.12	0.12
Skin	–	0.01
Stomach	–	0.12
Thyroid	0.03	0.05
Remainder	0.30	0.05

Example: Assume every organ listed in Table 8-2 (considering “remainder” as a single organ), receives a dose of 1 rem each. The effective dose to the whole body would then also be 1 rem. On the other hand, if the bone surface was to receive 100 rem (1 Sv) and all other organs received none, the effective dose would again be 1 rem, using the ICRP-60 organ weighting factors.[92]

A term similar to effective dose is committed effective dose (formerly, the committed effective dose equivalent, or CEDE, a term still used), which is the predicted dose from internal exposures over the remaining life of the individual, normally taken to be 50 years for adults, or 70 years for children; it also does not include external exposures. Committed effective dose is thus a subset of effective dose. However, as with equivalent dose compared with committed equivalent dose, confusion has arisen in that some incorrectly use effective dose to refer to only external radiation, because committed effective dose refers only to internal radiation. A new term, total effective dose equivalent (TEDE), is now used to indicate the sum of the external (short-term) and the internal (committed, long-term) effective doses (10 CFR Part 20). TEDE is called the TED in ICRP-60 and current calculations are for TED.

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[92] This example is for illustration only as no accident would give dose to only one internal organ.

Doses arise from both internal and external exposures, as noted above. Per DOE-STD-3009-2014, the only internal exposures of concern consist of inhalation from being immersed in the plume, except when the water pathway could significantly contribute to the overall radiological consequences. The external exposures are from cloudshine, groundshine, and prompt (direct) radiation from a criticality event. These are discussed individually below.

8.2.2 INHALATION (PLUME) DOSE

Inhalation dose from immersion in a plume to a given organ or tissue from a given isotope, i, is the product of the amount of respirable radioactive material released, or the source term ST, atmospheric dispersion factor χ/Q, breathing rate BR, and dose conversion factor DCF_i

$$\text{Dose}_i = ST_i \times \chi/Q \times BR \times DCF_i \qquad \textbf{Equation 8-8}$$

assuming the receptor remains exposed for the duration of the plume passage. The total dose to the organ or tissue is the sum over all isotopes inhaled. The source term (ST_i) is the product of the MAR, DR, ARF, RF, and LPF, as discussed in Chapter 5. The χ/Q is discussed in Chapter 6 and the breathing rate and dose conversion factors are discussed below. The breathing rates for the "reference man" for various activities, as have been used in accident analyses for the past several years at many DOE sites, are given in Table 8-3 (ICRP-2 and ICRP-30, *Limits for Intakes of Radionuclides by Workers*). ICRP-66, *Human Respiratory Tract Model for Radiological Protection,* gives revised breathing for the "reference man."[93] These are also shown in Table 8-3. Still other breathing rates are appropriate for other individuals, such as infants, the elderly, and the infirm, and for other levels of activity (ICRP-66).

Table 8-3. "Reference Man" Breathing Rates for Various Levels of Activity.

Activity Level	Breathing Rate (m^3/s)
ICRP-2, ICPR-30	
Chronic	2.66E-4
Light	3.33E-4
Heavy	3.47E-4
ICRP-66	
Sleep	1.25E-4
Rest, sitting	1.50E-4
Light exercise	4.17E-4
Heavy exercise	8.33E-4

DOE-STD-3009-2014, Section 3.2.4.2 requires a breathing rate of 3.3E-4 m^3/s. This value was initially developed for "light activity" based on data and methods from ICRP-2 / ICRP-30 DCFs, and is equivalent to "light work" as defined in ICRP-68, *Dose Coefficients for Intakes of Radionuclides by Workers,* using ICRP-66 data. ICRP-68 has revised the 8-hour day breathing rates as follows: light work is defined as 2.5 hr sitting (inhalation rate 0.54 m^3/hr [1.5E-4 m^3/s], breathing frequency 12/min) and 5.5 hr light exercise (inhalation rate 1.5 m^3/hr [4.17E-4 m^3/s], breathing frequency 20/min). NNSA SD G 1027, *Hazard Categorization and Accident Analysis Techniques for Compliance with DOE Order 5480.23, Nuclear Safety Analysis Reports to Address Areas in Need of Clarification and Improvement* (Admin

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[93] The reference man is a male, 30 years old, height 176 cm (5 ft, 9 in.), and weight 73 kg (161 lb). ICRP-89 provides additional data for other factors related to breathing rate, including age, gender, and race.

Change 1, May 2014) has added significant figures (to bring it to 3.3333E-04 m^3/s), although this added precision does not materially change the dose result.

Once radioactive material enters the respiratory tract, it begins to migrate to other parts of the body. A portion is transferred directly to the blood and another portion to the gastrointestinal (GI) tract. Transfer of the material directly from the respiratory tract into the blood depends upon where in the respiratory tract it is deposited and how soluble it is. Material is also cleared from the respiratory tract by means of the body's mucociliary mechanism and then swallowed, thus entering the GI tract. The fraction f_1 of the material that passes from the GI tract into the blood, primarily from the small intestine, depends on the solubility of the material. For some radionuclides, such as iodine, the transfer to the blood is nearly complete ($f_1 = 1.0$). For other radionuclides, such as plutonium, the portion transferred to the blood is much less than 1 percent; the remainder is excreted. Once the material enters the blood, it can be carried to any part of the body. From there, it may preferentially attach to a given organ or tissue, as determined by the chemical properties of the radioactive material and of the organ or tissue. For example, plutonium and americium become preferentially attached to bone surface. The amount of biological damage that radioactive material may inflict on an organ or tissue is given by the DCF mentioned above. For inhalation, this is expressed in units of Sv/Bq (or rem/Ci), which can be converted to Sv/g (or rem/g) by multiplying by the specific activity. An example of tables of DCFs for a large number of radionuclides are given in Federal Guidance Report (FGR)-11 (EPA FGR-11). The DCFs take into account the migration of the radioisotope within the body, the decay of the radioisotope, and the formation of daughter isotopes that may be radioactive.

The residence time of a radioactive particle in the lungs depends in part upon the solubility of the material. Older DSAs use the residence times from ICRP-30 whereas more recent DSAs use the residence times from ICRP-68. Three broad categories for use with ICRP-30 or *Limiting Values of Radionuclide Intake and Air Concentration and Dose Conversion Factors for Inhalation, Submersion, and Ingestion* (EPA FGR-11) DCFs have been defined.

Y: Radionuclides in insoluble compounds remain in the lungs for a long time; these are of Solubility Class Y (for years), also called Lung Clearance Class Y.

W: Radionuclides in moderately soluble compounds remain in the lungs for weeks; these are of Solubility Class W (for weeks), also called Lung Clearance Class W.

D: Radionuclides in soluble compounds remain in the lungs for only a short time; these are of Solubility Class D (for days), also called Lung Clearance Class D.

According to EPA FGR-11, plutonium compounds can be Class Y (the oxides[94]) or Class W (all other Pu compounds); there are no Class D Pu compounds. Americium compounds are only Class W. Uranium compounds can be Class Y (UO_2 and U_3O_8), Class W (UO_3, UF_4, and UCl_4), or Class D (UF_6, UO_2F_2, and $UO_2(NO_3)_2$). Fission products are of all three lung clearance classes.

Should these compounds be involved in a fire, their chemical nature may change. For example, a plutonium salt, as in certain residues, which is Class W, may change to an oxide (Class Y) in a fire. High-fired plutonium oxide is an example of Class Y. However, conversion of a salt in a fire will probably not be complete. Accordingly, it may be appropriate to assume that the resultant chemical form

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[94] Plutonium hydroxides have subsequently been added to Class Y.

is the one that gives the largest dose. In the case of plutonium salts, for example, Class W for plutonium salts may apply.

Newer biokinetic models of the human respiratory system (ICRP-68) give DCFs for plutonium and americium that are notably smaller than those used in ICRP-30. The following differences can be noted between these two databases.

1. The DCFs for fission products are similar between the two databases, but those of the actinides are much smaller in ICRP-68 than in ICRP-30.

2. The ICRP-68 values do not use the D, W, and Y solubility classes. Instead, they use "F (Fast)," "M (Moderate)," and "S (Slow)," which are broadly equivalent to D, W, and Y.
   a. "Fast" refers to those compounds that dissolve quickly and are absorbed into the respiratory tissue where they are initially deposited, or directly into the blood, in minutes to hours. There is virtually no time for these compounds to be transported to other respiratory sites.
   b. "Moderate" refers to those compounds that dissolve more slowly. Only a small portion (modeled as 10 percent) is absorbed directly into respiratory tissue at the initial deposit site, or directly into blood; the remainder is transformed (in a period of weeks) into a more soluble compound. While in this transformed state, it can be transported to other respiratory tissues. It eventually is dissolved into the blood and thus is available for transport to other parts of the body.
   c. "Slow" refers to those compounds that are essentially insoluble. Almost none of this material is absorbed directly into the tissue at the initial deposit site, or directly into the blood. It is slowly transformed into a more soluble compound (on a time scale of years). While in this transformed state, it can be transported to other respiratory tissues. It eventually is dissolved into the blood and thus is available for transport to other parts of the body.

3. The DCFs of ICRP-68 are given for two particulate size distributions, centered at 1 μm and 5 μm. These sizes are referred to as AMAD, the median diameter of a lognormal size distribution. In contrast, the ICRP-30 values were only for one particulate size distribution, 1-μm AMAD.

ICRP-68 recommends that the 5-μm AMAD DCFs be used unless the analyst can justify the use of the DCFs for the 1-μm AMAD; such as the case in which the particulates had passed through HEPA filtration. Federal agencies have accepted the use of 1 um AMAD for consequence management response actions (e.g., Federal Radiological Monitoring and Assessment Center Assessment Manual calculations). DCFs generally are larger for smaller particle sizes. HEPA filters are least efficient at about 0.3 -μm-sized particles for which the DCF would be larger than for either 1 -μm or 5 -μm. On the other hand, very small particles tend to agglomerate and stick to surfaces. The DCF chosen for a given scenario needs to be technically justified if other than the value for 1-μm or 5-μm. Refer to ICRP-68 Annex F for assigning lung clearance type to different compounds. ICRP-72 has a an even more detailed discussion.

ICRP-68 was developed for assessing potential doses to workers and can be used to evaluate the postulated dose to the CW. For the MOI consequence assessment, the adult dose conversion factors from

ICRP-72, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides, Part 5,*[95] is used as described in DOE-STD-3009-2014, Section 3.2.4.2.

8.2.3 CLOUDSHINE DOSE

The amount of gamma radiation (and beta, if appropriate) received by a receptor from a plume of radioactive material depends upon the location of the receptor relative to the plume. The greatest dose would be received by a receptor in the plume centerline and DCFs have been developed for such a receptor. The assumptions made in deriving these DCFs are that (1) the plume is uniform and semi-infinite[96] and (2) the receptor is standing upright on the ground. The dose received from a given radionuclide is the product of the concentration of the radionuclide and the DCF, integrated over the duration of the plume. The doses from all the radionuclides are then be summed. The DCFs for cloudshine are given in FGR-12, *External Exposure to Radionuclides in air, Water, and Soil*. Information for ordering this report is given in the EPA internet web site http://www.epa.gov/radiation/federal/index.html. Cloudshine DCFs are expressed in units of (Sv-m^3)/(Bq-s). FGR-11 also gives DCFs for cloudshine but these have been superseded by those of FGR-12.

The cloudshine doses calculated using the DCFs from FGR-12 are conservative because of the assumptions that the receptor is standing upright in a uniform, semi-infinite cloud. The plume is neither uniform nor semi-infinite, the receptor may not be at the plume centerline, the plume may be elevated, the receptor may be sheltered, and the receptor may not be standing up; each of these factors would tend to reduce the dose. Corrections for finite cloud size and distribution (Gaussian) and for receptor locations off-centerline are included in several computer models of atmospheric dispersion and consequence assessment (see Section 6.12.2). The safety analyst should also consider additional dose reduction factors associated with sheltering.

8.2.4 GROUNDSHINE DOSE

The amount of gamma radiation received by a receptor from radioactive material deposited on the ground through deposition (see Section 6.8.4) depends upon the location of receptor relative to the fallout. The greatest dose would be received by a receptor at the center of the deposition, and DCFs have been developed for such a receptor. The assumptions made in deriving groundshine DCFs are: (1) the material is uniformly distributed on the surface or in the soil for an infinite distance in every horizontal direction azimuth); and (2) the receptor is standing upright on the ground. The dose received from a given radionuclide is the product of the concentration of the radionuclide on, or in, the ground and the DCF, integrated over the duration of the exposure (how long the receptor is present to receive groundshine). The ground shine doses from all the radionuclides are then summed. The concentration to be used in the calculation is either an areal concentration (Bq/m^2), if the material is only on the surface, or a volume concentration (Bq/m^3), if mixed with the soil. The dose rate is the product of the concentration and DCF. Groundshine DCFs are expressed in units of either (Sv-m^2)/(Bq-s) for surface contamination, or (Sv-m^3)/(Bq-s) for soil contaminated down to a specified depth. The DCFs for groundshine are given in FGR-

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[95] DOE-STD-1196-2011, Appendix A includes dose coefficients for adults consistent with ICRP-72 dose coefficients. DOE has determined that the adult dose coefficients are appropriate for hazard scenario consequence estimates. However, in other situations such as determining collective dose to the public from a release, reference person coefficients from DOE-STD-1196-2011 are more appropriate. That standard includes gender and age weighted dose coefficients that are appropriate for estimating doses to the general public resulting from chronic exposures. These dose coefficients may be appropriate when assessing doses from residual radioactive material over the long-term.

[96] “Semi” because the plume extends upward from the ground, but not downward.

12. The depths of soil contamination considered in these tables are for 1-cm, 5-cm, 15-cm, and an infinite depth. Groundshine DCFs for other depths of soil contamination can be found by interpolation among these tables.

The groundshine doses calculated using the DCFs from FGR-12 are conservative because of the assumptions that the receptor is standing upright on a uniformly contaminated, infinite plane. The deposition is neither uniform nor infinite and the receptor may not be the middle of it. Furthermore, surface morphology irregularities (uneven terrain) tend to shield the receptor, the receptor may be sheltered, and the receptor may be elevated or more distant from the groundshine; each of these factors would reduce the dose. The safety analyst may also wish to consider additional dose reduction factors associated with sheltering or surface roughness/unevenness.

In calculating groundshine doses, the time variation of the ground concentration at the receptor's location is considered. In the early stages of plume passage, the ground concentration is increasing; the concentration reaching a peak at the end of plume passage. Resuspension (see Section 6.8.4) of the particulates then erodes the amount of contamination. The DOE-STD-3009-2014 recommended exposure duration is up to 8 hours. In calculating groundshine doses, the time variation of the ground concentration at the receptor's location is considered. In the early stages of plume passage, the ground concentration is increasing; the concentration reaching a peak at the end of plume passage. Refer to the toolbox code manuals for details of how each code treats this.

8.2.5 PROMPT (DIRECT) DOSE

Prompt doses from criticality accidents arise exclusively from neutrons and gamma rays from fissions and fission products and capture gamma rays from fission neutrons (see Appendix B). The prompt dose depends directly upon the number of fissions in the criticality accident, the distance to the receptor, and the amount of intervening shielding material, such as steel, concrete, or water. NUREG/CR-6504, *An Updated Nuclear Criticality Slide Rule*, gives curves of unshielded dose as a function of distance, number of fissions, and time after the criticality accident.

Shielding is expressed in terms of the amount of intervening concrete or the equivalent if other shielding materials are involved. Shielding dose reduction factors may be determined from the following relationships, which are taken from NUREG/CR-6504.

Steel Dose Reduction Factor:	neutrons = exp (-0.256 × steel thickness in inches)
	gammas = exp (-0.386 × steel thickness in inches)
Concrete Dose Reduction Factor:	neutrons, = exp (-0.240 × concrete thickness in inches)
	gammas = exp (-0.147 × concrete thickness in inches)
Water Dose Reduction Factor:	neutrons = exp (-0.277 × water thickness in inches)
	gammas = exp (-0.092 × water thickness in inches)

Prompt doses from criticality accidents need to be compared with the Safety Significant (SS) Structure, System, and Component (SSC) guidelines for the FW (Chapters 2 and 10). These guidelines state that "prompt death" or "serious injury" is a high consequence. These refer to deterministic health effects, not cancer. A prompt dose of 450-rad from a criticality accident is considered lethal to 50% of the people within 30 days, a dose labeled $LD_{50/30}$. A dose of about half of this would cause serious injury but not death to most individuals. It is recommended that if the prompt dose exceeds 400 rad it be considered lethal (prompt fatality or "high consequence"). A prompt dose between 200 and 400 rad would cause serious injury (also a "high consequence") and a prompt dose below 200 rad would not be a serious injury for a healthy worker. See Section 8.3. For a criticality event producing 1E+17 fissions first spike, a dose of 400 rad would be received by an unshielded worker about three meters from the accident.

The total radiation dose from a criticality accident, including inhalation, cloudshine, and from prompt exposure, is included in the assessment of consequences to the CW. However, the prompt dose may be determined to not be significant based on distance and/or shielding, and not included in the total dose estimate. The unmitigated analysis may credit shielding from passive design features such as concrete walls, and their safety significance evaluated per the DOE-STD-3009-2014 guidance on ICs.

8.2.6 PLUTONIUM EQUIVALENT CURIES

For simplification of accident analysis calculations it is beneficial to introduce the concept of surrogate compositions of MAR, based on isotopic-specific DCFs. For example, the concept can be used to establish a common inventory or tracking basis for a dose calculation. It can provide a process for accepting new material while remaining within the bounds of the accident analyses, thus allowing operational flexibility while complying with the safety basis and source strength administrative control limits.

This is commonly done for materials composed of several isotopes of plutonium. For accident analysis purposes and safety system classifications, EGs are in units of TED, which is indifferent to the dose pathway or the kinds of radionuclides involved. The dose equivalent curie concept effectively converts radiological consequences for individual isotopes or mixes of isotopes to the same consequences from a corresponding amount of a base isotope. For example, for Pu-239, a plutonium equivalent curie (PE-Ci) is defined as the summation of the curies of each isotope multiplied by its dose equivalence factor:

$$PE\text{-}Ci = \Sigma\,(dose\ equivalence\ factor)_n \times (curies)_n \qquad \textbf{Equation 8-9}$$

where n is the index for the isotopes included in the mix. In the case of Pu-239, dose equivalence is a method of normalizing the radiotoxicity of various radionuclides to Pu-239 for use in determining relative hazard of radioactive materials. The normalization is often based on the inhalation pathway only. It is derived from the ratio of the inhalation committed effective dose for each radionuclide to that of Pu-239. The inhalation DCFs are based on ICRP-72 for the public receptor and are usually more conservative than ICRP-68 DCFs which were developed for facility worker dose commitments. This ratio is the dose equivalence factor of the isotope per curie of isotope. This approach should not be used for radionuclides that can pose a non-negligible external dose.

8.3 HEALTH RISKS

Although not required for the DSA accident analysis, radiological doses may be converted to health risks for other special assessments, such as comparison to the DOE Safety Goal in DOE P 420.1. For regulatory decision-making, the linear, no threshold (LNT) risk model provides a starting point for calculating stochastic risk factors for low-dose LET radiation. These risk factors do not apply to high doses and have great uncertainty at low doses (less than a few Rad) and low dose rates. This may be done by multiplying doses by stochastic risk factors for comparative purposes. However, the preferred approach is to apply risk coefficients from FGR-13, *Cancer Risk Coefficients for Environmental Exposure to Radionuclides*, directly to the radionuclide intake or exposure (DOE/EH-412/0015/0802; ISCORS Tech. Report 1; EPA FGR-13). Latent cancer fatalities (LCFs) are the (chronic) health risks of most interest. The term "latent" indicates that the estimated cancer fatalities would occur sometime in the future, within the next 50 years for adults, or the next 70 years for the general population, which includes children. One can also estimate latent cancer occurrences (fatal plus non-fatal) or genetic effects, but these are not normally evaluated in safety analyses. The stochastic risk factor depends upon the type of radiation and the organ considered. The following subsections address health risks from high-LET radiation (alpha particles) and low-LET (beta particles and gamma rays) radiation.

8.3.1 HIGH-LET RADIATION

In the case of alpha emitters, such as plutonium and uranium, the only organs of importance for cancer risk are the lungs, liver, and bone surface as discussed in NUREG/CR-4214, *Health Effects Models for Nuclear Power Plant Accident Consequence Analysis, Modification of Models Resulting From Addition of Effects of Exposure to Alpha-Emitting Radionuclides*. The stochastic risk factors for cancer fatalities for these organs are shown in Table 8-4. For these three organs, the stochastic risk factors are linear and continuous. Earlier models, based on ICRP-26, used a linear-quadratic model. The new model, based on ICRP-60), is linear but may be discontinuous for some radionuclides. The values from NUREG/CR-4214 differ from the earlier ICRP-26 values): the lung factor is about four times larger, the bone skeleton factor is about ten times smaller, and liver factor is about three times smaller than the earlier values. The values in Table 8-4 are for high-LET radiation (alpha particles). Table 8-4 does not give the stochastic risk factor for committed effective dose, as the total cancer risk should be calculated as the sum of the individual organ cancer risks [Σ (dose × stochastic factor)]. The other organs of the body do not contribute significantly to cancer risk from exposure to alpha radiation and have been ignored.

Table 8-4. Stochastic Risk Factors for Alpha-Emitters (NUREG/CR-4214).

Organ	**Risk Factor** (LCF/rem)
Bone surface	6.0E-7
Lungs	8.0E-5
Liver	1.5E-5

8.3.2 LOW-LET RADIATION

For low-LET radiation (beta and gamma radiation), the latent cancer risk may be estimated for regulatory decisionmaking from the committed effective dose, although the individual organ cancer risks could also be summed. ICRP-60 recommends using a stochastic risk factor of 5.0E-04 LCF/rem (5.0E-02 LCF/Sv) for the whole population,[97] or 4.0E-04 LCF/rem (4.0E-02 LCF/Sv) for adult workers, based on the committed effective dose.[98] The stochastic risk factor for the public is higher than for adult workers because the public consists of a mixture of individuals with varying degrees of resistance to hazardous materials, including children, the elderly, and the infirm. This factor includes the cancer risk to all organs, unlike the treatment of alpha radiation, which considers only the three organs of Table 8-4 to be important for cancer risk.

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[97] This ICRP-60 recommendation was adopted by the DOE in 1993 for the evaluations of Environmental Assessments and Environmental Impact Statements, but was increased slightly to 6.0E-04 LCF/rem in the current DOE guidance (DOE/ESH, 2004).

[98] The ISCORS Technical Report No. 1 (ISCORS, 2002) cites a slightly higher risk factor of 6.0E-2 LCF/Sv (6.0E-4 LCF/rem) without distinguishing between the public and workers.

8.3.3 ACUTE HEALTH RISKS

Doses received in a short time period (acute doses) may cause acute health risks, if large enough. A dose from gamma or neutron radiation, such as from a criticality event, is the primary concern. Table 8-5 (taken from Table 3-2 of EPA-400/R-17/001, *PAG Manual, Protective Action Guides and Planning Guidance for Radiological Incidents*) summarizes the health effects associated with varying levels of gamma radiation.

Table 8-5. Acute Radiation Effects for Gamma Radiation[*]

Feature or Illness	**Effects of Whole Body Absorbed Dose from External Radiation or Internal Absorption, by dose range in Rad (Gray)**				
	0-100 (0-1 Gy)	100-200 (1-2 Gy)	200-600 (2-6 Gy)	600-800 (6-8 Gy)	>800 (>8 Gy)
Nausea, Vomiting	None	5-50%	50-100%	75-100%	90-100%
Time of onset		3-6 hr	2-4 hr	1-2 hr	< 1 hr to minutes
Duration		< 24 hr	< 24 hr	< 48 hr	< 48 hr
Lymphocyte Count	Unaffected	Minimally Decreased	<1000 at 24 hr	< 500 at 24 hr	Decreases within hours
Central Nervous System Function	No Impairment	No Impairment	Cognitive impairment for 6-20 hr	Cognitive impairment for > 20 hr	Rapid incapacitation
Mortality	None	Minimal	Low with aggressive therapy26	High	Very High: Significant neurological symptoms indicate lethal dose

[*] Percentage of people receiving whole body doses within a few hours expected to experience acute health effects. Original source as cited in EPA-400/R-17/001: *Medical Management of Radiological Casualties*, Second Edition, Armed Forces Radiobiology Research Institute, U.S. Department of Defense. Bethesda, MD, April 2003.

An acute dose from inhalation of plutonium or uranium, the dose received in a few hours or days, is normally very small. All of the isotopes of plutonium and uranium have half-lives of many years; therefore, the inhalation dose received by a person during the first few days following inhalation will only be a tiny fraction of the lifetime committed dose. Accordingly, an acute health effect requires a very large amount of plutonium or uranium to be released. For example, in order for a person at a distance of about 2 km from the release site to get a dose large enough to cause pneumonitis, the first prompt health effect to occur, an airborne release of about 100 kg of respirable plutonium-239 would be required (Peterson, 1993). Such a large release is not physically possible. Therefore, acute health effects to the public need not be considered for releases of plutonium or uranium isotopes.

9 CHEMICAL DISPERSION AND CONSEQUENCE ANALYSIS

9.1 INTRODUCTION

Chapter 6 discussed atmospheric dispersion analysis with its main focus on radiological releases, and Chapter 8 discussed radiological consequence analysis. Many of the atmospheric dispersion principles associated with radiological releases of neutrally-buoyant gases discussed in Chapter 6 are also applicable to neutrally-buoyant toxic chemical releases. Wherever there was commonality between radiological and toxic chemical dispersion and consequence analysis, it was so indicated in that chapter.

There are many types of toxic chemical releases that require a more comprehensive treatment than steady-state releases of neutrally-buoyant gases. These analyses involve more specialized source term phenomenological models and atmospheric dispersion models to address their emission into and redistribution in the atmosphere. In addition, the human health effect metrics of toxic chemicals are far more complex than the metrics associated with radiological health effects. Each of these differences are identified and treated in this chapter.

As discussed in Section 2.3.3, DOE-STD-3009-2014 requires assessment of toxic chemical hazards as part of a DSA hazard evaluation, either qualitatively or quantitatively. This chapter addresses the quantitative analysis of toxic chemical releases applying accident analysis methodologies.

As in Chapter 6, this chapter addresses the evaluation of releases of toxic chemicals and associated concomitant health risks to the facility worker, CW, and the MOI. However, it also discusses the different types of chemical release phenomenology and the factors to consider when estimating the health effects that these toxic chemicals can have on the human body and its target organs. Once the toxic chemical source term phenomenology is established and the appropriate atmospheric dispersion model selected, the resultant health risks associated with each toxic chemical needs to be evaluated at each important receptor and compared to the appropriate chemical health indicators.

NSRD-2015-TD01 concluded:

> Similar to calculations for the radiological releases, the chemical release calculations showed that the default χ/Q value is conservative for chemical releases for nearly all cases, except the situations where the building wake cannot be credited or where a building is smaller than that assumed in NUREG-1140. For these situations the default χ/Q value may not provide a conservative estimate of dispersion.

This chapter addresses both the atmospheric dispersion of chemical materials and their consequences in terms of exposure concentrations to meet the requirements of Section 3.2.4.3, Chemical Source Term and Consequence, of DOE-STD-3009-2014, once the source term (ST) either as a release rate (mg/s) or total release quantity (mg) over a release duration (s) is estimated as described in Chapter 5. For safety analysis purposes, the dispersion analysis is used to estimate chemical consequences in terms of a peak air concentration that occurs any time during the duration of the release to the MOI and CW.

The following is the general approach for the atmospheric dispersion and chemical consequence analysis:

1. From the accident scenario, as defined by applying Chapter 3 guidance, identify parameters (ground level, buoyant, elevated stack, discharge temperature) relevant to evaluating releases to the environment.
2. Select the appropriate dispersion methodology (e.g., DOE Toolbox code, manual spreadsheet calculation).
3. Analyze appropriate weather data and convert to a format for the selected methodology.
4. Apply the dispersion methodology, justifying input values as affected by the accident scenario, unique site conditions, or recommended default values from the most recent guidance documents, such as those for the DOE Toolbox codes or this chapter.
5. Calculate the chemical concentration to the MOI and CW.

This Chapter goes through each of these steps. However, before doing so it begins with some fundamentals of chemical consequence assessment and other topics that support the DSA analysis of chemicals. Specifically this Chapter provides information on:

- Chemical Consequence Assessment Fundamentals;
- Chemical Screening Criteria;
- Chemical Health Effects on the Human Body;
- Toxic Chemical Release Phenomenology and Subsequent Atmospheric Transport And Diffusion;
- Meteorological Parameters Affecting Toxic Chemical Consequence Analysis;
- Toxic Chemical Atmospheric Transport and Diffusion Models;
- Toxic Chemical Consequence Scoping Methodology to Exceed PAC/TEEL Values; and
- Example Toxic Chemical Calculations.

9.2 CHEMICAL CONSEQUENCE ASSESSMENT FUNDAMENTALS

There are a number of ways in which the consequence assessment of toxic chemicals differ from that of radioactive materials; thus requiring more comprehensive treatment. The most fundamental difference is that unlike radiological exposures whose health effects have been normalized to a common scale of rem measurement, each particular toxic chemical insults the human body in its own unique way; enormously complicating the health effects evaluation portion of the assessment process. For a facility with an inventory of many different chemicals, consequence assessment can quickly become a cumbersome process. Accordingly, chemical hazard assessment makes extensive use of a screening process to focus on those chemicals of sufficient quantity and toxicity to present a clear potential threat to the facility worker, CW, MOI, and the public. Without this screening process, the amount of effort to perform chemical consequence assessments would be untenable.

Toxic impacts of most of the chemicals of concern for this handbook are associated with a threshold dose or concentration, usually defined for most toxic chemicals below which no adverse effects are expected. In contrast, the effects elicited by radioactive materials on the human body addressed in this handbook are assumed to occur over a dose continuum. Chemicals that have chronic carcinogenic, mutagenic and teratogenic effects are similar to those of radioactive materials in that they are considered non-threshold events but are only briefly addressed in this accident analysis handbook because those chemicals are not within the scope of 10 CFR § 830.204(b)(3).

Other consequence assessment differences include the physical and temporal characteristics associated with the release phenomenology, the atmospheric characteristics of the plume, and the nature of the health and environmental effects. For chemicals that have a higher molecular weight than that of the atmosphere (i.e., 28.97 g/mol), density differences can produce dense gas gradients, resulting in airborne plumes that remain near the ground and flow downhill in response to local topography. In addition, liquid pools that are physically much colder than the environment, termed cryogenic, may also exhibit dense gas characteristics. Lastly, the quantity of the release is another important discriminator, as the release has to be sufficiently large to create its own dense gas dispersion environment. The Bulk Richardson number is used by dense gas models (e.g., ALOHA) to determine the nature of the dispersion environment. NRSD-2015-TD01 Section F.6 and Section 7.5.3 of this Handbook present additional discussion on dense gas dispersion. Chemical reactions in contact with air and upon exposure to sunlight and atmospheric moisture can also alter the human toxicity characteristics of a plume by changing its chemical composition and concomitant health effects.

9.3 CHEMICAL SCREENING CRITERIA

The evaluation of toxic chemical hazards often involves the consideration of many chemical substances. The DSA can be simplified with a negligible loss in conservatism and scientific integrity by limiting the chemical hazard evaluation to toxic chemicals that constitute the most significant safety concerns. This simplification can be accomplished through a systematic chemical pre-screening process. DOE-STD-3009-2014, Section A.2, provides the most recent chemical screening guidance for DSA hazard evaluations, such as excluding chemicals that are commonly available and used by the general public, or small-scale use quantities of chemicals. Moreover, SIHs should also be screened out per the guidance presented in Section 2.2.4, Exclusion of Standard Industrial Hazards and Other Hazardous Materials, of this Handbook. The following discussions provide additional clarifications and guidance related to the toxicity guidance addressed in DOE-STD-3009-2014, Section A.2.

The factors that determine the degree of hazard that any given chemical represents include:

- Physicochemical properties that contribute to dispersibility, reactivity, and toxicity;
- Significant quantities of chemicals that may displace oxygen in the air as simple asphyxiants;
- Incompatibility with other chemicals; and,
- Conditions under which the chemical is stored and/or used, including the quantity involved.

Specific questions to determine which chemicals to include in a DSA are presented in Table 9-1 below.

Table 9-1. Identification of Chemicals in the Prescreening Process: Baseline Criteria.

A) Is a particular chemical on any of the following lists? This is the first level of screening in or screening out of any chemical. Note that the TPQ and RQ values should not be used for quantitative screening.
• EPA list of extremely hazardous substances and threshold planning quantities (TPQs) (40 CFR § 355)
• EPA list of hazardous substances and reportable quantities (RQs) (40 CFR § 302)
• OSHA list of highly hazardous chemicals, toxic chemicals and reactive chemicals (29 CFR § 1910.119 Appendix A)
• EPA list of regulated substances and thresholds for accidental release prevention Threshold Quantities (40 CFR Part 68)
B) Is there any indication that the particular chemical exhibits significant toxic properties in Safety Data Sheets (SDSs), required by OSHA Hazards Communication, 29 CFR § 1910.1200?
C) Have any short-term acute exposure limits been derived for a particular chemical?
• EPA Acute Exposure Guideline Limits (AEGLs)
• AIHA Emergency Response Planning Guidelines (ERPGs)
• DOE/NA-41 PAC/TEELs
D) Does a particular chemical have a National Fire Protection Association Health Hazard Rating of 2, 3 or 4? See DOE-STD-3009-2014, Section A.2.
E) Is a particular chemical extremely reactive or flammable? F) Is a particular chemical in close physical proximity to other incompatible chemicals, which could result in the release of toxic reaction products in an accident?
G) Is a particular chemical readily volatilized (i.e., having a high vapor pressure) upon release to the atmosphere?
H) Does a particular chemical generate toxic combustion products?
I) Does a particular chemical act as a simple asphyxiant which reduces the available oxygen below 19.5 percent, per OSHA 29 CFR 1926.55 Appendix A? Additional simple asphyxiant guidance is provided in ANSI Z88.2-1992 and DOE-HDBK-1046-2016.

SDSs are required from chemical manufacturers to meet hazard communications requirements in OSHA's rule 29 CFR § 1910.1200. These SDSs also provide valuable chemical exposure health effects information relative to chemical screening, as follows:

- Section 2: Hazards identification inclusive of target organs, routes of entry, acute effects, chronic health effects, carcinogenic, mutagenic and teratogenic effects
- Section 10: Stability and reactivity
- Section 11: Toxicological information

All chemicals that are not screened out are evaluated in the DSA hazard evaluation as discussed in Section 2.3.2.

9.4 CHEMICAL HEALTH EFFECTS ON THE HUMAN BODY

The following subsections address chemical concentration, exposure modes and exposure time, and the various PAC/TEELs[99] to establish acute human health effects from toxic chemicals. Toxicity is defined as the degree to which a chemical substance or a particular mixture of substances can damage an organism. DSAs only require the assessment of the acute effects of toxic chemicals. Therefore, chronic chemical exposure effects are only briefly addressed in Section 9.4.5.

9.4.1 CHEMICAL CONCENTRATIONS AND EXPOSURE TIME

9.4.1.1 CHEMICAL EXPOSURE TIME

Chemical exposure concentrations may be expressed in either units of mg/m^3 or parts per million volume (ppmV). The latter represents a volume ratio of parts of toxic chemical per million parts of clean air, while mg/m^3 units are commonly used for aerosol (i.e., particulates or droplets of non-volatile liquid) release evaluations. For releases involving gases or vapors from volatile liquids, units of mg/m^3 can be used but ppmV units are more commonly used. Equation 9-1, which is based on the equation of state of an ideal gas, can be used to convert concentrations in units of mg/m^3 to units of ppmV, assuming a standard pressure of one atmosphere (101,325 N/m^2) and an ambient temperature of 25°C; the latter recommended in 40 CFR § 68.22.

$$\boldsymbol{C[ppm] = C\left[mg/m^3(air)\right] \times 10^6\left[m^3(air)/10^6 m^3(air)\right] \times \left\{\frac{R \times T}{MW \times P \times 1000}\right\}\left[m^3/mg\right]} \quad \textbf{Equation 9-1}$$

Where,

10^6 = ppmV conversion factor [units of m^3(air)/10^6·m^3(air)]

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[99] PAC/TEEL values for emergency planning for chemical release events are based on the following exposure limits, given in terms of airborne concentration, expressed as ppm or mg/m^3:

1. AEGL values published by the EPA.
2. ERPG values produced by AIHA.
3. TEEL values developed by the DOE Subcommittee on Consequence Assessment and Protective Actions (SCAPA).

AEGLs, ERPGs, and TEELs have three common benchmark values for each chemical (i.e., PAC/TEEL-1, -2, and -3). Each successive benchmark is associated with an increasingly severe effect that involves a higher level of exposure. The DOE policy for its facilities and activities established irreversible health effects (the "-2" level) as the protective action criterion benchmark for chemical releases in Table 1 of DOE-STD-3009-2014. ERPGs refer to exposure durations of 1 hour (with shorter periods for some chemicals). While AEGLs are developed for five time periods the PAC database includes the AEGL one-hour value. TEELs have been standardized to one-hour. PAC values are developed to take into account all factors potentially causing a human health affect caused by exposure to the defined chemical. Refer to https://sp.eota.energy.gov/pac/.

R = Universal gas constant [8.314 N·m/gmol·K]

MW = Molecular weight [g/gmol]

P = Standard atmospheric pressure [101,325 N/m^2]

T = Temperature [K]

1000 = Mass conversion factor [units of "mg/g"]

The term enclosed by the large brackets represents the specific volume (reciprocal of density) of the chemical, which is directly proportional to ambient temperature.

Chemical health impacts are based on total exposure, which is a function of both the chemical concentration at the receptor and the exposure time at this concentration. Ten Berge, et al., (1986) developed a technique to account for exposure time on dose, and the ALOHA toolbox code has an algorithm that calculates dose as a function of exposure time using Ten Berge's equations. According to Ten Berge, if the concentration varies during the exposure period, this dose factor may be expressed as $[c(t)]^n dt$], where c(t) is the concentration as a function of time during exposure and n is a chemical-specific dimensionless exponent:

$$[c(t)]^{n}\, dt$$ **Equation 9-2**

Ten Berge presents values of the exponent, n, for 20 specific chemicals. For n=1, the effects are assumed to be a function of dose. The developers of AEGL values, which vary from 10-minute to 8-hour exposure times, used empirical data to evaluate the exponent n.

For toxic chemical aerosols and gases with a density approximately that of air, standard Gaussian atmospheric dispersion may be used to estimate chemical consequences. If the toxic material is released at some average rate over some period of time, the peak concentration at the receptor is obtained directly from the definition of the steady state χ/Q

$$\mathrm{C} = \mathrm{Q}'\left(\frac{\chi}{\mathrm{Q}'}\right)$$ **Equation 9-3**

Where,

C = peak concentration (mg/m^3)
Q' = toxic material release rate (mg/s)
χ/Q = relative concentration (s/m^3)

> Note that in plume dispersion modeling, χ represents the concentration in the atmosphere, while for determining health effects, C denotes concentration of the chemical species.

Equation 9-3 represents a single, steady-state concentration that can be compared to the PAC/TEEL values presented in Section 9.4.1.2. In some cases, the release rate may be temporally variant, and needs to be evaluated as changing over time throughout the duration of the accident. This will result in concentrations at the receptor changing over time, creating a need to modify the time-varying concentration into a single value so it can be compared to the PAC/TEEL values. This can be accomplished using the time weighted average (TWA) concept. The toxicity characteristics of the toxic chemical and duration of the plume exposure both factor into the time basis for the TWA as discussed in Section A.2 of DOE-STD-3009-2014. The plume exposure duration is generally assumed to be the same as the release duration of the source term.

Some consequence assessment dispersion codes will calculate the desired maximum 15-minute average concentration directly by allowing the analyst to specify the averaging period. To determine the average concentration manually, the following equation may be used:

$$\mathrm{TWA} = \frac{C_1T_1+C_2T_2+\cdots+C_nT_n}{T_1+T_2+\cdots+T_n} \qquad \textbf{Equation 9-4}$$

Where:

C = Concentration (ppmV or mg/m^3)
T = Time period of exposure (min)
n = Number of time segments

For short-duration releases (e.g., less than 15 minutes), the concentration at the receptor may be calculated as the TWA over the release period, but for no less than 1 minute. Since concentration varies with time due to the time-dependent release rate (Q') and long-wave atmospheric turbulence (i.e., plume meander), concentrations based on one-minute segments do not credit plume-meander; consistent with the concept of determining a peak TWA that is not smeared by time averaging effects.

For release durations longer than 15 minutes, the peak 15-minute average concentration during the duration of the release is used. For the peak 15-minute TWA, the 15-minute period of maximum exposure (concentration) is selected and input as 15, one-minute segments, into Equation 9-4. For exposure periods of less than 15 minutes, the product of C_xT_x may equal zero during the exposure period. Individual time intervals less than one minute are not appropriate for use in the numerator of the above formula for calculating the TWA. This assumption is conservative for “instantaneous” types of releases (e.g., container puncture of powders, over-pressurization of container). However, the use of a shorter averaging duration than 15 minutes, such as the actual exposure period but not less than one minute, may be warranted depending on the acute toxicity of the chemical of interest and the peak concentration observed.

If sufficient physiochemical information is available, the release rate of a toxic chemical can be directly calculated based on the phenomenology of the release and the properties of the chemical. For example, the rate of evaporation from a pool of a spilled chemical may be directly estimated, as discussed in Sections 9.5.4, 9.8.2, 9.9.3 and 9.9.4 of this handbook.

9.4.1.2 PROTECTIVE ACTION CRITERIA FOR RELEASES OF A SINGLE CHEMICAL

Section A.2 of DOE-STD-3009-2014 establishes the need for chemical PACs. Exposure to an air concentration greater than the toxic chemical PAC/TEEL criteria for safety SS control selection is assumed to confer a certain health detriment to the exposed individual. Although a duration of exposure is implicit in the PAC/TEEL definitions, shorter exposures to higher concentrations of some chemicals can have comparable effects. Accordingly, averaging the concentration from a short-duration release over 30 or 60 minutes may significantly under-predict the hazard. On the other hand, averaging over a very short time (e.g., a minute or two) represents the peak concentration more conservatively; however, the validity of any comparison between the calculated “peak” concentration PAC/TEEL value is questionable. It is therefore useful to calculate a TWA concentration at the receptor location for some period less than that implied by the PAC/TEEL definition but long enough that the results can be viewed as having relevance to the criteria.

To address both concerns, TWA concentration at the receptor location is usually calculated for some period less than that implied by the PAC/TEEL definition, but long enough that the results can be accepted as having some relevance to the criteria. For example, EPA-550-B-99-009 which specifies ERPG-2 values (one of the human health criteria for establishing the PAC/TEEL-2) as primary toxic endpoints for their evaluation, assumes a 10-minute release averaging time in its determination of distance to the endpoint for worst-case analyses of toxic chemicals even though the ERPG-2 values are based on 60 minutes.

The DOE PAC/TEEL concentrations are based on different durations as defined by their concentration limit definitions from EPA or the chemical industry. To standardize releases from gases, liquids, and particulates, the hazard evaluation and/or accident analysis may assume a peak 15-minute, TWA chemical concentration for comparison to the PAC/TEEL values for SS control designation. There is no adjustment of the PAC/TEEL value or the calculated concentration to account for differences between the recommended 15-minute exposure time and the exposure time implicit in the definition of the PAC/TEELs.

9.4.1.3 PROTECTIVE ACTION CRITERIA FOR RELEASES OF MULTIPLE CHEMICALS

For chemical mixtures and concurrent releases of different substances, consequences are assessed using the (CMM) “Hazard Index” approach recommended by the DOE Office of Emergency Management, SCAPA Chemical Mixtures Working Group.[100] A brief explanation of this approach and the published journal article are available on the SCAPA website, https://sp.eota.energy.gov/EM/SitePages/SCAPA-CMM.aspx, under Health Code Numbers. The link also provides access to the CMM Wizard that automates the implementation of the approach for up to 30 chemicals. Although not in the Central Registry toolbox, this capability has undergone a rigorous SQA process. Even so, the analyst should check that this modeling tool is acceptable for use on a particular project by checking the approved software list for that project, or determine what site-specific QA requirements may apply.

Concurrent releases should be analyzed if a plausible scenario exists by which quantities of different substances could be released from the same location at the same time. Concurrent releases of dissimilar substances that, because of separation by distance or physical barriers, could result only from catastrophic events (such as major fires, aircraft crashes, severe NPHs) should be analyzed in accordance with the guidance for DBA scenarios. Concurrent releases of dissimilar substances caused by extreme malevolent acts need not be analyzed.

9.4.2 MODES OF EXPOSURE AND ROUTES OF ENTRY OF TOXIC CHEMICALS THAT RESULT IN HEALTH EFFECTS

Acute health effects from short-term exposures to toxic chemicals differ with respect to mode of exposure or route of entry into the human body. Since the inhalation pathway is also considered the most impactful for toxic chemical exposures, most toxic chemical consequence assessments focus on inhalation exposures. Other chemical exposure pathways (e.g., skin absorption) generally result in less severe health effects than the inhalation pathway. Accordingly, for aerosol-type releases, an inhalation only analysis should be adequate using conservative parameters; thus precluding any unnecessary analyses of alternate

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[100] SCAPA: DOE Subcommittee on Consequence Assessment and Protective Actions. SCAPA has several working groups, which include the Chemical Exposures Working Group that developed the PAC/TEELs, and the Chemical Mixtures Working Group that developed the CMM.

pathway exposure. Impacts from chemical ingestion are generally chronic in nature and can be prevented by water and food interdiction management measures or mitigated by chelation processes.

DOE-HDBK-1046-2016, *Temporary Emergency Exposure Limits for Chemicals: Method and Practice,* provides an excellent discussion on all modes of exposure and routes of entry and also discusses each pathway inclusive of inhalation, skin absorption, inter-peritoneal, and ingestion, associated with acute effects of chemicals on human health. These form the toxicological basis for the PAC/TEELs. This Handbook also provides an excellent discussion on which organs are targeted by specific chemicals from the Health Indices and Health Code Numbers of the CMM. The CMM can be used if the analysis involves the release of up to 30 different chemicals.

9.4.3 TOXIC CHEMICAL ACUTE EXPOSURE LIMITS

There are three types of PACs available to the analyst:

(1) AEGLs for five different exposure periods developed by EPA for about 300 specific chemicals;
(2) ERPGs for about 150 chemicals for an approximate one-hour exposure period developed by the AIHA; and
(3) PAC/TEELs developed by the DOE Office of Emergency Response and Policy Implementation (DOE/NA-41) for 3386 specific chemicals.

The following briefly discusses each of these toxic chemical human health criteria.

9.4.3.1 EPA ACUTE EXPOSURE GUIDELINE LEVELS

EPA’s Office of Prevention, Pesticides and Toxic Substances established the National Advisory Committee for Acute Exposure Guideline Levels (NAC/AEGL) for hazardous substances to develop AEGLs. They are intended to assist Federal and State Agencies and private sector organizations with their needs for short-term hazardous chemical exposure information.

Final and interim AEGLs for about 300 chemicals have been published by EPA and are essentially comparable to ERPGs. Unlike ERPGs, AEGLs are calculated for five relatively short exposure periods (10 minutes, 30 minutes, one hour, four hours, and eight hours) dictated by the severity of the toxic effects caused by the exposure, with all levels based above which it is predicted that the general population could experience, including susceptible individuals. The levels are based on the following health effects resulting from exposure to a chemical substance:

- AEGL-1: Notable discomfort, irritation, or certain asymptomatic non-sensory effects. However, the effects are not disabling and are transient and reversible upon cessation of exposure.
- AEGL-2: Irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.
- AEGL-3: Life-threatening health effects or death.

The principle advantage of AEGLs is that they have been established for eight exposure times ranging from 10 minutes to 8 hours. AEGLs have a high technical pedigree, since the AEGL process involves an exhaustive search for data, careful analysis, thorough documentation, and expert review. The disadvantage is that they are available for only a limited number of chemical substances. It should be noted that only the one-hour AEGL is used in accident analysis.

9.4.3.2 AIHA EMERGENCY RESPONSE PLANNING GUIDELINES

The AIHA began developing ERPGs for use in evaluating the health effects of accidental chemical releases on the general public. These ERPGs are developed and published annually through a rigorous peer review process conducted by the AIHA Emergency Response Planning (ERP) Committee. The ERPG development process results in high-quality community exposure limits that are recognized and used both nationally and internationally.

For specific chemicals, ERPGs are estimates of concentration ranges above which acute exposure would be expected to lead to adverse effects.

- ERPG-1: The maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 hour without experiencing other than mild transient adverse health effects or perceiving a clearly defined objectionable odor.
- ERPG-2: The maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 hour without experiencing or developing irreversible or other serious health effects or symptoms that could impair their abilities to take protective action.
- ERPG-3: The maximum airborne concentration below which it is believed that nearly all individuals could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.

9.4.3.3 DOE PAC/TEELS

Many of the toxic chemicals of interest at DOE/NNSA sites lack ERPGs and AEGLs. In response to this need, the DOE Office of Emergency Response and Policy Implementation developed a TEEL methodology in 1992 to provide interim guidance for chemicals of interest. TEELs estimate the concentrations at which most people will begin to experience health effects if they are exposed to a hazardous airborne chemical for a given duration. TEELs are used for emergency management in similar situations as the one-hour AEGLs and one-hour ERPGs.

TEEL-1, TEEL-2, and TEEL-3 have similar definitions as the equivalent ERPGs and one-hour AEGLs. A chemical may have up to three TEEL values, each of which corresponds to a specific tier of health effects. The three TEEL tiers are defined as follows (PAC, 2016):

- TEEL-1 is the airborne concentration (expressed as ppm or mg/m3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience notable discomfort, irritation, or certain asymptomatic, non-sensory effects. However, these effects are not disabling and are transient and reversible upon cessation of exposure.
- TEEL-2 is the airborne concentration (expressed as ppm or mg/m3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience irreversible or other serious, long-lasting, adverse health effects or an impaired ability to escape.
- TEEL-3 is the airborne concentration (expressed as ppm or mg/m3) of a substance above which it is predicted that the general population, including susceptible individuals, when exposed for more than one hour, could experience life-threatening adverse health effects or death.

The methodology for assigning TEELs was originally based on hierarchies of commonly available published and documented concentration-limit parameters, particularly occupational exposure limits, later expanded to include other published concentration limits and then further expanded to include the use of published toxicity parameters. The current TEEL hierarchy, taken from Table 3.1 of DOE-HDBK-1046-2016 and presented in Table 9-2 is based on 9 concentration exposure indicators and 6 toxicity indicators from 11 technical sources. DOE-HDBK-1046-2016 not only documents the process of how the PAC/TEELs were developed, but provides insights as to how the analyst should apply them to chemical consequence assessments.

Table 9-2. TEEL Data Selection Hierarchy.

TEEL-i	TEEL Data	Data Source
TEEL-3	EEGL (30-min)	NRC
	IDLH (1990 values)	NIOSH
	Other	Various
	LC50	HSDB/SAX/RTECS
	LCLO	HSDB/SAX/RTECS
	LD50	HSDB/SAX/RTECS
	LDLO	HSDB/SAX/RTECS
TEEL-2	EEGL (60-min)	NRC
	LOC	EPA
	TLV-C	ACGIH
	WEEL-C	AIHA
	PEL-C	OSHA
	REL-C	CDC
	MAK-C	GRF
	Other	Various
	TCLO	HSDB/SAX/RTECS
	TDLO	HSDB/SAX/RTECS
TEEL-1	TLV-STEL	ACGIH
	WEEL-STEL	AIHA
	PEL-STEL	OSHA
	REL-STEL	CDC
	MAK-STEL	GRF
	Other	Various

TEEL-i	TEEL Data	Data Source

TEEL Concentration Exposure Indicators

C – Ceiling Limit
EEGL - Emergency Exposure Guidance Level
IDLH – Immediately Dangerous to Life and Health
LOC – Level of Concern
MAK – Maximale Arbeitsplatz-Konzentration
PEL – Permissible Exposure Level
REL – Recommended Exposure Level
STEL – Short-Term Exposure Limit
TLV – Threshold Limit Value
WEEL - Workplace Environmental Exposure Limit

TEEL Toxicity Indicators

LC_{50} - Lethal Concentration that kills 50% of population
LC_{LO} – Lowest reported lethal concentration
LD_{50} - Lethal Dose that kills 50% of population
LD_{LO} – Lowest reported lethal dose
TC_{LO} – Toxic Concentration Lowest
TD_{LO} – Toxic Dose Lowest

TEEL Data Sources

ACGIH – American Conference of Government Industrial Hygienists
AIHA – American Industrial Hygiene Association
CDC – Centers for Disease Control and Prevention
EPA – Environmental Protection Agency
GRF – German Research Foundation
HSDB – Hazardous Substances Data Bank
NIOSH – National Institute for Occupational Safety and Health
NRC – Nuclear Regulatory Commission
OSHA – Occupational Safety and Health Administration
RTECS – Registry of Toxic Effects of Chemical Substances
SAX – Dangerous Properties of Industrial Materials

As can be seen from ubiquity of Table 9-2, the PAC/TEELs represent the current most comprehensive compendium of acute exposure guidelines. Revision 29 (PAC, 2016), issued in May 2016 can be accessed at http://sp.eota.energy.gov/pac. ERPG values for various substances are revised annually by the AIHA ERP Committee. The newly published ERPG values for a particular chemical will replace its PAC/TEEL values. EPA is no longer developing AEGLs. If EPA resumes its AEGL development effort, when an AEGL value for a particular chemical is newly published, it will replace ERPG or TEEL values. Accordingly, the PAC/TEEL database will be periodically updated and presented in a subsequent revision which can be accessed in the aforementioned link. Safety analysts are encouraged to consult that link prior to completing their chemical consequence analyses to ensure that they use the latest PAC/TEEL values.

For chemicals that are not toxic, but can act as simple asphyxiants at high concentrations that reduce ambient oxygen to levels where human health can be compromised, the PAC/TEELs for that chemical establishes concentrations that will result in various levels of human health insult and incapacitation:

- PAC/TEEL-1 represents a concentration where oxygen levels are reduced to 19.5%; the OSHA limit for respiratory protection.
- PAC/TEEL-2 represents a concentration where oxygen levels are reduced to 16%. At this level, a threshold is reached for the onset of impaired coordination, perception, and judgment; sufficient to compromise a person's ability of self-protection and escape.
- PAC/TEEL-3 represents a concentration where oxygen levels are reduced to 12.5%, the threshold for causing very poor judgment and coordination, followed by unconsciousness and death.

Elemental uranium and its compounds are radiological hazards that are evaluated for radiological consequences using the techniques in Section 6. However, elemental uranium and its compounds also pose a significant toxicological risk to the MOI, CW, facility worker and the public and accordingly, its chemical consequences are also evaluated. In some cases, uranium toxicological risks exceed its radiological risks. Table 9-3 presents the Revision 29 PAC/TEELs for uranium and its compounds that are the health endpoints an analyst should be informed of when performing a uranium toxic chemical consequence assessment.

Table 9-3. Uranium Compound PAC/TEELs.

Chemical	CASRN#	PACs (mg/m^3)		
		PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
Sodium uranium oxide monohydrate; (Sodium urinate (VI) monohydrate)	10135-92-9	0.82	6.8	41
Uranium	7440-61-1	0.6	5	30
Uranium hexafluoride; (Uranium fluoride)	7783-81-5	3.6	9.6	36
Uranium hydride; (Uranium (III) hydride)	13598-56-6	0.61	5	30
Uranium oxide; (Triuranium octaoxide)	1344-59-8	0.71	10	50
Uranium telluride	12138-37-3	1.2	10	62
Uranium telluride (U3Te4)	12138-37-3a	1	8.5	51
Uranium trioxide	1344-58-7	0.045	0.5	3
Uranium dioxide; (Uranium(IV) oxide)	1344-57-6	0.68	10	30
Uranyl acetate; (Uranium oxyacetate)	541-09-3	0.98	5.5	33
Uranyl fluoride; (Uranium oxyfluoride)	13536-84-0	0.78	4.3	26

Chemical	CASRN#	PACs (mg/m^3)		
		PAC/TEEL-1	PAC/TEEL-2	PAC/TEEL-3
Uranyl nitrate (solid); (Bis(nitrato-O,O') dioxouranium)	10102-06-4	0.99	5.5	33
Uranyl nitrate (yellow salt)	36478-76-9	0.99	5.5	33
Uranyl nitrate hexahydrate	13520-83-7	1.3	7	42

9.4.4 CHEMICAL MIXTURE METHODOLOGY

Effects from exposure to multiple chemicals can be addressed by using the CMM, also developed by the DOE Office of Emergency Response and Policy Implementation. The CMM approach determines whether effects of multiple chemicals are synergistic or antagonistic on various target organs.

The CMM provides recommended default emergency exposure guidelines for mixtures of chemicals. The CMM makes extensive use of HCNs to examine the additive impact that each chemical component in a chemical mixture may have on specific target organs. The CMM is a more realistic predictor of potential human health impacts than can be obtained using the:

(1) Non-conservative method of separately analyzing the consequences of each chemical component; or
(2) Overly-conservative method of adding the exposures from each chemical together regardless of the human organ targeted by the chemical.

The CMM is recommended for potential use in emergency planning hazards assessments, DSAs, and in emergency response circumstances. The CMM and its workbook can be downloaded from https://sp.eota.energy.gov/EM/SitePages/SCAPA-CMM.aspx .

The CMM approach that involves adding all exposures from each chemical, regardless of the target-organ effects of the chemicals, tends to overestimate impacts and therefore be over-conservative. The health impacts from chemicals that target different organs are often not simply additive to all target organs.

When using the CMM, a hazard index (HI) is calculated for each component of a chemical mixture at the chosen receptor point. The "HI_i" is the concentration of chemical "i" ($Conc_i$) divided by the concentration limit for chemical "i" ($Limit_i$), as shown in Equation 9-5:

$$HI_i = Conc_i/Limit_i$$ **Equation 9-5**

A $HI_i < 1$ means that the limit for that single chemical "i" has not been exceeded. However, if the hazard indices for all chemicals in a mixture are summed, and the cumulative HI is greater than one, then an unacceptable condition may exist and mitigating strategies may need to be considered. Unless the health effects of the components are known to be independent, the toxic consequences of all components should, as an initial step in an assessment, be considered to be additive. This represents the most conservative upper-bound approach for assessing exposures to mixtures. If this upper-bound approach produces unacceptable results, the next step is to classify the chemicals in the mixture according to their toxic consequences. The toxicological classification of specific chemicals can be accomplished using the HCNs established for each chemical.

HCNs are used in the CMM to identify the target-organ effects of each chemical in the mixture. Any chemicals that targets the same or similar organs or operates by the same acute or chronic mode of toxicity should be considered additive to that target organ or by that same mode of toxicity. Target-organ effects and modes of toxicity are considered simply as target organ effects.

HCNs are similar to medical diagnostic codes in that they are code numbers that identify a particular target organ or health effect to enable classification of chemicals by target organ toxicity. Summation of HIs for all chemicals in a mixture having the same toxic consequences (same or similar HCNs) enables determination of the acceptability or unacceptability of exposure to any specific mixture of chemicals using this more realistic approach.

HCNs also offer a convenient way of performing this exposure addition by numerically “binning” identical or similar target organ effects. All of the individual exposure HIs that are binned into the same or similar HCN bin are added together to yield an “HI sum” for that target organ bin. Any of the individual HI sums that exceed a value of 1.0 indicate that the exposure limit has been exceeded and that some kind of mitigating action should be taken to reduce the exposure to that specific target organ below the applicable limit.

The latest version of the CMM Workbook, which can process up to 30 chemicals in a given mixture, is in CMM Revision 29.

9.4.5 CHRONIC HEALTH EFFECTS OF TOXIC CHEMICALS ON THE HUMAN BODY: CARCINOGENICITY, MUTAGENICITY, AND TERATOGENICITY

Although DOE has a few large inventories of carcinogenic chemicals, DOE DSAs do not evaluate carcinogenic effects but focus on documenting consequences of chemicals with acute exposure effects. The evaluation of cancer effects from chemical releases is not required by DOE-STD-3009-2014 or DOE-STD-1189-2016. The DOE Safety Goal related to LCFs for radiological releases is with respect to 50-mile radius population doses and not to the facility worker, CW, or MOI. There is no analogous DOE Safety Goal associated with carcinogenic chemicals. The following provides some information on where to obtain chronic chemical health effect information should there be a need for a qualitative evaluation.

Dose-response curves for non-carcinogenic chemicals are characterized by the existence of threshold exposure levels below which no toxic effects will be observed. Due to a fundamental difference in the mechanism of action, the dose-response curves for carcinogens are considered as LNT representations.

Known or suspected human carcinogens are identified in the EPA data bases Integrated Risk Information System and Health Effects Assessment Summary Tables, the National Institute for Occupational Safety and Health Pocket Guide to Chemical Hazards, and International Agency for Cancer Research publications.

Per 1986 EPA guidance, confirmed or suspected human carcinogens are treated differently from those compounds eliciting only acute toxic effects. Incremental cancer risk (ICR) can be calculated using the

Integrated Risk Information System database values for the chemical-specific slope factor.

9.5 TOXIC CHEMICAL RELEASE PHENOMENOLOGY AND SUBSEQUENT ATMOSPHERIC TRANSPORT AND DIFFUSION

Unlike radiological releases, which are generally assumed to be continuous and of the same magnitude throughout the accident sequence, there are a large number of variables that need to be accounted for to characterize toxic chemical releases and their effects on the facility worker, CW, and the MOI. Although most chemical releases are associated with complex phenomenology, some of them are continuous steady-state and thus chemical health effects can be determined by simple atmospheric dispersion models. It should be noted that radiological releases can also be subjected to the same phenomenology, but in practice, analysts do not commonly take this into consideration. Phenomenological releases, as described in Chapter 5, and special atmospheric transport and diffusion considerations that are specific to the release of toxic chemicals include, but are not limited to:

- Temperature, pressure, and state of the chemical in its storage container;
- Type of storage container (tank, vessel, pipe);
- Density, temperature and quantity of the substance released that determines whether it will disperse as a positively-buoyant gas, neutrally-buoyant gas, or a dense/heavy gas;
- Phenomenology of release (e.g., guillotine pipe break, small hole);
- Speed of chemical leaving its container through an orifice relative to the speed of the sound (choked flow versus non-choked flow);
- Energy associated with the release, such as thermal energy of a fire;
- Chemical transformations resulting from the effects of fire or reaction with water vapor in the atmosphere (e.g., uranium hexafluoride release into a humid atmosphere); and
- Synergistic and antagonistic effects of a multiple chemical release and the cumulative effects on target organs (see Section 7.4.4).

The following subsections present a discussion on toxic chemical release phenomenology.

9.5.1 PRESSURIZED LIQUIDS: TWO-PHASE FLOW TOXIC CHEMICAL RELEASE

Pressurized liquid releases are the most complex of non-energetic single chemical releases, as two-phase flow needs to be accounted for. The initial portion of the liquid release flashes to a gas, due to its rapid depressurization at the point that it encounters the atmosphere. The flashed portion of this type of release is usually of short duration (a puff) which requires a three-dimensional Gaussian puff model to determine its fate and transport.

The remaining chemical that does not flash forms a liquid puddle, or gaseous area source for a sublimating chemical (e.g., carbon dioxide). The liquid puddle evaporates as a non-pressurized sub-cooled liquid release behind the puff requiring a conventional two-dimensional Gaussian code similar to what would be used on a liquid release that evaporates. This evaluation may also need to be performed in an iterative manner since the source term varies with time.

Pressurized liquid releases from a tank through a pipe adds one additional level of complexity as the rapid depressurization of the chemical when it reaches the atmosphere at the point of the pipe break causes a choked flow condition, discussed in Section 9.5.2, upstream of the pipe. Thus, the flashing of the liquid occurs inside the pipe before discharge, and this choked flow limits the mass release rate. Analysis of this phenomenology is a highly complex time-dependent process as the fluid near the discharge experiences a pressure drop and flashes, while the fluid upstream does not sense the break and stays in liquid form. Therefore, an oblique pressure wave travels upstream resulting in a greater fraction of the liquid flashing inside the pipe. For this type of chemical release, the vapor mass fraction needs to be calculated in an iterative manner to determine the time-varying chemical source term. Therefore, the analyst accounts for the phenomenology of pressurized liquid releases using techniques such as those in Section 9.5.1.1.

The Hazard Prediction and Assessment Capability (HPAC) ITRANS source term module provides a comprehensive methodology to establish chemical release quantities; especially for pressurized liquid chemical releases. HPAC has dense gas modeling capabilities, and a sub-code, Second-Order Closure Integrated PUFF (SCIPUFF) (Sykes, 1998), that can also address positively-buoyant gases quantifying its liftoff after release.

The following subsections provide the analyst with some of the complex equations associated with pressurized liquid releases to calculate the flashing fraction and aerosol formation, and for two-phase release of chlorine from a pipe.

9.5.1.1 FLASHING FRACTION AND AEROSOL FORMATION

Section 9.5.1 discusses the complex phenomenology associated with the release of pressurized liquids to the atmosphere. The initial portion of the liquid release flashes to a gas, due to its rapid depressurization at the point that it encounters the atmosphere. The flashing fraction may be calculated by means of a heat balance across the outlet orifice where the decrease in latent heat of vaporization and increase in heat capacity are accounted for as the initial temperature approaches the critical temperature. This fraction is expressed as shown in Equation 9-6.

$$\boldsymbol{f = 1 - exp^{-2.63}\frac{C_l(T_b)}{L(T_b)}(T_c - T_b)\left\{1 - \left[\frac{(T_c - T_l)}{(T_c - T_b)}\right]^{0.38}\right\}}$$ **Equation 9-6**

Where,

f = flashing fraction (dimensionless);

$C_l(T)$ = liquid heat capacity at temperature T (J/kg °K);

$L(T)$ = latent heat of vaporization at temperature T (J/kg);

T_c = critical temperature (°K);

T_b = liquid boiling temperature at one atmosphere pressure (°K); and,

T_l = liquid temperature (°K).

Generally, a superheated liquid jet or spray needs to be present to achieve significant quantities of liquid droplets suspended in the initial cloud. As the discharge pressure decreases, some of the liquid will flash immediately to vapor, while the remaining non-flashed liquid will either be suspended as liquid droplets (i.e., finely distributed aerosols), or fall to the ground forming a pool that will boil or evaporate over time.

The distribution of droplet sizes is required before the rainout fraction can be calculated. Kitamura et al., 1986 and Bettis et al., 1987 have experimentally observed that the droplet sizes are log-normally distributed, as shown in Equation 9-7.

$$\boldsymbol{p(d) = \frac{exp^{1/2}\sqrt{[ln(d)-ln(<d>)]/ln(\sigma_g)}}{\sqrt{2\pi\, ln(\sigma_g) d}}}$$ **Equation 9-7**

Where,

d = random droplet diameter (m);

p(d) = probability distribution as a function of drop diameter d (dimensionless);

σ_g = geometric variance (dimensionless) (assume σ_g=1.3; Iannello et al., 1989); and,

<d> = mean droplet diameter (m).

The mean droplet diameter may be estimated by means of the Nukiyama-Tanasawa equation (see Tilton and Farley, 1990), as shown in Equation 9-8.

$$\boldsymbol{< d > 585 \frac{\sqrt{\sigma_l}}{u_e\sqrt{\rho_l}}}$$ **Equation 9-8**

Where,

σ_l = liquid surface tension (dyne/cm);

ρ_l = droplet liquid density (kg/m^3); and,

u_e = axial spray velocity at end of discharge region (m/s),

where the droplet diameter is μm units. Using the values for each of the salient parameters germane to anhydrous chlorine yields, a droplet diameter distribution is obtained.

Since an instantaneous release directly into the ambient wind field is postulated for this analysis, the axial spray velocity is assumed identical to the ambient wind speed. The criterion for droplet rainout is satisfied when the inclination of the droplet trajectory, β_d, with respect to the vertical direction is greater than the half angle of jet expansion at the start of entrainment. The subsequent droplet settling velocity (V_d) may be calculated by solving the balance equation expressing the equality between the force of gravity on the droplet and the upward-acting viscous and drag forces, as depicted in Equation 9-9.

$$\boldsymbol{\frac{\pi}{6} d^3 (\rho_l - \rho_g) g = C_d\, \rho_g \frac{V_d^2}{2} \left(\frac{\pi}{4} d^2\right)}$$ **Equation 9-9**

With,

$\boldsymbol{\rho_g}$ = vapor density after expansion (kg/m^3); and,

$\boldsymbol{C_d}$ = friction factor including both viscous and drag losses (dimensionless).

Where, Equations 9-10 and 9-11 show:

$$C_d = \frac{24}{Re_d} + \frac{6}{1+\sqrt{Re_d}} + 0.4$$

Equation 9-10

$$Re_d = \frac{\rho_g V_d d}{\mu_g}$$

Equation 9-11

Where, μ_g denotes the viscosity of vapor in units of Pa·s.

Therefore, the final expression, which V_d satisfies, is given by Equation 9-12:

$$3V_d\left[\frac{24\mu_g}{\rho_g V_d d} + \frac{6}{1+\sqrt{\frac{\rho_g V_d d}{\mu_g}}} + 0.4\right] - 4d(\rho_d - \rho_g)g = 0$$

Equation 9-12

The critical droplet diameter (d_c) satisfies the criterion in Equation 9-13:

$$\tan\beta_{d_c} = \frac{V_{d_c}}{U_e} = \tan\beta_e$$

Equation 9-13

Any droplet trajectory possessing an angle of inclination, β_d, with respect to the horizontal that is greater than the spray half-angle, β_e, will drop out of the vapor-aerosol plume and rainout onto the ground surface to form a pool. Observing that as V_d increases, tan β_d also increases for $u_e>0$ fixed, and the solution is therefore unique and given by Equations 9-14 and 9-15:

$$V_{d_c} = U_e \tan\beta_e$$

Equation 9-14

$$f'(d_c) = 3V_{d_c}\left[-\frac{24\,\mu_g}{\rho_g V_{d_c} d_c^2} + \frac{3\sqrt{\rho_g V_{d_c}}}{\sqrt{\mu_g d_c}\left(1+\sqrt{\frac{\rho_g V_{d_c} d_c}{\mu_g}}\right)^2}\right] - 4(\rho_d - \rho_g) - g$$

Equation 9-15

Finally, the solution to d_c may be obtained using Newton's method by way of the two functional relationships in Equation 9-16:

$$f(d_c) = 3V_{d_c}\left[-\frac{24\,\mu_g}{\rho_g V_{d_c} d_c} + \frac{6}{1+\sqrt{\frac{\rho_g V_{d_c} d_c}{\mu_g}}} + 0.4\right] - 4d_c(\rho_d - \rho_g)g = 0$$

Equation 9-16

Using a model for a spherical droplet in laminar flow, which is not to be confused with turbulent jet flow during droplet formation, a critical drop diameter, d_c, can be calculated.

Droplets possessing a diameter exceeding this value experience a sufficiently large gravitational force to induce the beginning of rainout. Using a value of β_e=9.1° (Wheatley, 1987), the critical drop diameter has been determined to be 25 microns. The fraction of liquid that rains out, f, is then calculated implicitly from Equations 9-17 and 9-18.

$$f_p = 1 - \int_{-\infty}^{d_c} \rho\,(\xi) d\xi = \frac{1}{2}[1 - erf(X_c/2)]$$ **Equation 9-17**

Where,

$$X_c = \frac{ln(d_c) - ln(< d >)}{ln(\sigma_g)};$$

$$erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-\xi^2}\, d\xi$$

Equation 9-18

In this case, since f_p=0.05, essentially all of the aerosol component remains airborne and evaporates right above the pool as the aerosol particles are transported downwind.

It should be noted that a great deal of uncertainty lies in the estimate of exactly how much of the non-flashed liquid is entrained into the air as a suspended aerosol. Large-scale experiments indicate that the mass of aerosol produced is very roughly equal to the mass of superheated liquid which immediately flashed to vapor when the flashing fraction is less than one-third (Lees, 1996). Since the flashing fraction is below one-third for the chlorine release, the initial aerosol mass is assumed to be equal to the mass of liquid flashed to vapor.

When the release initially results in a dense gas slumping cloud, note that the dispersing medium within the dense gas cloud consists only of the sub-cooled vapor (i.e., vapor evaporated from the pool) component. No clear causal relationship exists between the dense cloud and droplets of liquid raining out of the cloud. Therefore, the model treats these two phenomena separately; specifically the mass fraction of the release which remains suspended as aerosol, and that which falls onto the ground to form a boiling or evaporating pool. A portion of the remaining liquid will either be suspended as liquid droplets or finely distributed aerosol. Any liquid entrained into the vapor cloud as a suspended aerosol is characterized in terms of the liquid mass evaporation rate and temperature as a function of time.

The suspended liquid aerosol droplets evaporate as the ambient air flows past them. The computational model of Papadourakis et al., 1991, is applied to determine the rate at which a droplet of 1000-micron diameter would evaporate in an ambient wind of 5 mph (2.22 m/s) and a temperature of 100°F (37.8°C), using an initial spray velocity of approximately 12 m/sec. A 1,000-micron diameter particle was selected since it represents a 95 percent confidence bound on aerosol particulate size. Only five percent of aerosol droplets formed are expected to have a diameter greater than 1,000 microns for a typical droplet spectrum.

Details of the underlying equations in the model describing the conservation of mass, energy, and momentum are not included in this discussion as they are beyond the scope of this discussion. The final numerical results demonstrate that the entire droplet mass undergoes complete evaporation within 12.25 m of the liquid release point. Therefore, as a conservative and bounding simplifying assumption, the analyst can assume that all-aerosol component evaporates in the near vicinity of the residual liquid pool with no initial dilution and the mass of vapor is then added to the vapor source term.

9.5.1.2 TWO-PHASE RELEASE OF CHLORINE FROM A PIPE

In this specific example, there is conversion of some of the chlorine liquid to vapor within the pipe itself. This change in upstream composition subsequently causes a reduction in the mass release rate and an increase in outflow velocity.

The variation in these release parameters can be calculated from Equation 9-19, which is the Fauske equation found in *Loss Prevention in the Process Industries* (Lees, 1996):

$$G = A_e \left[\frac{-k}{T_1+T_2+T_3}\right]^{1/2}$$ **Equation 9-19**

Where,

$$T_1 = (1 - x + kx)xdv_g/dP$$ **Equation 9-20**

$$T_2 = \left[v_g(1 + 2kx - 2x) + v_l\left(2kx - 2k - 2xk^2 + k^2\right)\right]dx/dP$$ **Equation 9-21**

$$T_3 = k\left[1 + x(k - 2) - x^2(k - 1)\right]dv_1/dP$$ **Equation 9-22**

$$dx/dP = -(dh_f/dP + xdh_{fg}/dP)/h_{fg}$$ **Equation 9-23**

Where,

G = release rate (kg/s);

A_e = effective area of the orifice (m^2);

x = mass fraction of vapor in the mixture (dimensionless);

v_g = specific volume of the gas (m^3/kg);

v_l = specific volume of the liquid (m^3/kg);

k = $(v_g/v_l)^{1/2}$

P = saturation pressure (Pa);

h_f = enthalpy of the saturated liquid (cal/g); and,

h_{fg} = latent heat of vaporization (cal/g).

The equation was evaluated using an Antoine equation (Antoine, 1888) for saturated vapor pressure and ideal gas conditions were assumed. Table 9-4 presents the results, which show the percentage of gas mass fraction. The percentage of liquid mass fraction is defined as 1 - gas mass fraction.

Table 9-4. Calculated Variation of Chlorine Jet Release Parameters as a Function of Upstream Gas Mass Fraction (Mills And Paine, 1990).

Gas Mass Fraction	Mass Release Rate (kg/s)	Release Velocity (m/s)	Initialization Temperature (degrees K)	Density (kg/m^3)	Effective Droplet Diameter (mm)
0.1	81.8	71	239	11.8	0.352
0.2	63.3	101	239	9.2	0.295
0.3	51.8	120	239	7.5	0.270
0.4	43.8	134	239	6.3	0.256
0.5	38.0	144	239	5.5	0.247
0.6	33.6	152	239	4.8	0.241
0.7	30.1	158	239	4.3	0.236
0.8	27.3	163	243	3.9	0.233
0.9	24.9	167	243	3.6	0.231

The table shows that the mass release rate is inversely proportional to the gas mass fraction and the release velocity is proportional to the gas mass fraction. As the fraction of the fluid in the pipe that flashes from liquid to gas at the outlet increases, choked flow upstream in the pipe results, and the resultant mass release rate decreases. This is a very interesting case where pressurized liquid two-phase flow from a pipe also exhibits pressurized gas choked flow characteristics.

The aforementioned equations in Sections 9.5.1.1 and 9.5.1.2 are limited to the assumptions in their derivation and/or the conditions under which they were developed. Prior to employing these equations to determine the phenomenology of a specific system or process, the analyst should demonstrate that the application domain of the equations is not exceeded.

9.5.2 PRESSURIZED GASES: CHOKED FLOW TOXIC CHEMICAL RELEASE

The release of pressurized gases is either under choked flow or non-choked flow depending on the internal pressure and the size of the orifice; both of which affect the speed at which the gas escapes through the orifice.

Pressurized gaseous non-energetic single chemical releases (e.g., hole in a cylinder containing gas stored at several atmospheres pressure) also cannot be addressed by steady-state Gaussian models since the source term is never steady-state; always varying with time. This is the result of the internal pressure decreasing with time as the gas escapes through the orifice and the remaining unreleased gas undergoing Joule-Thompson cooling, which affects its temperature and volume. As the internal pressure decreases with time, the release rate will decrease accordingly.

For highly-pressurized gases that are released through a very small orifice, additional complexities associated with choked flow need to be accounted for. Choked flow occurs when the released gas attempts to exit its storage container at a rate that exceeds the speed the sound, which itself is a function of ambient temperature. Accordingly, a gas cannot travel outside of its containment at a speed greater than the speed of sound, which is a physically limiting factor. Therefore, the analyst needs to account for choked flow until the internal pressure is reduced to a subsonic level, where the flow becomes and remains non-choked. Pressurized gases escaping through an orifice at speeds less than the speed of sound will do so under non-choked flow.

ALOHA Version 5.4.6 incorporates LEAKR algorithms (Belore and Buist 1986) to establish the release rate of gases from orifices, holes and short pipes. It initially determines whether gas flow will be supersonic (choked) or subsonic (unchoked) from the ratio of tank to atmospheric pressure, ratio of hole width to tank length, and critical pressure ratio for sonic flow. Should the pressure difference be large enough, ALOHA models flow as supersonic until the pressure drops to the point at which flow reaches subsonic speeds. From that point onward, ALOHA computes a subsonic release rate tank pressure, which has been reduced to atmospheric pressure. The estimated rate of gas release gets smaller over time since tank or pipe pressure is expected to drop as gas exits and adiabatic expansion from Joule-Thomson cooling, cools the tank contents, further reducing pressure. To account for the phenomenology of pressurized gas releases, use techniques such as those presented in Sections 9.5.2.1 through 9.5.2.5.

The following subsections provide the analyst with some of the complex equations associated with pressurized gas releases to calculate vapor outflow from a pipeline, spherical tank, cylindrical tank, and other type of vessel. Guidance provided by the EPA (EPA-550-B-99-005, Section 8.1.1, Equation 11) offers a method for estimating the maximum emission rate for an unmitigated release of gas from a vessel.). The expression does not account for the decrease in the release rate as the pressure in the tank decreases. A method for determining the time-dependent mass release rate from a pressure vessel is presented in Section 9.5.2.1.

9.5.2.1 TIME-DEPENDENT VESSEL GAS BLOW DOWN MODEL

In the case where the onset of gas release occurs under choked, or sonic, flow conditions, the time-dependent mass release rate is given by

$$\boldsymbol{w(t) = w_o[F(t)]^{(\gamma+1)/(\gamma-1)}} \qquad \textbf{Equation 9-24}$$

Where,

t	time [s];
w	sonic mass release rate [kg/s];

w_o is the initial sonic mass release rate [kg/s] given by

$$\boldsymbol{w_o = C_d A_d \sqrt{\gamma \rho_o P_o [2/(\gamma+1)]^{(\gamma+1)/(\gamma-1)}}} \qquad \textbf{Equation 9-25}$$

C_d	coefficient of discharge [dimensionless];
A_d	outlet (orifice) area [m^2];
g	specific heat ratio [dimensionless];
r$_o$	initial fluid density inside the vessel [kg/m^3];
P_o	initial fluid pressure inside the vessel [Pa].

The time dependent function in the relationship, F(t), is given by Equation 9-26, below:

F(t) = 1/(1+At) **Equation 9-26**

Where,

$$A = w_o(\gamma - 1)/2m_o$$ **Equation 9-27**

and,

m_o represents the initial mass inside the vessel (kg).

Equation 9-26 is valid only for the conditions of choked (sonic) flow, namely when the internal system pressure, P_o, exceeds a physical constant referred to the critical pressure $P_{critical}$ defined as:

$$P_{critical} = P_{ambient}\left(\frac{\gamma+1}{2}\right)^{\gamma/(\gamma+1)}$$ **Equation 9-28**

Where, $P_{ambient}$ is the ambient pressure outside of the vessel.[101]

Although most of the tank inventory will be discharged in sonic flow, it is possible to calculate the time at which the flow becomes subsonic or unchoked. Assuming ideal gas behavior, the initial mass release rate from the vessel under unchoked (sub-sonic/sub-critical) flow conditions when $P_o \leq P_{critical}$ is given by Equation 9-29, taken from *Perry's Chemical Engineers' Handbook (Eighth Edition)* (Green and Perry, 2007):

$$m_r(0) = A_d C_d \left\{2\frac{P_{ambient}^{2/\gamma}}{P_o^{1-2/\gamma}}\rho_v \frac{\gamma}{\gamma+1}\left[1 - \left(\frac{P_{ambient}}{P_o}\right)^{(\gamma-1)/\gamma}\right]\right\}^{1/2}$$ **Equation 9-29**

Where,

$m_r(0)$ = gas mass release rate at time zero [kg/s];
M_w = gas molecular weight [kg/kg·mole]; and,
P_o = gas pressure upstream of the orifice [Pa].

Where, r_v denotes the vapor density [kg/m^3] at standard temperature and pressure. Again, Equation 9-29, just as in the case of w_o appearing in Equation 9-26, is an expression of the maximum mass release rate under their respective release regimes.

Alternatively, the following time-dependent expression for the mass outflow may be used to obtain the average mass release rate:

$$m_r(t) = \frac{A_o C_o P_o}{Z\,R\,T_o}\left[1 + \tau\left(\frac{\gamma-1}{2}\right)\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}}\right]^{2\gamma/(1-\gamma)}$$ **Equation 9-30**

---

[101] $P_{critical}$ should not be confused with the critical pressure, P_c, associated with the critical point on a temperature-volume diagram for a particular substance.

Where,

$$\boldsymbol{\tau = \frac{A_o}{V}(\gamma\, R\, T_o)^{1/2} t}$$ **Equation 9-31**

and,

t = time following the beginning of unchoked flow [s],
Z = compressibility factor [dimensionless];
R = gas constant [8314.39 N/m·kg-mole·K];
T_o = gas temperature upstream of the orifice [K];
V = internal tank volume [m^3].

The *average* vapor release rate, $E\ \{m_r\,(t)\}$ in the time period [0,T] is then computed by evaluating Equation 9-32.

$$\boldsymbol{E\{m_r(t)\} = \frac{1}{T}\int_o^T m_r(t)dt\ = \frac{2\,A_oC_oP_o}{Z\,R(1+\gamma)T_o}\left(\frac{\gamma+1}{2}\right)^{\frac{\gamma+1}{2(\gamma-1)}}\left\{1-\left[1+\right.\right.}$$
$$\boldsymbol{\left.\left.\frac{A_o}{V}(\gamma R\, T_o)^{1/2}\, T\left(\frac{\gamma-1}{2}\right)\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{2(\gamma-1)}}\right]^{2\gamma/(1-\gamma)}\right\}}$$ **Equation 9-32**

The expressions presented above for the vapor mass rate of outflow are applicable only to tanks where the inner diameter is much greater than the diameter of the outlet orifice. If the analysis involves leakage from a length of process pipe, then the model described below should be used to estimate the vapor mass outflow rate.

9.5.2.2 VAPOR OUTFLOW FROM BREACH OF A PIPELINE

$$\boldsymbol{m_r(t) = \frac{m_r(0)}{1+\alpha_P}e^{-\frac{t}{(\alpha_P^2\beta_P)}} + \frac{W_o}{\beta_P}e^{-\frac{t}{\beta_P}}}$$ **Equation 9-33**

The time-varying release rate of gas or vapor from a pipeline rupture is estimated using the following expression (Bell, 1978; Wilson and Angle, 1979):

Where,

$m_r(t)$ = gas mass release rate at time t [kg/sec];
t = time since the pipeline rupture [sec];
W_o = total mass of gas in the pipe length [kg]; and,
b_p = a constant expressed as

$$\boldsymbol{\beta_P = 2(\gamma f)^{1/2}L^{3/2}/3v_oD^{1/2}}$$ **Equation 9-34**

f = pipe friction factor [dimensionless];
D = pipe diameter [m];
L = pipe length [m]; and,
v_o = speed of sound in the pipeline gas [m/s]

$$\boldsymbol{v_o = \left(\gamma RT_f/M_w\right)^{1/2}}$$ **Equation 9-35**

T_f = final temperature of gas release just after leaving the orifice [°K];
a_p = dimensionless parameter given as:

$$\boldsymbol{\alpha_p = W_o/\left[\beta_p m_r(0)\right]}$$ **Equation 9-36**

W_o = total initial mass of gas [kg] given by

$$\boldsymbol{W_o = \pi\, D^2\, P_o\, L\, M_w/(4\, R\, T_o)}$$ **Equation 9-37**

The variable T_f represents the final temperature of the gas as it first accelerates towards the sonic velocity at the orifice, and then decelerates after passing into the atmosphere. If the gas is assumed to exhibit ideal behavior, there will be no Joule-Thompson cooling; hence $T_f = T_o$.

To calculate the *average* vapor release rate, $E\{m_r(t)\}$, in the time period $[0,T]$, use Eq. 9-38 below.

$$\boldsymbol{E\{m_r(t)\} = \frac{1}{T}\int_o^T m_r(t)dt \;=\; \frac{m_r(0)\alpha_p^2\beta_p}{T(1+\alpha_p)}\left(1 - e^{-\frac{T}{(\alpha_p^2\beta_p)}}\right) + \frac{W_o}{T}\left(1 - e^{-\frac{T}{\beta_p}}\right)}$$ **Equation 9-38**

When loss of liquid containment results from a localized breach in a self-contained storage vessel, the mass flow rate of liquid out of the orifice may be computed as a function of the upstream pressure. This time-dependent pressure term, in turn, depends on:

- Vapor partial pressure;
- Hydrostatic head above the leak; and
- Pressure head induced externally by a mechanical device such as a compressor.

Assuming that the system pressure input to the code, P_{sys}, reflects the pressure head from the compressor, the first two pressure terms may be calculated. An upper bound on the release duration may be obtained by neglecting terms (1) and (3), which permits some reasonable values for the time intervals to be established.

9.5.2.3 OUTFLOW FROM A CYLINDRICAL TANK

The time-dependent mass flow rate of an incompressible fluid out of an upright cylindrical tank can be derived. Beginning with the Bernoulli equation expressed in the form:

$$\boldsymbol{\frac{\Delta u_b^2}{2} + g\Delta z + \frac{\Delta p}{\rho} = 0}$$ **Equation 9-39**

Where, in the MKS system, g_c becomes (kg)(m)/(N)(sec^2) or $g_c \equiv 1$, and g denotes the local value for the acceleration of gravity. The variables u_b, z, r, and P represent the fluid bulk speed, fluid free surface elevation above ground level, fluid density, and pressure experienced at the orifice centerline, respectively.

<u>Note:</u> Δz denotes the distance between the fluid free surface level within the tank and the orifice elevation above ground, and by the convention chosen, the D operator represents the difference in going from the interior of the vessel to the outer ambient environment. For the sake of simplicity, it is assumed that internal and external pressure terms remain constant throughout the release duration. Therefore:

$$\Delta u_b = u_{b_{inside}} - u_{b_{outside}}$$
$$\Delta z = z - z_o$$
$$\Delta p = p_{inside} - p_{outside} = p_{system} + p_{vapor} - p_{ambient}$$

Equations 9-40 through 9-42

with the orifice elevation denoted by z_o and the system pressure, saturated vapor pressure, and ambient pressure represented by P_{system}, P_{vapor}, and $P_{ambient}$, respectively.

Further assuming that u_b within the tank as well as all pressure terms are constant with respect to time, Equations 9-40 through 9-42 may be cast into a differential form with respect to time *t*:

$$-u_b \frac{d_{u_b}}{dt} + g\frac{dz}{dt} = 0$$

Equation 9-43

Where, u_b now represents the bulk fluid outflow speed.

$$\frac{dm_o}{dt} = \rho A_o u_b - \frac{du_b}{dt} = \frac{1}{\rho A_o}\frac{d^2 m_o}{dt^2}$$

Equation 9-44

The quantity of greatest interest is the total mass outflow m_o as a function of time. In order to recast the equation as a differential equation in m_o, the first step is to recognize that the mass release rate dm_o/dt may be expressed in terms of the instantaneous flow velocity, as shown in Equation 9-44, with A_o representing the cross-sectional area of the orifice. Once an expression is obtained for dz/dt in terms of differentials of m_o, the equation may be cast into the form of an ordinary differential equation.

Equation 9-45 represents the formula for computing the volume of liquid inventory remaining in the tank at time t:

$$V_l(t) = \frac{\pi D^2 z_l(t)}{4} = \frac{m_l}{\rho} - \frac{dz_l}{dt} = -\frac{4}{\rho\pi D^2}\frac{dm_l}{dt} = \frac{4}{\rho\pi D^2}\frac{dm_o}{dt}$$

Equation 9-45

Where, $V_l(t)$ and $m_l(t)$ represent the volume and mass inventory of liquid remaining inside the tank, respectively, at time *t* while r and D denote the liquid density and diameter of the tank. Substituting this last expression obtains:

$$\frac{1}{\rho A_o^2}\frac{dm_o}{dt}\frac{d^2 m_o}{dt^2} - \frac{4g}{\pi D^2}\frac{dm_o}{dt} = 0$$

Equation 9-46

$$\frac{d^2 m_o}{dt^2} = \frac{-4g\,\rho\,A_o^2}{\pi D^2}$$

Equation 9-47

Final reconfiguration of this equation yields Equation 9-47.

In order to solve the above second order differential equation, two initial conditions are required. One condition is that at time zero, $m_o\,(t{=}0) = 0$. The other condition is derived by solving the Bernoulli equation directly for the special case at time zero since $z\,(t{=}0) = z_i$ representing the initial liquid level above the outlet centerline axis is given, yielding:

$$\left.\frac{dm_o(t)}{dt}\right|_{t=0} = \rho\, A_o \sqrt{2\left[g(z_i - z_o) - \frac{\Delta p}{\rho}\right]} \qquad \textbf{Equation 9-48}$$

Now that the two initial conditions to the second order linear ordinary differential equation are known, the unique solution is given by Equations 9-49 and 9-50.

$$\frac{dm_o(t)}{dt} = -\frac{4g\,\rho\, A_o^2}{\pi D^2}t + \rho\, A_o \sqrt{2\left[g(z_i - z_o) - \frac{\Delta p}{\rho}\right]} \qquad \textbf{Equation 9-49}$$

$$m_o(t) = -\frac{2g\,\rho\, A_o^2}{\pi D^2}t^2 + \rho\, A_o \sqrt{2\left[g(z_i - z_o) - \frac{\Delta p}{\rho}\right]}\,t \qquad \textbf{Equation 9-50}$$

Only times for which $dm_o/dt>0$ are physically relevant, and since dm_o/dt is monotone decreasing we have the duration of the release given by $t=t_{max}$ satisfying

$$\left.\frac{dm_o(t)}{dt}\right|_{t=t_{max}} = 0 \qquad \textbf{Equation 9-51}$$

Solving for t_{max} in the Equation above yields:

$$t_{max} = \frac{\pi D^2}{4\,gA_o}\sqrt{2\left[g(z_i - z_o) - \frac{\Delta p}{\rho}\right]} \qquad \textbf{Equation 9-52}$$

9.5.2.4 OUTFLOW FROM A SPHERICAL TANK

Although a spherical tank is a seemingly benign perturbation away from a simple cylindrical tank, this particular geometry results in a much more complicated expression for the mass flow rate of liquid out of the vessel. The volume of liquid inventory as a function of liquid free surface elevation is given by:

$$V_l(t) = \frac{2}{3}\pi R^3 \int_0^{\alpha} \sin\varphi\, d\varphi + \frac{1}{3}\pi d^2(z - R) = \frac{2}{3}\pi R^2 z + \pi z(2R - z)(z - R) \qquad \textbf{Equation 9-53}$$

Where

$$\alpha = \cos^{-1}(1 - z/R)$$
$$(0 \le \cos^{-1}(x) \le \pi)\forall x \qquad \textbf{Equation 9-54}$$

and *R*, *z*, and *d* represent the tank radius, elevation of the liquid free surface above the bottom of the tank, and one half the chord length of the liquid free surface, or

$$d = \sqrt{R^2 - (R - z)^2} = \sqrt{z(2R - z)} \qquad \textbf{Equation 9-55}$$

The change in liquid level, *z*, can be related to the mass outflow rate using the time derivative of Equation 9-53:

$$\frac{dV_l(t)}{dt} = -\frac{1}{\rho}\frac{dm_o}{dt} = -\pi\left\{3z^2 - 6Rz + \frac{4}{3}R^2\right\}\frac{dz}{dt} \qquad \textbf{Equation 9-56}$$

or equivalently

$$\frac{dz}{dt} = \left[\pi\rho\left(3z^2 - 6Rz + \frac{4}{3}R^2\right)\right]^{-1}\frac{dm_o(t)}{dt} \qquad \textbf{Equation 9-57}$$

Finally, substituting Equation 9-57 and Equation 9-44 into Equation 9-43, yields

$$\frac{1}{\rho\, A_o^2}\frac{d^2m_o}{dt^2} - \frac{g}{\pi\left(3z^2-6Rz+\frac{4}{3}R^2\right)} = 0 \qquad \textbf{Equation 9-58}$$

By noting that the mass of outflow at time t is expressed as m_o=m_{tot} - r$V_l(t)$ where m_{tot} is the total mass of liquid inventory inside the vessel at time t=0 and inspecting the form of the expression for $V_l(t)$ given in Equation 9-53, m_o is a cubic polynomial in the variable z and hence a closed-form analytic solution exists for z as a function of m_o.

Therefore, Equation 9-58 can be recast into an ordinary differential equation in the one dependent variable, m_o. The resulting equation, however, is complicated, highly nonlinear in m_o, and does not lend itself to a solution without the use of rather involved numerical techniques.

An alternate approach is to compute an average flow rate by simply taking the total mass of liquid that can flow out of the vessel and divide by the time t_{max} required for the liquid level to fall from the initial elevation z_i to the elevation of the discharge orifice, z_o. This time is expressed in Equation 9-59.

$$t_{max} = \frac{\pi}{15C_oA_o}\sqrt{\frac{2(z_i-z_o)}{g}}\left(5D\,z_i + 10D\,z_o - 3z_i^2 - 4_{z_iz_o} - 8z_o^2\right) \qquad \textbf{Equation 9-59}$$

See Hart and Sommerfeld (1993) for additional details of this derivation.

The aforementioned equations in Sections 9.5.2.1 through 9.5.2.4 are limited to the assumptions in their derivation and/or the conditions under which they were developed. Prior to employing these equations to determine the phenomenology of a specific system or process, the analyst should demonstrate that the application domain of the equations is not exceeded.

9.5.2.5 OUTFLOW FROM PROCESS VESSELS OF OTHER VARIOUS SHAPES

Equations for the drainage time of vessels for other geometrical shapes are presented in Lee and Sommerfeld (1994). This is a starting point for safety analysts in establishing techniques for this type of problem.

9.5.3 DENSE GAS TOXIC CHEMICAL RELEASE AND DISPERSION

Toxic chemical releases are dense or heavy gas releases when their molecular weight is greater than that of air (28.97 g/mol for dry air), or the gas is cryogenic or very cold. Dense gas releases can potentially also occur with gases that have sufficient aerosol content. However, a gas with a molecular weight greater than that of air and/or exhibiting cryogenic properties does not always result in dense gas behavior. To exhibit dense gas behavior, the dense gas blanket needs to be of a sufficient volume to generate its own turbulence field. Therefore, the determination of whether a released material establishes a dense gas flow pattern requires the knowledge of a key parameter, the calculated Bulk Richardson number, which is a relative measure of the potential energy of the cloud with respect to the mechanical turbulent energy of the atmosphere. The Bulk Richardson number is the critical parameter that provides the benchmark for dense gas behavior. The criterion for dense gas dispersion is that the Bulk Richardson number has to be greater than 50; which is a function of volume, temperature and molecular weight of the gas relative to the gases in the atmosphere.

Initially, a dense gas cloud of material will be undiluted (not mixed with air) and will drop to the ground and flow along the topography downhill or in the direction of the wind, for the most part, although a small part of it may flow uphill or upwind as well, because of gravitational slumping. For this reason, an accurate depiction of the near-field local topography is extremely important to ensure meaningful results from dense gas modeling. Vertical dispersion will be severely restricted for a dense gas, due to gravitational effects, and ambient air will be entrained through the sides of the plume. Thus, the plume shape will take on a pancake-like appearance; further distorted by local topographic anomalies.

Early models of heavy or dense gas dispersion used the Gaussian Line Source model, in which the material was assumed to spread out from a line-source (i.e., formed into a plume), with a Gaussian distribution in the vertical and horizontal directions. The σ_y and σ_z values were assumed the same as given above. These models ignored many important physical phenomena, were generally unsatisfactory, and quickly fell into disuse. More modern models (e.g., DEGADIS, SLAB, HPAC, and HGSYSTEM) took into account phenomena that were not included in the Gaussian Line Source model. These phenomena include:

- Gravitational slumping of the heavy or dense gas and accompanying lateral spreading;
- Stratification of the heavy or dense gas, which tends to dampen turbulence and air entrainment; and
- Heat exchange between the cloud of gas and the ground, which may also cause phase changes.

A more exhaustive discussion of the equations describing the heavy gas model and their use is beyond the scope of this Handbook. Due to the complexity of dense gas dispersion, these codes should not be used as a “black box” without a thorough understanding of the phenomena governing dense gas flows.

The analyst is recommended to use one of the standard computer codes for evaluation of heavy gas dispersion, inclusive of ALOHA Version 5.4.6. The dense gas dispersion calculations used in ALOHA are based on the DEGADIS model (Havens and Spicer 1985, EPA-450/4-89-019). DEGADIS, in turn, is an adaptation of the Shell HEGADIS model described by Colenbrander (Colenbrander 1980, Colenbrander and Puttock 1983). It also incorporates some techniques used by van Ulden (van Ulden 1974, 1983). ALOHA incorporates a decision algorithm to choose between the dense gas and neutrally-buoyant Gaussian models, using the critical Richardson Number as the criterion for distinguishing between passive or non-passive dispersion. The critical Richardson Number is a function of the density of the pollutant, the wind speed, and the release rate. Therefore, the release needs to be of significant magnitude to exhibit dense gas characteristics. As the dense gas plume is dispersed downwind, neutrally-buoyant ambient air begins to mix in, and when the critical Richardson Number decreases to below 50, the plume begins dispersing as a neutrally buoyant gas; that is, entrainment of ambient air as the plume is transported downwind leads to the dense gas plume becoming a neutrally buoyant plume. ALOHA then switches to the neutrally-buoyant Gaussian model. Since the entrainment of air in the sides of the plume generates significant turbulence, dense gas dispersion is actually greater than neutrally buoyant dispersion at 95-percentile meteorological conditions of F stability and 1 meter/second. This is discussed in more detail in the Technical Report NRSD-15-TC01. Section F.8 of this report presented the following conclusions relative to the CW:

1. The ALOHA χ/Q values, considering the building wake effects, are consistent with the default radiological χ/Q value specified in DOE-STD-1189-2008.

2. The aerodynamic effect of buildings on dispersion is approximately an order of magnitude larger, and is much larger than the dry deposition effect;

3. The dispersion from negatively-buoyant, dense gas releases under light wind stable meteorological conditions is greater than neutrally-buoyant releases; and

4. The default χ/Q value is not sensitive to release durations.

Some dense gas models (e.g., HGSYSTEM, HPAC) can be used for area sources (e.g., pools) as well as line source applications.

9.5.4 NON-PRESSURIZED LIQUID RELEASE

Source term determinants from liquid releases (e.g., evaporation rate, aerosolization rate) have been addressed in detail in Chapter 3 and Chapter 5. For non-pressurized, non-energetic liquid chemical releases, it can be reasonably assumed that all aerosols immediately liquefy into a sub-cooled liquid puddle. For cryogenic non-pressurized liquids, dense gas dispersion principles still apply. The non-varying source term is commonly based on an evaporation rate, which is a function of wind speed, ambient temperature, solar insolation and an assumed puddle depth of 1 cm. This puddle depth is used in all chemical transport and diffusion codes that have evaporation algorithms and is considered a reasonable assumption by the technical community. Thus, the puddle surface area determines the amount of chemical available to be evaporated for subsequent atmospheric transport and diffusion, and this release continues until the puddle is totally evaporated.

Controls can be used to reduce the source term from this type of release. Impoundment basins allow the chemical depth to increase, thus reducing the surface area of the puddle and subsequent evaporation rate. Floating balls in such impoundment basins have also been used to further reduce the puddle surface area.

Non-pressurized, non-energetic liquid chemical releases with varying release rates cannot be as easily addressed by conventional Gaussian models since the source term can vary with time as the parameters that control evaporation may vary. However, an iterative technique can be applied through successive time steps to account for varying evaporation rates while keeping the atmospheric conditions that affect transport and diffusion constant.

ALOHA Version 5.4.6 has the capacity to calculate toxic chemical consequences from non-pressurized liquid releases, employing one of two methods for finding the evaporation rate depending upon whether or not the puddle is close to its boiling point. It applies Brighton’s formulation (Brighton 1985) when the average puddle temperature is sufficiently below its boiling point, and an energy balance method when the puddle approaches its boiling point. ALOHA also allows puddles to transition from boiling to non-boiling, or non-boiling to boiling. It constantly compares the evaporation rate calculated with the boiling puddle model with the evaporation rate calculated with Brighton’s model at its temperature limit, and then selects the method that yields the larger evaporation rate.

ALOHA calculates the magnitude of six energy sources to establish puddle temperature. These include:

- Net short wave solar flux into the puddle;

- Long wave radiation flux down from the atmosphere;
- Long wave radiation flux upward into the atmosphere;
- Heat exchanged with the substrate by thermal conduction;
- Sensible heat flux from the atmosphere; and,
- Heat lost from the puddle by evaporative cooling.

An example scenario for a tank release is provided in the ALOHA technical documentation (Example 1, Part 1, ALOHA, August 2013).

Section 9.5.1 discusses the complex phenomenology associated with the release of pressurized liquids to the atmosphere and this section discusses non-pressurized liquid releases. Both phenomenologies involve the evaporation of liquid from a pool. In the event of a boiling liquid pool, two simple expressions for obtaining a first-order conservative approximation to the mass evaporation rate are presented, namely, convective boiling and conductive boiling.

The following subsections provide the analyst with some of the complex equations to account for the phenomenology of the evaporation of a puddle formed by pressurized and non-pressurized liquid releases. In addition, various evaporation rate calculations are presented for nitric acid and carbon tetrachloride to emphasize the complexities of accurately assessing evaporation rates.

9.5.4.1 CONVECTIVE BOILING

Equation 9-60 presents a technique to calculate the mass evaporation rate (m_v) due to convective boiling:

$$\boldsymbol{m_v = k_{air}\frac{A_p}{L_p}Nu_L\frac{(T_{air}-T_b)}{H_v}} \qquad \textbf{Equation 9-60}$$

Where,

m_v = mass evaporation rate (kg/m^2 s);

k_{air} = thermal conductivity of air (kJ/m °K);

A_p = pool surface area (m^2);

L_p = pool effective diameter in the wind direction (m);

Pr = $\mu_{air}c_{p_{air}}/k_{air}$

μ_{air} = viscosity of air at ambient temperature (poise);

$c_{p_{air}}$ = heat capacity of air at constant pressure (kJ/kg °K);

T_{air} = air temperature (°K);

T_b = liquid ambient boiling temperature (°K); and,

H_v = liquid latent heat of vaporization (kJ/kg).

and,

$$Nu_L = \begin{Bmatrix} 0.664\, Pr^{1/3} Re_L^{1/2} for\ Re_L \leq 320{,}000 \\ 0.037\, Pr^{1/3}\ (Re_L^{0.8} - 15200) for\ Re_L > 320{,}000 \end{Bmatrix}$$ **Equation 9-61**

9.5.4.2 CONDUCTIVE BOILING

Equation 9-62 presents a technique to calculate the mass evaporation rate (m_v) due to conductive boiling:

$$m_v = \frac{k_s A_p (T_{air} - T_b)}{H_v \sqrt{\pi \varepsilon t}}$$ **Equation 9-62**

Where,

k_s = thermal conductivity of ground surface (kJ/m °K);

A_p = pool surface area (m^2);

t = time s;

T_{air} = air temperature (°K);

T_b = liquid ambient boiling temperature (°K); and,

T_g = ground surface temperature (°K);

ε = $k_s/(\rho_s c_{p_s})$

ρ_s = density of ground surface (kg/m^3);

c_{p_s} = heat capacity of ground surface at constant pressure (kJ/kg °K); and

H_v = liquid latent heat of vaporization (kJ/kg).

Conductive boiling, or conductive heat transfer from the ground, is generally the dominant driving mechanism for boiling in the case of most chemical liquids. However, in the case of some cryogenic releases (e.g., sub-cooled anhydrous ammonia, chlorine), the ground conduction is dramatically reduced if there is moisture present in the substrate since a layer of ice has a thermal conductivity much lower than that of most ground surface substances and it quickly forms at the base of the pool. Furthermore, a thin vapor film frequently forms at the interface between the ground surface and the pool, which further reduces the effective conductivity in that region and limits the amount of heat transfer into the pool. Therefore, Equation 9-62 is generally quite conservative during the majority of the boiling regime and most accurately reflects true vaporization conditions at the first instant that the liquid comes into contact with the ground surface. Conversely, Equation 9-60 is more representative of the steady-state vaporization of a pool once the ground surface temperature drops below the boiling temperature of the liquid.

9.5.4.3 NITRIC ACID AND CARBON TETRACHLORIDE POOL EVAPORATION RATES

An alternative correlation that is commonly used in estimating pool evaporation rates and that has been demonstrated to provide lower estimates of pool evaporation rate for a nitric acid and carbon tetrachloride spill is presented. Furthermore, example hand calculations have been provided for the same two releases based on simple models of heat and mass transfer and compared to the experimental correlations to obtain even a less conservative estimate for the pool evaporation rate.

The following calculations employ a relatively simple means of assessing the accuracy of the pool evaporation source term calculations. Illustrative examples are given that assume liquid nitric acid and liquid carbon tetrachloride spill onto the ground surface and form a pool that will be subject to evaporative sub-cooling. The mass evaporation rate is determined by the following factors:

1. Molecular diffusion and mass transport;
2. Conductive heat transfer;
3. Radiative heat transfer;
4. Convective heat transfer;
5. Bulk liquid heat transfer; and
6. Internal heat content.

The following detailed source term calculations treat provide an upper bound on the potential impact of an evaporating pool in the case that all six evaporation source term factors were considered.

9.5.4.3.1 Nitric Acid Pool Evaporation

Vapor is entrained by air flowing over the surface of the pool. The rate of mass transfer is expressed in Equation 9-63:

$$\boldsymbol{m_v = -\frac{k_m\,P_t\,M_w}{RT_s}\,ln\left[1-\frac{P_v}{P_t}\right]} \qquad \textbf{Equation 9-63}$$

Where,

k_m = mass transfer coefficient (m/s);

P_t = sum of atmospheric pressure and partial pressure of chemical vapor (Pa);

M_w = molecular weight of chemical (kg/mole);

R = ideal gas constant = 8.31424 J/mole·K;

T_s = pool surface temperature (K);

P_v = chemical vapor pressure at temperature T_s (Pa).

Kulmala (1988) and Barrett and Clement (1988) provide detailed derivations of this expression and Studer et al., 1988 provide a technique for practical use of this expression in the context of pool evaporation.

Equation 9-63 is a specific instance of the mass transfer due to diffusion through a transpired boundary layer. A more general form is presented in Kays and Crawford (1987). While the transpired boundary layer model is not needed for the low vapor pressure associated with HNO_3, CCl_4 evaporates much more rapidly and therefore the transpired boundary layer model is necessary. This will be shown in Section 9.5.4.3.2. It is convenient, then, to operate with the single model for CCl_4 and apply it to HNO_3 as a degenerate case. Mass evaporation equations are part of standard diffusion boundary layer literature and can be found in numerous texts (see Kays and Crawford, 1987; Bergman et al., 2001).

The mass transfer coefficient may be related to the Sherwood number (Sh), coefficient of diffusivity of the chemical in air (D_{ba}) and the effective path length of air flowing over the pool, which is usually the effective diameter of the pool (L), as shown in Equation 9-64:

$$k_m = Sh\frac{D_{ba}}{L} \qquad \textbf{Equation 9-64}$$

The diffusion coefficient may be approximated by a group contribution method attributed to Fuller et al. (Reid et al., 1987), as shown in Equation 9-65:

$$D_{ba} = \frac{10^{-3}T_a^{1.75}{M_{w_{ab}}}^{1/2}}{P_a\left[(\sum v)_a^{1/3}+(\sum v)_b^{1/3}\right]^2} \qquad \textbf{Equation 9-65}$$

where, the sums apply to the atomic diffusion volumes for each component in the chemical molecule and,

$$M_{w_{ab}} = \frac{M_{w_a}+M_{w_b}}{M_{w_a}\,M_{w_b}} \qquad \textbf{Equation 9-66}$$

The subscripts b and a, refer to the chemical species and air, respectively. In particular, M_{w_b} and M_{w_a} denotes the molecular weight of nitric acid and air, respectively.

Assuming the air temperature is 40 degrees °C (313.15 °K) and M_{w_b}=63.02 g/mole, M_{w_a}=28.97 g/mole, $(\sum v)a = 20.1$ and,

$$(\sum v)_b = v(H) + v(N) + 3v(O) = 1.98 + 5.69 + 3(5.48) = 24.11 \qquad \textbf{Equation 9-67}$$

and substituting the above values into Equation 9-65 yields Equation 9-68 for the diffusion coefficient and Equation 9-69 for the maximum pool length.

$$D_{ba} = 1.64 \times 10^{-6}\ m^2/s \qquad \textbf{Equation 9-68}$$

$$L_{max} = \sqrt{\frac{4x(pool\ area)}{\pi}} \qquad \textbf{Equation 9-69}$$

Instead of using the effective length (L), conservatively take L to be the diameter of the pool and assume a pool area of 91 m^2; L_{max} becomes 10.8 m.

The Sherwood number may be expressed as in Equation 9-70:

$$Sh = 0.037\left(Re_L^{0.8} - 15200\right)Sc^{1/3} \qquad \textbf{Equation 9-70}$$

Where, the Schmidt number (Sc), and the Reynolds number (Re_L) are expressed in Equations 9-71 and 9-72:

$$Sc = \frac{\mu_v}{\rho_v D_{ba}} \qquad \textbf{Equation 9-71}$$

$$Re_L = \frac{\rho_\infty u_\infty L}{u_\infty} \qquad \textbf{Equation 9-72}$$

With,

ρ_∞ = main stream density (kg/m^3);

u$_\infty$ = main stream ambient wind speed (m/s); and,

μ_∞ = main stream viscosity (poise).

The Schmidt number arises when considering a laminar boundary layer on a flat plate in which the diffusion was occurring as a result of some mass-transfer condition at the surface. The concentration and velocity profiles will have the same shape when the dynamic viscosity $\nu_\infty = \mu_\infty/\rho_\infty$ satisfies $\nu_\infty=D_{ba}$ or $\nu_\infty/D_{ba}=1$.

The Schmidt and Reynolds numbers are many times calculated with the fluid properties at infinity in boundary layer coordinates rather than vapor properties (see Bergman et al., 2011). Occasionally one will find the fluid properties calculated at the average of the infinity and wall values. Using the outer fluid properties will significantly affect the resultant value for the Sherwood number in the case of cryogenic spills, for instance, where the thermodynamic properties are sensitive to small changes in ambient conditions.

The above correlation for the Sherwood number in Equation 9-70 only holds true for Re>15,200. Furthermore, the mixed boundary layer, the Sherwood number correlation is not valid for Sc<0.6 (see Bergman et al., 2011). Although Equation 9-70 expression for the Sherwood number is commonly quoted in analyses studying the evaporation of liquids, it was derived from studying the heat transfer coefficient of a dry body. Therefore an alternative, and presumably more appropriate empirical technique to express for the Sherwood number in the event of a liquid spill based on the work of Smolsky and Sergeyev in the area of heat and mass transfer from free surfaces of liquids into a heated turbulent stream is shown in Equation 9-73:

$$\boldsymbol{Sh = 0.094\, Re^{0.8} Sc^{0.33} Gu^{0.2}}$$ **Equation 9-73**

Where,

$$\boldsymbol{Gu = \frac{T_\infty - T_w}{T_\infty}}$$ **Equation 9-74**

Gu denotes the Guhmann number with T_∞ and T_w denoting the mainstream and liquid surface temperature, respectively.

This expression is based on experimental studies of the heat and mass transfer from the free surfaces of various liquids into a heated turbulent air stream. Equation 9-74 is therefore recommended as the more appropriate estimate of the Sherwood number in the case of an evaporating pool. However, estimates of the Guhmann number are vulnerable to high degrees of uncertainty. In an effort to circumvent this issue, the Sherwood number should be estimated using Equation 9-70 with the dynamic viscosity evaluated as the average of the main steam (i.e., air) and boundary layer vapor (i.e., chemical) dynamic viscosities in the definitions of the Schmidt (Sc) and Reynolds (Re) numbers, as depicted in Equations 9-75 through 9-77:

$$\boldsymbol{\overline{Re}_L = \frac{u_\infty L}{\bar{v}}}$$ **Equation 9-75**

$$\boldsymbol{\overline{Sc} = \frac{\bar{v}}{D_{ab}}}$$ **Equation 9-76**

$$\overline{v} = \frac{1}{2}\left(v_{air} + v_{vapor}\right)$$ **Equation 9-77**

Applying a nitric acid vapor density of 2.18 kg/m^3, u_∞=5 m/s and, due to limited data on HNO_3, approximating the vapor viscosity by the gas viscosity for nitrous oxide at the pool surface temperature of 20°C given to be 1.46E-2 c_p or 1.46E-5 kg/m·s yields v_{vapor}= 6.7E-6 m^2/s. The outer fluid properties make use of v_{air}=1.72E-5 m^2/s, for air at 313K and standard atmospheric pressure, and the pool diameter length scale L_{max} = 10.8 m, the averaged Schmidt (Sc) and Reynolds (Re) numbers are recalculated as shown in Equation 9-78.

$$\begin{aligned}\overline{v} &= 1.19 \times 10^{-5}\\ \overline{Sc} &= 7.29\\ \overline{Re}_L &= 4.52 \times 10^{6}\end{aligned}$$ **Equation 9-78**

Finally, substituting all the above intermediate results into Equation 9-70 obtains:

$$Sh = 1.4 \times 10^{4}$$ **Equation 9-79**

The mass transfer coefficient therefore becomes the following from Equation 9-64.

$$k_m = 2.13 \times 10^{-3} m/s$$ **Equation 9-80**

Therefore, the mass transfer rate is estimated to be the following value as calculated from Equation 9-81:

$$\begin{aligned}m_{tran} &= \frac{-\left(2.11 \times 10^{-3} m/s\right)(101325\,Pa + 413.2\,Pa)(0.06302\,kg/mole)}{(8.314 J/mole\,°K)(293.15°K)}\, ln\left[1 - \frac{413.2\,Pa}{101325\,Pa}\right]\\ &= 2.29 \times 10^{-5} kg/m^2 s\\ &= 0.0229 g/m^2 s\end{aligned}$$ **Equation 9-81**

The total mass transfer rate is simply the product of m_{tran} and the pool area of 91 m^2, as shown in Equation 9-82:

$$m_v(HNO_3) = 2.08 g/s$$ **Equation 9-82**

9.5.4.3.2 CARBON TETRACHLORIDE POOL EVAPORATION

The diffusion coefficient can be estimated by means of the group contribution method detailed above, with

M_{w_b}=153.83 g/mole, M_{w_a}=28.9 g/mole, $(\Sigma v)_a$=20.1 and

$$\left(\sum v\right)_b = v(C) + 4v(Cl) = 16.5 + 4(19.5) = 94.5$$ **Equation 9-83**

Finally, substituting the above values into Equation 9-65 yields Equation 9-84.

$$D_{ba} = 8.93 \times 10^{-6} m/s$$ **Equation 9-84**

Assuming a pool area of 73 m^2, the length scale L_{max} becomes 9.64 m from Equation 9-69. Assuming a CCl_4 vapor density of 5.32 kg/m^3, u_∞=5 m/s, and the vapor viscosity at the pool surface temperature of 20°C determined to be 9.66E-3 c_p or 9.66E-6 kg/m·s yields v_{vapor}=1.82E-6 m^2/s.

The outer fluid properties, v_{air}=1.72E-5 m^2/s for air at 313K and standard atmospheric pressure, the averaged fluid properties Schmidt (Sc) and Reynolds (Re) numbers are calculated to be what is shown in Equation 9-85.

$$\boldsymbol{\overline{v} = 9.51 \times 10^{-6}}$$
$$\boldsymbol{\overline{Sc} = 1.06}$$
$$\boldsymbol{\overline{Re}_L = 5.07 \times 10^6}$$

Equation 9-85

Substituting all the above intermediate results into Equation 9-70 yields:

$$\boldsymbol{Sh = 8.15 \times 10^3}$$

Equation 9-86

The mass transfer coefficient therefore becomes:

$$\boldsymbol{k_m = 7.55 \times 10^{-3} m/s}$$

Equation 9-87

Therefore, the mass transfer rate is estimated to be what is shown in Equation 9-88.

$$\boldsymbol{m_{tran} = \frac{-(7.5 \times 10^{-3} m/s)(101325\,Pa + 2 \times 10^4\,Pa)(0.15383\,kg/mole)}{(8.314 J/mole\,°K)(293.15°K)} ln\left[1 - \frac{2 \times 10^4\,Pa}{101325\,Pa}\right] = 1.27 \times 10^{-2} kg/m^2s}$$
$$= 12.7 g/m^2 s$$

Equation 9-88

Using a pool area of 73 m^2, the total mass transfer rate is simply the product of m_{tran} and the pool area, as shown in Equation 9-89:

$$\boldsymbol{m_v(CCl_4) = 0.928 kg/s}$$

Equation 9-89

In contrast to nitric acid, the boiling temperature of CCl_4 is closer to that of ambient temperature and the effects of bulk liquid heat transfer and internal heat content play a more important role in the overall mass evaporation rate. Both of these factors serve to mitigate the release rate to some extent. However, because of the greater volatility of CCl_4, solar radiation and convective heat transfer have a significant effect in terms of increasing overall mass evaporation rate.

No simple correlation has the capabilities of accurately incorporating all the various thermal phenomena taking place in the event of a volatile liquid release. However, a simple correlation can provide a reasonable conservative estimate of the true evaporation rate.

Compare the evaporation correlation used in the CEI guidelines (TNO, 1979), as shown in Equation 9-90.

$$\boldsymbol{\dot{m} = 9 \times 10^{-4} A_p^{0.95} \frac{(MW)P_v}{T+273}}$$

Equation 9-90

Where,

$\dot{m}$ = pool evaporation rate (kg/hr);

A_p = pool area (m^2);

MW = chemical molecular weight (g/mole);

P_v = vapor pressure of the chemical at the characteristic temperature (kPa); and

T = characteristic pool temperature (°C).

with a similar closed-form expression described by Clewell (1983), as shown in Equation 9-91:

$$\dot{m} = 8 \times 10^{-2} u^{3/4} A_p Z \left(1 + 4.3 \times 10^{-3} T^2\right) \quad \textbf{Equation 9-91}$$

Where, Z is the volatility factor of species x with respect to hydrazine expressed as such in Equation 9-92.

$$Z = \frac{(MW)_x P_{v_x}}{(MW)_{hydrazine}\, P_{v_{hydrazine}}} \quad \textbf{Equation 9-92}$$

Predicted evaporation rates for nitric acid and carbon tetrachloride at various ambient temperatures with a fixed pool surface area of 1 m^2 and an ambient wind speed of 5 m/s are provided in Figure 9-1 and Figure 9-2, respectively.

In the turbulent boundary layer, the mass transfer coefficient is proportional to $u^{0.8}$ and $L^{1.8}$, while in the TNO correlation, the mass transfer coefficient is proportional to $u^{0.8}$ and $L^{1.9}$. Accordingly, the TNO expression will be become progressively more conservative as the pool area increases and as the laminar region, where Sh is proportional to $Re^{1/2}$, increases.

As for the additional modes of heat transfer, evaporative cooling offsets heating effects due to ground conduction and solar radiation. For volatile liquids such as CCl_4, Clewell suggests a pool temperature decrease of 10-20 °C is not unreasonable due to evaporative cooling (Clewell, 1983). By setting the pool temperature equal to the air temperature, a conservative evaporation rate is maintained. This is equivalent to assuming a very large convective heat transfer coefficient between the pool and the air.

The standard turbulent boundary layer calculation also suffers from lack of data as the diffusion coefficients for CCl_4 vapor is calculated based on the chlorine diffusion volume, which, according to Perry's *Chemical Engineers' Handbook* (2008), is based on very little data. No data was found to directly compare to the calculated diffusion coefficients for HNO_3 as well.

Table 9-5 compares the results for the hand calculations, the TNO model, and the Clewell model in the case of the nitric acid and carbon tetrachloride evaporation rates. Although there is relatively good comparison among all three models in the case of nitric acid, there is a disparity among results in the case of carbon tetrachloride. The hand calculation is in itself conservative, but even after allowing for pool cooling and other mitigating features, the question as to whether simple correlations can be relied upon to yield conservative results for a wide class of chemicals remains unanswered.

The aforementioned equations in Sections 9.5.4.1 through 9.5.4.3 are limited to the assumptions in their derivation and/or the conditions under which they were developed. Prior to employing these equations to determine the phenomenology of a specific system or process, the analyst should demonstrate that the application domain of the equations is not exceeded.

These examples were chosen to dramatize the point that one should never blindly place faith in experimental correlations based on limited data.

Table 9-5. Comparison of Results for Three Evaporation Models as Applied to HNO_3 and CCl_4.

Model	HNO_3 Evaporation Rate (g/sec)	CCl_4 Evaporation Rate (g/sec)
Hand Calculation	**2.08**	**928**
TNO	**1.53**	**342**
Clewell	**2.82**	**606**

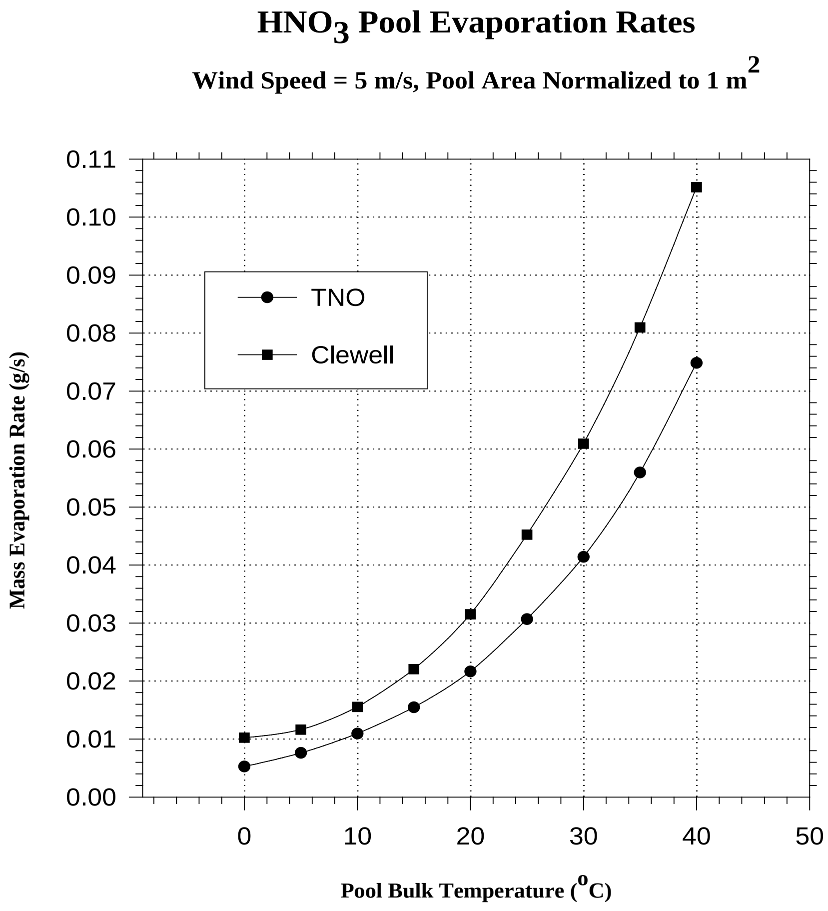

Figure 9-1. Comparison of Evaporation Rate Predictions for 60 Percent Solution of Nitric Acid with a 1 m^2 Pool Surface Area.

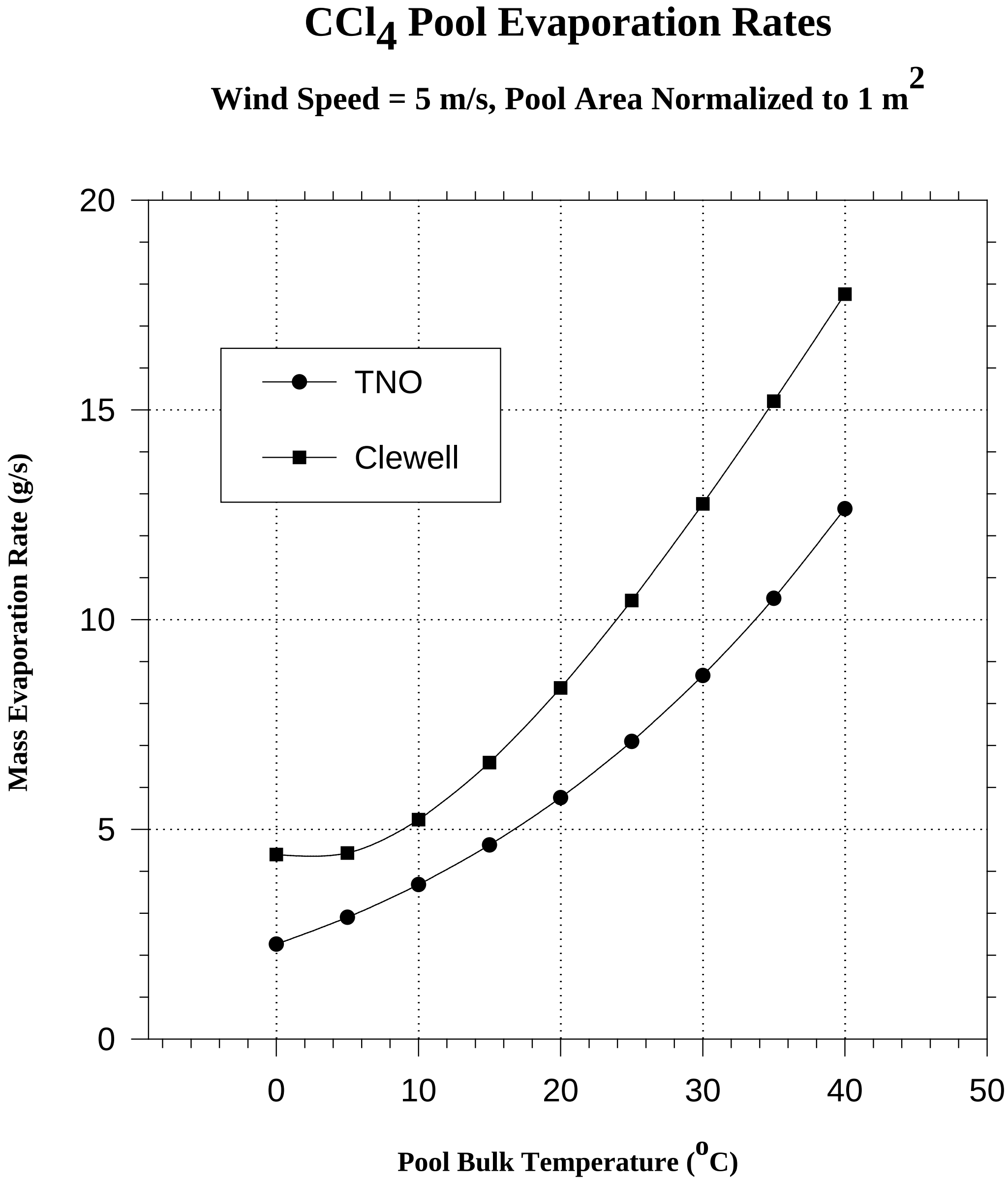

Figure 9-2. Comparison of Evaporation Rate Predictions for Carbon Tetrachloride with a 1 m^2 Pool Surface Area.

9.5.5 ENERGETIC EVENTS: FIRES, DEFLAGRATIONS, DETONATIONS, DELAYED IGNITION EXPLOSIONS, AND BLEVES

For toxic chemical dispersion and consequence energetic events analysis, the initial phase of such an event releases a volume of hot gases under high pressure. Hot gases rise through its' own buoyancy and expand rapidly until reaching equilibrium with atmospheric pressure, determining the plume initial dimensions and effective height of release. After reaching equilibrium with the ambient atmosphere, conventional atmospheric redistribution processes act on this plume, carrying it downwind as it continues to expand through turbulent diffusion in the horizontal and vertical planes.

Energy associated with the release, which includes a fire, deflagration, detonation, delayed ignition detonation, and BLEVE, require special analytical treatment. A BLEVE occurs during a fire event where the contained liquid in a vessel expands due to the sensible heat transfer to the inside of the vessel and eventually reaches a point where the internal pressure from the expanding vapor in the vessel exceeds the vessel's structural integrity and a violent explosion occurs.

Few atmospheric dispersion codes in common use at DOE facilities model atmospheric dispersion from energetic events. ERAD, applicable to radionuclide releases from HE, has been discussed in Chapter 6.

Special techniques and codes have been developed to determine the radiant heat and other impacts resulting from fires, deflagrations, and detonations. Deflagrations differ from detonations in that for deflagrations the pressure wave expands at less than the speed of sound. When chemical fires propagate at a speed that exceeds the speed of the sound, the propagation causes an overpressure in the atmosphere, which essentially moves the ambient atmosphere at a faster speed to a point downwind than it would normally move causing a compression wave, or overpressure. The detonation overpressure, which is measured in atmospheres, can be quite destructive. Detonations can be an immediate phenomenon, or can result hours after the release of a flammable gas when the chemical disperses to a concentration between its upper and LFLs and encounters an ignition source. The effects of overpressures on the CW, MOI and the public from either a delayed ignition detonation or immediate detonation are a function of its overpressure magnitude, the distance from the detonation (i.e., attenuation), and other mitigating factors (e.g., shielding from buildings).

Hydrogen is a by-product of radiolysis, and build-up of this lighter-than-air gas can lead to either deflagrations or detonations. Given this complexity, determination of the physics underlying hydrogen deflagrations or detonations has undergone much research. Table 4-2 and Section 4.3 provide some guidance on determining whether the hydrogen-air mixture is explosive, whether the propagation speed is sufficient to become a detonation, calculation of its energy and peak Chapman-Jouget pressure, and the consequences of a hydrogen detonation on SSC integrity and the health and safety of the facility worker, CW and the public. MELCOR and FLUENT codes can be employed to establish initial conditions and gas distribution of the detonation calculations.

ALOHA Version 5.4.6 and other peer-reviewed techniques and codes are required to determine the overpressures from a delayed ignition detonation, an immediate detonation, or a BLEVE. This version of ALOHA is in the DOE Central Registry and is capable of addressing the energetic events discussed in this subsection. It has the capacity to calculate toxic chemical consequences from pool fires, BLEVEs, flash fires or vapor cloud explosions, and jet fires.

ALOHA Version 5.4.6 only models combustion reactions and estimates the blast wave from unconfined vapor cloud explosions (e.g., fast deflagrations, detonations). Confined vapor cloud explosions generally produce more damaging blast waves than unconfined or partially confined explosions.

The overpressure calculation utilizes the Baker-Strehlow-Tang (BST) model (Pierorazio et al. 2005), employing non-dimensional, empirically-derived blast curves to establish overpressure. Overpressure magnitude is a function of the flame front propagation speed and the mass of fuel involved in the reaction.

ALOHA Version 5.4.6 also models flame hazards associated with the combustion of liquids and gases. However, fire scenarios involving chemicals with flashpoints exceeding 300°F cannot be modeled. Two types of combustion are addressed in ALOHA: (1) a fuel mixed with air to form a cloud with concentrations within the flammability range; and (2) an overly-rich core of fuel that burns at its outer edges. Different methodologies are applied for estimating the threat zones for these two types of combustion events. ALOHA Version 5.4.6 employs solid flame models to compute thermal radiation hazards from fireballs, jet fires, and pool fires, where the flux of thermal radiation emitted from the surface of the flame is computed and the radiation impinging upon a distant target is determined.

ALOHA Version 5.4.6 has a BLEVE-fireball model based on studies of fireballs resulting from BLEVEs (CCPS, 1994). A fire thermally stresses a vessel causing the internal pressure to rise beyond the capacity of pressure relief valves, leading to a tank explosion. The tank contents are rapidly released and quickly flash boil as they depressurize, and both liquid droplets and gas ignite. Since the substance is too rich to burn; a fire burns at the surface where sufficient air can mix with the fuel resulting in a fireball that burns for tens of seconds. The flux of thermal radiation emitted from the burning surface is computed, and the radiation impinging upon a distant target is determined.

Example scenarios for pool fires (Example 1 Part 2), BLEVEs (Example 2 Part 1), flash fires or vapor cloud explosions (Example 2 Part 2), and jet fires (Example 2 Part 3) are provided in ALOHA Example Scenarios.

If a small quantity of chemical is spilled or released in a fire or explosion, the resultant plume can be approximated with the Gaussian plume model, as long as the additional plume buoyancy and explosion overpressures are addressed in other codes. EPIcode has an explosion sub-model that addresses this type of release, calculating a virtual point of release in three-dimensional space before applying Gaussian modeling techniques.

Other complicating factors, such as chemical reactions and chemical transformations within the plume, should be addressed on a case-by-case basis using the dispersion modeling protocol in Section 6.1.9. See Section 4.3 on explosions for additional information on energetic release phenomenology, chemical reactions, and chemical transformations.

Section A.2 of DOE-STD-3009-2014 states that the DSA does not evaluate decomposition of chemicals from accidental fires, nor establishes SSCs or SACs based on the hazards of these toxic products. Accordingly, this technical area is not included in this Handbook.

9.6 METEOROLOGICAL PARAMETERS AFFECTING TOXIC CHEMICAL CONSEQUENCE ANALYSIS

The discussions in Section 6 on the meteorological parameters of wind speed, wind direction, sigma theta, temperature, and precipitation are also applicable to toxic chemical releases. For these meteorological variables, the atmosphere does not operate any differently whether the release is a radionuclide or toxic chemical, or a combination of both. Turbulence typing for chemical dispersion and consequence analysis is the same as for radiological releases that was also described in Section 6. In calculating plume concentrations, both “typical” and “unfavorable” dispersion conditions are of special interest in accident analyses.

Several meteorological variables, namely temperature and humidity, are specific to analyzing the consequences of toxic chemical releases. A brief discussion on each follows.

9.6.1 TEMPERATURE EFFECTS

The atmospheric variables of temperature and moisture (e.g., relative humidity, wet-bulb temperature) do not directly affect the magnitudes of the atmospheric dilution and diffusion for radionuclide release evaluations. However, for releases of toxic chemicals, these variables play a significant role in determining the thermodynamics in establishing rates of flashing, aerosolization, and puddle evaporation.

Section 9.5.4 provides a discussion of puddle evaporation algorithms and heat balance including conduction from the ground surface. It also provides a discussion of impoundment basins and how they limit the surface area of the puddle and therefore reduce evaporation rate.

9.6.2 RELATIVE HUMIDITY EFFECTS

Uranyl hexafluoride (UF_6) is a special case due to its disassociation into hydrofluoric acid (HF) and uranyl fluoride (UO_2F_2) in a humid environment. A special code developed by Hanna in the 1980s, HGSYSTEM-UF6, and a recent version of the NRC code, RASCAL, has an algorithm to model the conversion rate of UF_6 to UO_2F_2 and HF over time and subsequently disperses both compounds.

Some chemical releases are also sensitive to ambient relative humidity; especially chemicals that are deliquescent and absorb water. An interesting situation is the release of ammonia (NH_3) in a dry environment, where it remains as a positively buoyant gas; while in a humid environment it becomes ammonium hydroxide (NH_4OH), which behaves as a dense gas.

The release of elemental tritium is also very sensitive to the amount of water vapor in the atmosphere at the time of release as it will convert to tritium oxide rapidly in a moist environment. There are significant differences in the DCFs between elemental tritium and tritium oxide.

9.7 TOXIC CHEMICAL ATMOSPHERIC TRANSPORT AND DIFFUSION MODELS

Many codes are available for evaluating toxic chemical releases, atmospheric dispersion, and concomitant consequences to the CW, MOI, and the public. It has been estimated that in the 1980s, there were as many as 250 atmospheric dispersion modeling codes available both internationally and within the private and public sectors of the United States. However, codes need to be maintained and improved in order to remain viable, so this number has decreased with time.

In 1995, SCAPA published “*Atmospheric Transport Modeling Resources*” (Mazzola and Addis, 1995), in which information about various aspects of 94 distinct atmospheric transport models were catalogued and presented in an easy-to-use format. In March 1999, the Office of the Federal Coordinator for Meteorological Services and Supporting Research (OFCM) published a much more comprehensive version of this document for 64 frequently used atmospheric dispersion models. This latter work is available electronically by accessing the technical documents section of the OFCM web page (www.ofcm.gov). In addition, the APAC Methodology Evaluation Program analyzed 15 radiological dispersion models (Working Group 5) (APAC5, 2003) and 25 chemical dispersion models (Working Group 6) (APAC6, 1997) in significant detail.

Some models have undergone extensive SQA inclusive of verification and validation. Other codes are available and may be more appropriate for some applications but were not included in those summaries because they are not commonly accessible or require specialized knowledge for their proper use.

DOE-STD-3009-2014, Section 3.2.4.3 states: "Atmospheric dispersion for hazardous chemicals may be modeled in a manner similar to radioactive material dispersion where the material transport characteristics are similar." As indicated in Section 6.1.10, three options are given in DOE-STD-3009-2014 to evaluate atmospheric dispersion and the resulting χ/Q:

- Option 1: Follow a process based on NRC Regulatory Guide 1.145;
- Option 2: Use a DOE-approved toolbox code and apply the conservative parameters; or
- Option 3: Use site-specific methods and parameters as defined in a site/facility specific DOE-approved modeling protocol.

Since Option 1 is only applicable to radiological consequences, for toxic chemical releases, use either Options 2 or 3. The Section 6.11 dispersion modeling protocol is applicable to both radiological and toxic chemical releases.

9.7.1 NEUTRALLY-BUOYANT GAUSSIAN MODELS

Gaussian models, due to their relative simplicity and ease of application, are the most common atmospheric dispersion models employed by analysts to determine consequences from toxic chemical releases. There are two chemical dispersion models (e.g., ALOHA, EPIcode) in the DOE CR, ALOHA meets all DOE O 414.1D and DOE G 414.1-4A SQA guidance, and although EPIcode does not, it is still determined to be adequate for safety analysis. The codes and their latest version in the CR are listed below.

- Areal Locations of Hazardous Atmospheres (ALOHA) Version 5.4.6, an EPA and National Oceanic and Atmospheric Administration (NOAA)-sponsored code (ALOHA, 2013); and,
- Emergency Prediction Information code (EPIcode), Version 8.0.2 (EPIcode, 2015).

ALOHA is the more versatile of the two toolbox codes as it contains both dense-gas and neutrally-buoyant dispersion models, and it can address various chemical release phenomenology and energetic events. During an ALOHA neutrally-buoyant dispersion model execution, the code selects one model based on the environment in which the release is occurring, the nature of the release, the toxic chemical being analyzed and the source-receptor distance of interest. For dense gas releases, ALOHA calculates the dispersion within the dense gas "blanket" and with each succeeding time step, evaluates whether the plume, which is gradually entraining ambient neutrally-buoyant air, still will disperse as a dense gas. Once the plume parameters no longer support the definition of a dense gas as it moves further downwind, ALOHA switches to the neutrally-buoyant Gaussian model. In contrast, EPIcode is based only on the neutrally-buoyant atmospheric dispersion model, but allows the user to vary the release time and deposition velocity, as well as implement a building wake effect model.

9.7.1.1 ALOHA

The ALOHA code was jointly developed by EPA and the hazardous materials division of NOAA. It is part of the Computer-Aided Management of Emergency Operations (CAMEO) suite of codes and is used primarily for emergency response situations and for training. As such, it is user-friendly, allowing easy data input and convenient output of areal maps with contours of concentration of toxic chemicals using the MARPLOT feature. Many of the internal features of the code are hidden from the user in order to make it more user-friendly. The full suite of ALOHA modeling capabilities can be referenced in NOAA Technical Memorandum NOS OR&R 43, ALOHA technical documentation (ALOHA, 2013).

Unlike some radiological dispersion codes (e.g., MACCS2, GENII, Hotspot), ALOHA does not have the capability to incorporate hourly, site-specific meteorological data and calculate 95th percentile levels consequences based on meteorological variability. EPIcode Version 7.0 has been recently upgraded to execute with hourly meteorological data files. For ALOHA applications, a single combination of atmospheric stability and wind speed is input instead of hourly meteorological data files. For dispersion analysis, 40 CFR § 68.22(b) specifies that poor dilution and diffusion conditions of 1.5 m/sec wind speed and F atmospheric stability class should be assumed.[102] Related conditions of ambient temperature and relative humidity, as may be needed, are recommended from the prescription also identified in 40 CFR § 68.22(b).[103]

ALOHA is intended for the evaluations of the consequences of toxic chemical releases. If the chemical released is a heavy gas, a heavy-gas model (i.e., a stripped-down version of DEGADIS) is used; otherwise, a neutrally-buoyant Gaussian model is used. ALOHA computations represent a compromise between accuracy and speed: it has been designed to produce good results quickly enough to be of use to first responders.

ALOHA Version 5.4.4 has the following attributes:

- Since evaporation of volatile chemicals is especially time-variant, ALOHA can calculate the time-dependent evaporation source term and resulting plume concentration;
- It can determine the extent of dense gas behavior and the distance of transition to neutrally buoyant gas behavior;
- It can predict the rates at which chemical vapors may escape into the atmosphere from broken gas pipes, leaking tanks, and evaporating puddles;
- It can address energetic events such as BLEVEs, vapor cloud explosions, detonations, delayed ignition detonations, and radiant heat effects of flash fires and jet fires;
- Its chemical library contains information about the physical properties of about 3,000 common toxic chemicals;

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[102] **Wind speed and atmospheric stability class**. “For the worst-case release analysis, the owner or operator shall use a wind speed of 1.5 m per second and F atmospheric stability class. If the owner or operator can demonstrate that local meteorological data applicable to the stationary source show a higher minimum wind speed or less stable atmosphere at all times during the previous three years, these minimums may be used. For analysis of alternative scenarios, the owner or operator may use the typical meteorological conditions for the stationary source” (40 CFR §68.22(b)).

[103] **Ambient temperature and relative humidity**. “For worst-case release analysis of a regulated toxic substance, the owner or operator shall use the highest daily maximum temperature in the previous 3 years and average humidity for the site, based on temperature/humidity data gathered at the stationary source or at a local meteorological station; an owner or operator using the Risk Management Program Offsite Consequence Analysis Guidance may use 25 °C and 50 percent humidity as values for these variables. For analysis of alternative scenarios, the owner or operator may use typical temperature/humidity data gathered at the stationary source or at a local meteorological station” (40 CFR §68.22(c)).

- It has a Site Acquisition of Meteorology (SAM) option, where an instrumented meteorological tower can provide input directly to the code; and
- It permits changes in the wind direction parameter every fifteen minutes when the SAM component is applied. This is known as the segmented Gaussian plume. When used in this mode, changes in wind direction allow the plume to bend in the downwind direction.

ALOHA Version 5.4.4 has the following limitations:

- It does not calculate plume rise for ground level releases, so it cannot realistically account for the enormous buoyancy effects of fires and energetic releases;
- It only addresses pure chemicals and consequently is not capable of analyzing the complexities of atmospheric chemistry associated with chemical reactions and mixtures of chemicals;
- It does not have any algorithms that account for dry deposition, wet deposition, plume depletion, and resuspension. Therefore, it does not do particularly well for releases that contain particulates;
- It is a segmented Gaussian plume model, which limits its ability to address complex flows associated with topography; and
- Like all Gaussian models that are steady-state by definition, is not reliable for very low wind speeds, for very stable atmospheric conditions, for shifting winds and terrain-steering situations, or for concentration patchiness.

9.7.1.2 EPICODE

EPIcode was originally developed at the Lawrence Livermore National Laboratory (LLNL) to provide emergency response personnel and emergency planners with a software tool to help evaluate downwind concentrations from atmospheric releases of toxic substances. It can also be used for safety analysis planning purposes for facilities handling toxic chemicals.

EPIcode has many similarities to ALOHA, in that it is a straight-line Gaussian model with an extensive chemical library. However, unlike ALOHA, it can only address direct and evaporating puddle chemical release situations since it does not contain pipe and tank sub-models.

The version of EPICode that is in the DOE Central Registry is EPICode Version 7.0. Attributes and limitations of a more recent version are presented below:

EPIcode Version 8.0.2 (EPIcode, 2015) has the following attributes:

- It can assess area releases, fire releases, and explosion releases; but not the energetics associated with these accidents;
- Its chemical library is slightly smaller than that in ALOHA, but it still addresses more than 600 specific chemicals;
- It has algorithms for dry deposition;
- It allows fast estimation and assessment of chemical release scenarios associated with accidents from industry and transportation;
- It is menu-driven and user friendly, requiring minimal user training;
- It contains a good graphics package; and
- Its User Manual also contains 11 case studies showing how the code can assess a wide range of chemical accident scenarios.

EPIcode Version 8.0.2 has the following limitations:

- It has a very simple evaporation rate algorithm.
- It only addresses pure chemicals and consequently is not capable of analyzing the complexities of atmospheric chemistry associated with chemical reactions and mixtures of chemicals;
- It does not have any algorithms that account for wet deposition and resuspension;
- It is a straight-line Gaussian model, which limits its ability to address complex flows associated with topography; and
- Like all Gaussian models that are steady-state by definition, is not reliable for very low wind speeds, for very stable atmospheric conditions, for shifting winds and terrain-steering situations or for concentration patchiness.

9.7.1.3 CHEMICAL DISPERSION ANALYSIS WITH ALOHA AND EPICODE

A parametric study from a very limited data set, provides insight to important sensitivities related to modeling evaporative chemicals with earlier versions of ALOHA and EPIcode and analysis of the concentrations at a 100-m distance (Thoman et al., 2006). This study, summarized in Table 9-6, yielded the following conclusions for ALOHA:

- Class F stability at 1 m/s wind speed for a rural region of transport is bounding relative to urban conditions for both EPIcode and ALOHA. The same conclusion holds for the results comparing the Class D stability at 2 m/s results; and
- ALOHA dense gas results for Class D stability at 2 m/s wind speed bounds the Gaussian neutrally-buoyant gas results for both rural and urban regions of transport, and the rural terrain dense gas results for Class D stability at 2 m/s wind speed are bounding relative to the urban terrain dense gas results.

Table 9-6. ALOHA Results for Evaporative Releases of Four Selected Chemicals.

Chemical Released	Dispersion Model[104]	Region of Transport	Stability class/ wind speed (m/s)	Release rate (g/s)	Concentration at 100 m (mg/m^3)
Nitric Acid	GNB	Rural	F/1	5.3	2.3 E2
	DG	Rural	F/1	5.3	8.8 E1
	GNB	Urban	F/1	5.3	4.8 E1
	DG	Urban	F/1	5.3	6.1 E1
Nitric Acid	GNB	Rural	D/2	9.1	3.2 E1
	DG	Rural	D/2	9.1	7.3 E1
	GNB	Urban	D/2	9.1	1.3 E1
	DG	Urban	D/2	9.1	4.9 E1
Chlorine	GNB	Rural	F/1	2100	2.1 E4
	DG	Rural	F/1	2100	3.0 E3
	GNB	Urban	F/1	2100	4.4 E3
	DG	Urban	F/1	2100	1.5 E3
Chlorine	GNB	Rural	D/2	2800	2.4 E3
	DG	Rural	D/2	2800	2.6 E3
	GNB	Urban	D/2	2800	9.5 E2
	DG	Urban	D/2	2800	1.6 E3
Benzene	GNB	Rural	F/1	9.6	4.3 E2
	DG	Rural	F/1	9.6	1.3 E2
	GNB	Urban	F/1	9.6	9.0 E1
	DG	Urban	F/1	9.6	9.1 E1
Benzene	GNB	Rural	D/2	17	4.9 E1
	DG	Rural	D/2	17	1.1 E2
	GNB	Urban	D/2	17	2.0 E1
	DG	Urban	D/2	17	7.4 E1
Ammonia	GNB	Rural	F/1	400	6.9 E3
	DG	Rural	F/1	400	7.6 E2
	GNB	Urban	F/1	400	1.4 E3
	DG	Urban	F/1	400	6.7 E2
Ammonia	GNB	Rural	D/2	540	8.6 E2
	DG	Rural	D/2	540	1.3 E3
	GNB	Urban	D/2	540	3.5 E2
	DG	Urban	D/2	540	8.7 E2

For the same chemical release under evaporative conditions, the neutrally-buoyant Gaussian model ALOHA results for the F stability conditions and 1 m/s wind speed for a rural region of transport bounds

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[104] GNB = Gaussian neutrally-buoyant; DG = Dense Gas or heavy gas

all other dense gas results in both rural and urban regions of transport and all other neutrally-buoyant Gaussian model results. For example, the Gaussian neutrally-buoyant nitric acid result of 230 mg/m^3 for F stability and 1 m/s wind speed bounds the other seven chlorine results obtained using the ALOHA model. Chemical release concentrations for the three other toxic chemicals also showed the same bounding value for Class F stability conditions and 1 m/s wind speed for a rural region of transport.

Both EPIcode and ALOHA allow the evaporative source term and dispersion calculations to be coupled such that the plume exposure time reflects the time over which the evaporation release occurs. For EPIcode, an evaporation rate that is constant with time is modeled. ALOHA calculates a time–varying evaporative release rate that is reflected in downwind concentrations that are observed to vary with time as shown in Figure 9-3.

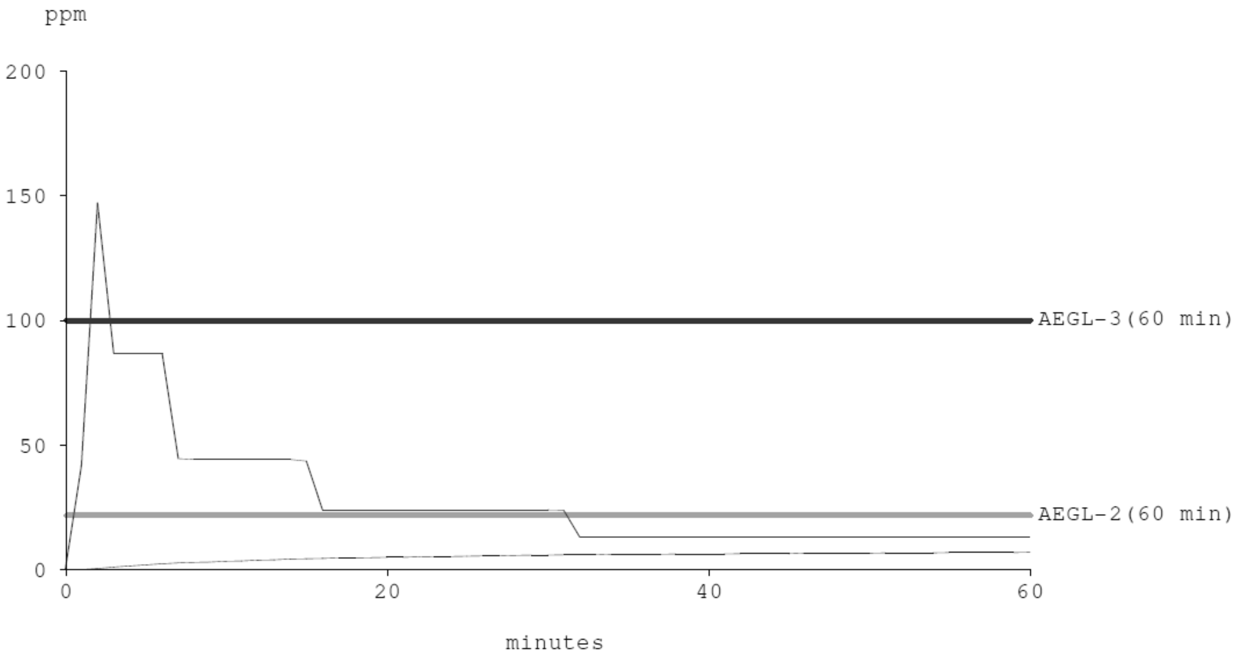

Figure 9-3. Example of ALOHA concentration output from an evaporative pool of hydrogen chloride.

It should be emphasized that this parametric study is based on a limited data base and its results should not be overly generalized.

9.7.2 DENSE GAS DISPERSION MODELS

Practically all of the hazardous chemicals that are stored and/or used at DOE facilities have densities greater than dry air. Some exceptions include anhydrous ammonia, nitric oxide and carbon monoxide.

Several heavy gas or dense gas codes have been developed to analyze the slumping effects of an accidental release of a dense gas. Each of these codes has been recommended for application in a broad range of safety basis documentation by APAC Working Group 6 (APAC6, 1997).

9.7.2.1 ALOHA

ALOHA can also be executed in heavy gas mode, if not bypassed by the user, for a release of a chemical with a molecular weight of greater than the molecular weight of dry air (28.97 g/mol) given that the critical Bulk Richardson number criterion is fulfilled during release conditions. ALOHA contains a stripped down version of the DEGADIS code to address the effects of heavy gases.

ALOHA can be run in Gaussian mode or dense gas mode. For dense gas applications, the dense gas model operates until the critical Bulk Richardson number is reached as the dense gas plume gradually entrains ambient air into the blanket. Once sufficient ambient air is within the dense gas blanket, it becomes neutrally-buoyant and ALOHA switches to the Gaussian model.

NSRD-2015-TD01 concluded:

> The ALOHA neutrally-buoyant Gaussian model results for a rural region of transport bounds all other dense gas results in both rural and urban regions of transport, as well as all other neutrally-buoyant Gaussian model results.

This is applicable to ground-level chemical releases and the health impact at a CW at 100 m for meteorological conditions of 1.0 m/s and F stability class.

9.7.2.2 DEGADIS

Version 1 of the Dense Gas Dispersion (DEGADIS) model was developed by the University of Arkansas for the United States Coast Guard and the Gas Research Institute in 1985. In 1988, Havens (1988) interfaced Ooms’ 1974 jet model to develop Version 2.0. The present Version 2.1 was established in 1989 through the work of Spicer and Havens (EPA-450/4-89-019).

EPA lists DEGADIS as an “Appendix B” refined air quality model that may be considered for individual regulatory applications on a case-by-case basis. It presently manages the maintenance of the model (EPA-450/4-88-006a; EPA-450/4-89-019). Updates can be accessed through the EPA Support Center for Regulatory Atmospheric Modeling bulletin board: http://www.epa.gov/scram001/tt22.htm#degadis.

Although the model is relatively easy to run, the analyst should take special care to fully understand the user options and the data input requirements, for example, distinctions between isothermal and non-isothermal simulations.

DEGADIS has the following attributes:

- It can address the transport and diffusion of many types of dense gas releases and account for a variety of surface roughness elements; and
- It can also simulate atmospheric transport and diffusion of pure chemical releases in passive-dispersion flow regimes.

DEGADIS has the following limitations:

- It does not have a front-end chemical library that the ALOHA and EPIcode models have. Correspondingly, the analyst should couple the DEGADIS dispersion results with chemical source terms generated from other models; and

- It cannot address buoyant plumes, although it is usually chosen for application for cases where the plume slumps due to its own density.

9.7.2.3 HGSYSTEM

Heavy Gas (HG) SYSTEM was developed for the American Petroleum Institute in 1990. Its current version, 3.0, was released in 1994.

Unlike DEGADIS and SLAB, HGSYSTEM is able to generate its own chemical source terms and therefore does not need to be supplied with an additional modeling technique.

HGSYSTEM has the following attributes:

- It can efficiently handle time-dependent dispersion by an internal automated selection of advection and averaging time; and
- It can also treat multi-component mixtures and vapor-aerosol generation.

HGSYSTEM has the following limitations:

- Proper training is needed. Although not as complex as a research-grade model, the user needs prior experience and familiarity with the code’s features since there are a large number of alternative options available that need to be fully understood; and
- It also has had difficulty in appropriately quantifying evaporation under low exit velocity release conditions and very stable low wind speed meteorological conditions.

A specially designed HGSYSTEM-UF_6 model has been developed for use in the accident analysis of Oak Ridge facilities to quantify the chemical consequences from a release of uranium hexafluoride.

9.7.2.4 SLAB

SLAB was developed from basic research involving experiments with chemical releases at China Lake, CA and the Nevada Test Site in the early 1980s (Ermak, 1990).

SLAB has the following attributes:

- It is not only easy to use, but it can be applied to a wide range of chemical release scenarios. These include application to jets released at any angle to evaporative area sources to instantaneous sources.; and
- It also contains a unique averaging time algorithm that allows application of the model to time-varying source emissions.

SLAB has the following limitations:

- Like DEGADIS, it does not have a front-end chemical library that the ALOHA and EPIcode models have;
- The analyst should couple the SLAB transport and diffusion results with chemical source terms generated from other models; and
- SLAB cannot address buoyant plumes.

9.7.3 VARIABLE TRAJECTORY DISPERSION MODELS

The frame of reference of all steady-state two-dimensional Gaussian-type models is Eulerian, meaning that the receptor is on a fixed coordinate system and receives no impact until the plume front reaches it. For sites that are located in regions that experience three-dimensional flows due to complex terrain (such as valley-mountain wind regimes) or due to temperature differences at land-water interfaces (such as sea breezes, lake breezes), the application domain of Eulerian codes is severely limited.

For the evaluation of chemical releases at locations with complex air flows, three-dimensional Lagrangian mass-consistent codes, (e.g., codes developed at NARAC) need to be considered for toxic chemical releases. Since the distance to the CW is sufficiently close enough where airflow trajectory reversals have not yet begun to occur, there is no practical need to be concerned with these complex terrain effects for this application. However, since the public is usually far enough away to experience the effects of airflow trajectory reversals, which are common at some DOE sites (Y-12, ORNL, NNSS, LANL, Hanford, INL), for that evaluation, a three-dimensional Lagrangian mass-consistent variable trajectory model would provide more accurate results than a Gaussian model that provides more bounding results. Several models have been developed to characterize atmospheric dispersion in regions of complex terrain. A few of these models that can be applied to address the effects of chemical as well as radiological releases in mountain-valley and sea breeze topographic settings include:

- NARAC codes;
- HYSPLIT;
- HYRAD;
- AERMOD; and
- CTDMPLUS.

9.7.4 RESEARCH-GRADE DISPERSION MODELS

Several research grade atmospheric dispersion models are applicable to chemical consequence analysis. The APAC Working Groups reviewed several of these codes, which include:

- HOTMAC/RAPTAD;
- FEM3C;
- SCIPUFF;
- VDI; and
- VLSTRACK.

The analyst is referred to the APAC Working Group 6 (APAC6, 1997) report for further information regarding the applicability of any of these codes to specific problem solving.

9.8 TOXIC CHEMICAL CONSEQUENCE SCOPING METHODOLOGY TO EXCEED PAC/TEEL VALUES

As discussed in Section 2.3.2, Chemical Hazard Evaluation and Section 9.3, Chemical Screening Criteria, chemical hazards are screened for further hazard evaluation by applying criteria such as in Section A.2 of the DOE-STD-3009-2014. For some of those hazards that are not screened out, a qualitative evaluation of toxic chemical consequences is generally sufficient to provide a basis for comparison to the qualitative consequence thresholds in Table 2-8, Consequence Thresholds, of this Handbook. However, for some of those hazards that are not screened out, a quantitative evaluation may be necessary to determine impacts to CWs, the MOI, and the public, when the toxic chemical hazards have the potential to exceed the SS control selection criteria.

This section provides a simplified quantitative scoping methodology for determination of toxic chemical quantities that are sufficient to challenge the screening criteria. This scoping methodology is based on EPA-550-B-99-009 for liquid evaporation, and from a 2007 calculation, "Chemical Threshold Quantities for Safety Basis Categorization," for gas, powder, and solid releases. PAC/TEEL-2 and PAC/TEEL-3 values were adjusted for Revision 29 values (PAC, 2016). Note that this is only one type of methodology receiving a positive review. Other equivalent methodologies may be acceptable.

This scoping methodology is applied to the following toxic chemical releases:

- Gas, powder, and solid release (Section 9.8.1); and
- Evaporation of a liquid release (Section 9.8.2).

Section 9.8.3 compares the scoping methods to applicable PAC/TEEL values for the MOI high consequence case.

9.8.1 GAS, POWDER, AND SOLID RELEASE MODEL

For all of the cases presented, the downwind toxic chemical concentration, C(x), in mg/m^3, can be described by Equation 9-93:

$$\boldsymbol{C(x) = Q' \times \chi/Q(x)} \qquad \textbf{Equation 9-93}$$

Where,

Q' = release rate (mg/s)
χ/Q (x) = atmospheric dispersion factor at receptor of interest distance (x) (s/m^3)

The distinction between powders and solids is based on how they are treated in the DOE-HDBK-3010-94, and Chapter 5 of this Handbook. For gas, powder, and solid releases, the model to calculate the release rate, (Q') of a toxic chemical (i.e., MAR) that will exceed applicable PAC/TEEL values is calculated by Equation 9-94:

$$\boldsymbol{Q' = ST/t} \qquad \textbf{Equation 9-94}$$

Where,

ST = source term released to air (mg)
t = release duration (s)

Assume 900 s for 15-min (900 s) TWA as discussed in Section 9.4.1.1, Chemical Exposure Time.

The five-factor ST formula from Equation 5-1 can be reduced to ST = MARxARF based on a conservative assumption for the unmitigated analysis that all of the MAR is released or spilled (DR = 1.0), all released MAR is of respirable size (RF = 1.0)[105], and all of the airborne release within a facility is released to the environment (LPF = 1.0)[106]. Combining this conservative ST equation with Equations 9-

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[105] EPA-550-B-99-009 allows <100 µm fraction with 1.0 ARF for powders released over 10 minutes. However, this is not used in this screening calculation

[106] EPA-550-B-99-009 allows a LPF = 0.55 for in-facility deposition. However, this is not used in this screening calculation.

93 and 9-94, the MAR quantity released or spilled is presented as a function of the concentration, release duration, ARF, and atmospheric dispersion factor in Equation 9-95:

$$\boldsymbol{MAR = [C(x) \times t]/[ARF \times \chi/Q(x)]}$$ **Equation 9-95**

For this scoping calculation, estimates of ARF based on a similar logic applied for nuclear hazard categorization determinations, are assumed to be bounding for particular chemical and potential accident stresses being evaluated as follows:

ARF = 1.0 for a gas
ARF = 0.01 for a powder
ARF = 0.001 for a solid[107]

9.8.2 LIQUID EVAPORATION SCOPING CALCULATION MODEL

This EPA technique is for a 15-minute average evaporation rate. Should the analyst need to address time-varying evaporation, this technique is not recommended, as the application domain of the EPA model is insufficient. More comprehensive techniques which were presented in Section 9.5.4 are recommended.

For sub-cooled liquids, where no heated correction factor is required, the evaporation model used to calculate the release rate, Q’, is from EPA-550-B-99-009, Equation D-1 (see the EPA reference for its derivation and English to metric unit conversions that are reflected in the constants in the Equation 9-96), which is based on surface area and volume of the spill, density, vapor pressure, and molecular weight of the liquid; and wind speed; as shown in Equation 9-96:

$$\boldsymbol{Q' = \left[0.284 \times u^{0.78} \times MW^{2/3} \times A \times VP\right]/[82.05 \times T]}$$ **Equation 9-96**

Where,

Q’ = release rate (lb/min)
U = wind speed (m/s)

Assume U = 1.0 m/s, Class F Stability to be consistent with 95th percentile χ/Q.

MW = molecular weight
A = V/h = unconfined surface area of pool (1 cm depth per EPA-550-B-99-005), converted to ft)
h = dike height for confined pool (ft)
V = MAR/ρ = volume of liquid spilled (ft^3)
ρ = density of liquid = specific gravity × 1.0 g/cm^3
VP = vapor pressure at ambient temperature (mm Hg)

$$\boldsymbol{VP = [VP_{data}/T_{data}] \times 298°K\ [25℃]}$$ **Equation 9-97**

T = liquid temperature (K)

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[107] EPA-550-B-99-009 evaluates powder in solution, or solids in molten form, with different methods.

Equation 9-97 is based on the method from the calculation that adjusts the VP for temperatures other than 25°C[108] by the Ideal Gas Law.[109] VP is the most sensitive parameter for application of Equation 9-96, and can be obtained from the PAC/TEEL website for pure chemicals, or for lesser concentrations, can be obtained from chemical references such as Green and Perry (2007). As an alternate method to Equation 9-96, Figure 9-4 illustrates how the vapor pressure varies as a function of the liquid temperature for a 70 wt% nitric acid water solution. The vapor pressure data are from Table 3-16 of the Chemical Engineers' Handbook (Green and Perry, 2007), and from EPIcode predictions from a site-specific evaluation.

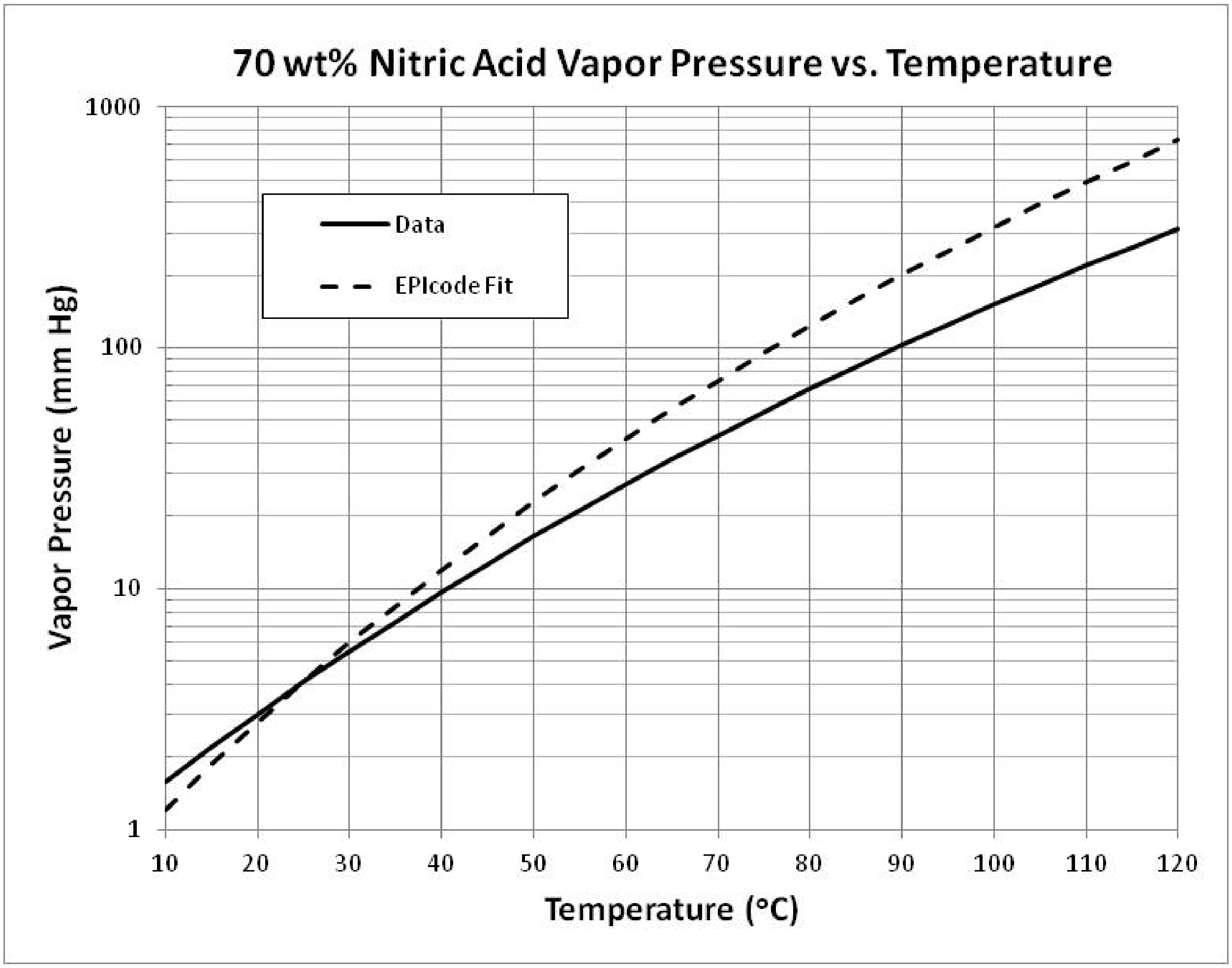

Figure 9-4. Comparison of Vapor Pressure Data vs. EPIcode Fit for 70 wt% Nitric Acid.

A recommended release rate correction factor (CF) to account for liquids with high vapor pressure at ambient T of 298°K (25°C) is shown in Eq. 9-98.

$$CF = -[P_a/VP] \times [ln(1 - VP/P_a)]$$ **Equation 9-98**

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[108] That calculation was based on 20°C, which has been revised to 25°C per the EPA methodology used for this scoping calculation.
[109] According to the linear function from zero at 0° K to the tabulated vapor pressure and temperature from a chemical reference.

Where,

P_a = 760 mm Hg ambient pressure @ Standard Temperature and Pressure, or local ambient P_a

For liquids with high vapor pressures, the corrected release rate (mg/s) becomes:

$$\boldsymbol{Q''/A = CF \times \left[0.284 \times u^{0.78} \times MW^{2/3} \times VP\right]/[82.05 \times T]}$$ **Equation 9-99**

The spill temperature, *T*, should be selected considering the range of possible liquid temperatures, consistent with the storage/operating temperature or the temperature of the environment. For common operational spills of liquids, not resulting from fire events, if conditions differ significantly from the default 25°C (77 °F) from EPA-550-B-99-009, the spill temperature should be selected as the greater of: (1) the maximum storage/operating temperature; or, (2) the highest maximum daily temperature for the previous three years (40 CFR § 68.25(d)(2)). The EPA-550-B-99-009 guidance assumes meteorological conditions for the worst-case scenario of Class F (stable atmosphere) and wind speed 1.5 m/s (3.4 mph), which is roughly equivalent to the 95th percentile dispersion condition required by DOE-STD-3009. For this conservative dispersion condition, EPA also allows use of an ambient air temperature of 25 °C (77 °F) for the worst case scenario when applying Equation 9-99, even if the maximum temperature at the site in the last three years is higher. However, an exception is provided if other methods and codes are being used). As an alternative, the analyst could consider whether an ambient temperature for conservative dispersion conditions consistent with their 95th percentile χ/Q calculation is a sufficiently conservative assumption for the spill temperature.

For spills of liquids under fire conditions where the fire is of sufficient size to cause bulk boiling of the spilled liquid, the spill temperature should be selected as the normal boiling point of the spilled material. Otherwise, the spill temperature should be selected as discussed above. Other corrections (such as VP, density) are also required as recommended in EPA-550-B-99-009.

The time to evaporate the entire MAR spilled or released, t_{evap}, is:

$$\boldsymbol{t_{evap} = [\rho \times h]/[Q''/A]}$$ **Equation 9-100**

Using Equations 9-99 and 9-100 with Equation 9-95, the quantity of toxic chemical MAR to exceed a specified concentration for high vapor pressure liquids, at a downwind distance can be calculated as shown in Equation 9-101:

$$\boldsymbol{MAR = [C(x) \times \rho \times h]/[Q''/A \times \chi/Q(x)] \times \left[900/minimum\ \left(t_{evap}, 900\right)\right]}$$ **Equation 9-101**

Note that the last term of Equation 9-101 adjusts for rapid t_{evap} < 900 s, or makes no adjustment for slow evaporation > 900 s. Thus, for evaporation that takes place over a >900 sec period, the last term is unity.

Lastly, the t_{evap} term can be modified by multiplying by % weight fraction of chemical concentration for liquids with impurities using Raoult's Law (Smith, J. M., et al., 2005).

9.8.3 SCREENING METHOD FOR MAXIMALLY-EXPOSED OFFSITE INDIVIDUAL (MOI) HIGH CONSEQUENCE

Since the release is assumed to be at ground-level, the MOI will be at the site boundary. For the MOI, the relevant inputs to Equations 9-95 and 9-101 are:

C (site boundary) =PAC/TEEL-2 (PAC, 2016)

χ/Q (site boundary) = normalized dispersion at site boundary for MOI (s/m^3)

The MOI MAR quantity of toxic chemical to exceed PAC/TEEL-2 is determined for high VP liquid releases and other releases applying Equations 9-102 and 9-103, respectively.

High VP liquid releases:

$$\boldsymbol{MAR = [PAC/TEEL-2 \times \rho \times h]/[Q''/A \times \chi/Q(site\ boundry)] \times [900/minimum\ (t_{evap}, 900)]}$$ **Equation 9-102**

Other liquid releases:

$$\boldsymbol{MAR = [PAC/TEEL-2 \times t]/[ARF \times \chi/Q(site\ boundary)]}$$ **Equation 9-103**

To estimate the MAR that could exceed the MOI moderate consequence threshold, the high consequence MAR can be multiplied by the PAC/TEEL-1/PAC/TEEL-2 ratio, or alternately, can be scaled by the moderate CW consequence MAR by the χ/Q (100 m)/χ/Q(site boundary) ratio.

The site-specific overall 95th percentile sector independent χ/Q or 99.5th percentile sector dependent χ/Q as determined by Section 6.1.10 of this Handbook, is applicable. Alternately, the following conservative assumptions can be made using the Tadmor-Gur rural dispersion factors for Class F stability and wind speed of 1 m/s, with a 3 cm surface roughness factor assumed in the modeling protocol. Note that this is the same as the reference value from the original experiments.

For illustration purposes, a minimum distance to the site boundary of 1 km is used in the following equations and in Section 9.9.

$$\boldsymbol{\sigma_z(x) = 0.2 \times x^{0.602} \times (surface\ roughness/3cm)^{0.2} = 12.79m\ at\ 1km}$$ **Equation 9-104**

$$\boldsymbol{\sigma_y(x) = 0.0722 \times x^{0.9031} = 36.97m\ at\ 1km}$$ **Equation 9-105**

$$\boldsymbol{\chi/Q\ (x) = \left[\pi \times u \times \sigma_y(x) \times \sigma_z(x)\right]^{-1} = 6.73\ E-4\ s/m^3\ at\ 1km}$$ **Equation 9-106**

9.9 EXAMPLE TOXIC CHEMICAL CALCULATIONS

Four example calculations, presented in Sections 9.9.1 through 9.9.4 representing a range of plausible release types and liquid release vapor pressures, are provided in the following subsections:

- Ammonia gas;
- Aluminum oxide powder;
- Liquid 70% nitric acid evaporation (unconfined spill); and
- Liquid 55% hydrofluoric acid evaporation (confined spill into a diked area).

These are based on the CW method, exceeding the PAC/TEEL-3 threshold. As previously indicated, these results can be scaled to estimate the quantity to exceed PAC/TEEL-2 moderate consequence for the CW or to exceed the MOI high PAC/TEEL-2 threshold or moderate PAC/TEEL-1 threshold. The last calculation in Section 9.9.4 looks at unmitigated and mitigated analyses for the CW and MOI for two PAC/TEEL criteria.

9.9.1 EXAMPLE 1: CALCULATE AMMONIA GAS QUANTITY THAT EXCEEDS PAC/TEEL-3 AT THE CW

Equation 9-103, modified for the CW χ/Q (100m) = 3.5E-3 s/m^3, applies to this example with the following inputs and assumptions:

C (100 m) = PAC/TEEL-3 at 100 m = 770 mg/m^3 [PAC, 2016] for ammonia CASRN 7664-41-7
t = 900 s [15 min TWA]
ARF = 1.0 for gaseous release
χ/Q (100m) = 3.5E-3 s/m^3

MAR = [PAC/TEEL-3 × t]/[ARF × 3.5 E-3 s/m^3]
MAR (100 m) = [(770 mg/m^3)(900 s)] / [(1.0)(3.5E-3 s/m^3)] × [lb/453.6 g × g/1,000 mg]

Conclusion: MAR = 4.37E+2 lb or greater of ammonia gas, needs to be released to exceed PAC/TEEL-3 at the CW.

9.9.2 EXAMPLE 2: CALCULATE ALUMINUM OXIDE POWDER QUANTITY THAT EXCEEDS PAC/TEEL-3 AT THE CW

Equation 9-103, modified for the CW χ/Q (100m) = 3.5E-3 s/m^3, applies to this example with the following inputs and assumptions:

C (100 m) = PAC/TEEL-3 at 100 m = 990 mg/m^3 [PAC, 2016] for aluminum oxide, CASRN 1344-28-1

t = 900 s [15 min TWA]
ARF = 0.01 for powder release
χ/Q (100m) = 3.5E-3 s/m^3

MAR = [PAC/TEEL-3 × t]/[ARF × 3.5E-3 s/m^3]
MAR (100 m) = [(990 mg/m^3)(900 s)] / [(0.01)(3.5E-3 s/m^3)] × [lb/453.6 g × g/1,000 mg]

Conclusion: MAR = 5.6E+4 lb or greater of aluminum oxide, needs to be spilled to exceed PAC/TEEL-3 at the CW.

9.9.3 EXAMPLE 3: CALCULATE LIQUID 70% NITRIC ACID QUANTITY THAT EXCEEDS PAC/TEEL VALUES AT 1 KM SITE BOUNDARY

Eq.9-102, modified for the CW χ/Q (100m) = 3.5E-3 s/m^3, applies to this example with the following inputs and assumptions: 70% nitric acid is a high vapor pressure release, and spill occurs at sea level under Standard Temperature and Pressure (STP) conditions. Note that ARF is not applicable to a liquid evaporation release, and the duration (t) is the evaporation time if less than the 15-min as used for the TWA calculation. References for the input data are included in [brackets].

PAC/TEEL-3 = 92 ppm = 240 mg/m^3 [2.58 mg/m^3/ppm from PAC, 2016] for nitric acid, CASRN 7697-37-2.

MW = 63.01 g/mol

VP = 4.49 mm Hg @ 26.4°C (299.4°K) [data provided by vendor specifications]

$VP = [VP_{data} / T_{data}] \times 298°K$

$VP = (4.49 \text{ mm Hg})/(299.4°K/298°K) = 4.47 \text{ mm Hg @ } 25°C\ (298°K)$

$SpG = 1.4134 \text{ @ } 20°C\ (293°K)$

$\rho = 1.4134 \text{ g/cm}^3$

T = temperature of liquid = ambient 25°C = 298°K

P_a = 760 mm Hg @ ambient STP

h = 1.0 cm; depth of unconfined puddle (EPA-550-B-99-005)

u = 1.0 m/s; wind speed [consistent with χ/Q wind speed assumption for Class F stability]

$Q' = [0.284 \times u^{0.78} \times MW^{2/3} \times A \times VP]/[82.05 \times T]$

$Q'/A = [0.284 \times u^{0.78} \times MW^{2/3} \times VP]/[82.05 \times T]$

$Q'/A = [0.284 \times (1 \text{ m/s})^{0.78} \times (63.01)^{2/3} \times (4.47 \text{ mm Hg})]/[82.05 \times 298K] = 8.22E\text{-}4 \text{ lb/min/ft}^2$

$CF = - [P_a / VP] \times [\ln (1 - VP/P_a)]$

$CF = - [(760 \text{ mm Hg})/(4.47 \text{ mm Hg})] \times [\ln (1 - (4.47 \text{ mm Hg})/(760 \text{ mm Hg})] = 1.003$

$Q''/A = CF \times [0.284 \times u^{0.78} \times MW^{2/3} \times VP]/[82.05 \times T]$

$Q''/A = (1.003)(8.22E\text{-}4 \text{ lb/min/ft}^2) = 8.24E\text{-}4 \text{ lb/min/ft}^2$

$Q''/A = (8.24E\text{-}4 \text{ lb/min/ft}^2)(453.6 \text{ g/lb})(\text{min}/60 \text{ s})(0.0328 \text{ ft/cm})^2 = 6.71E\text{-}6 \text{ g/s/cm}^2$

$t_{evap} = [\rho \times h]/[Q''/A]$

$t_{evap} = [(1.4134 \text{ g/cm}^3) \times (1.0 \text{ cm})]/[(6.71E\text{-}6 \text{ g/s/cm}^2)] = 2.1E{+}5 \text{ s } (\text{min}/60 \text{ s}) = 3.5E{+}3 \text{ min} > 15 \text{ min}$ (no adjustment =1).

$MAR = [PAC/TEEL\text{-}3 \times \rho \times h]/[Q''/A \times 3.5E\text{-}3 \text{ s/m}^3] \times [900/\text{minimum } (t_{evap}, 900)]$

$MAR = [(240 \text{ mg/m}^3)(1.4134 \text{ g/cm}^3)(1.0 \text{ cm})] / [(6.71E\text{-}6 \text{ g/s/cm}^2) \times (3.5E\text{-}3 \text{ s/m}^3)] \times [1] \times (\text{lb}/453.6 \text{ g}) \times (\text{g}/1{,}000 \text{ mg})$

Conclusion: MAR = 3.2E+4 lb or greater of 70% nitric acid needs to be spilled, to exceed PAC/TEEL-3 at the CW.

For perspective, a spill of 3.2E+4 lb of 70% nitric acid translates to:

Volume spilled = 2,666 gal

Puddle area = 81,271 ft^2

Puddle diameter = 322 ft

To exceed High MOI consequences at 1 km, Equation 9-102 applies with the following inputs:

PAC/TEEL-2 = 62 mg/m^3 [PAC, 2016]

χ/Q (site boundary) = 6.73E-4 s/m^3

MAR = [PAC/TEEL-2 × ρ × h]/[Q’’/A × χ/Q (site boundary)] × [900/minimum (t_{evap}, 900)]

MAR = [(62 mg/m^3)(1.4134 g/cm^3)(1.0 cm)]/[(6.71E-6 $g/s/cm^2$)(6.73E-4 s/m^3)] × [1] × (lb/453.6 g) × (g/1,000 mg)

Conclusion: MAR = 4.28E+4 lb or greater of 70% nitric acid needs to be spilled, to exceed PAC/TEEL-2 at a site boundary distance.

9.9.4 EXAMPLE 4: CALCULATE LIQUID 55% HYDROFLUORIC ACID QUANTITY THAT EXCEEDS PAC/TEEL VALUES AT 1 KM SITE BOUNDARY

Equation 9-102, modified for the CW χ/Q (100m) = 3.5E-3 s/m^3, applies to this example with the following inputs and assumptions: 55% hydrofluoric acid is a high vapor pressure release, and spill occurs at sea level under STP conditions. ARF is not applicable to a liquid evaporation release, and the duration (t) is the evaporation time if less than the 15-min as used for the TWA calculation. References for the input data are included in [brackets].

PAC/TEEL-3 = 36 mg/m^3 [PAC, 2016] for hydrofluoric acid, CASRN 7664-39-3.

MW = 20.01g/mol

VP = 50 mm Hg @ 25°C [data provided by vendor specifications]

VP = [VP_{data} / T_{data}] × 298°K

VP = (50 mm Hg)/(298°K/298°K) = 50 mm Hg

ρ = 100,000 lb /1,353 ft^3 = 73.91 lb/ft^3 [based on vendor specifications for design of a dike]
= 73.91 lb/ft^3 × 453.6 g/lb / 28,317 cm^3/ft^3= 1.184 g/cm^3

T = temperature of liquid = ambient 25°C = 298°K

P_a = 760 mm Hg @ ambient STP

h = 92.7 cm depth in dike [see liquid depth data]

u = 1.0 m/s wind speed [consistent with χ/Q wind speed assumption for Class F stability]

Q’ = $[0.284 \times u^{0.78} \times MW^{2/3} \times A \times VP]/[82.05 \times T]$

Q’/A = $[0.284 \times u^{0.78} \times MW^{2/3} \times VP] / [82.05 \times T]$

Q’/A = $[0.284 \times (1.0\ m/s)^{0.78} \times (20.01)^{2/3} \times (50\ mm\ Hg)]/[82.05 \times 298K] = 4.3E\text{-}3\ lb/min/ft^2$

CF = $-\ [P_a / VP] \times [\ln (1 - VP/P_a)]$

CF = - [(760 mm Hg)/(50 mm Hg)] × [ln (1 – (50 mm Hg)/(760 mm Hg)] = 1.034

Q''/A = CF × [0.284 × $u^{0.78}$ × $MW^{2/3}$ × VP]/[82.05 × T]

Q''/A = (1.034) (4.3E-3 lb/min/ft^2) = 4.4E-3 lb/min/ft^2

Q''/A = (4.4E-3 lb/min/ft^2)(453.6 g/lb)(min/60 s)$(0.0328 \text{ ft/cm})^2$ = 3.6E-5 g/s/cm^2

t_{evap} = [ρ × h]/[Q''/A]

t_{evap} = [(1.184 g/cm^3) × (92.7 cm)]/[(3.6E-5 g/s/cm^2)] = 3.05E+6 s (min/60 s) = 5.08E+4 min > 15 min (no adjustment =1).

MAR = [PAC/TEEL-3 × ρ × h]/[Q''/A × 3.5E-3 s/m^3] × [900/minimum (t_{evap}, 900)]

MAR = [(36 mg/m^3)(1.184 g/cm^3)(92.7 cm)]/[(3.6E-5 g/s/cm^2) × (3.5E-3 s/m^3)] × [1] × (lb/453.6 g) × (g/1,000 mg)

Conclusion: MAR = 6.9E+4 lb or greater of 55% hydrofluoric acid, needs to be spilled to exceed PAC/TEEL-3 at the CW.

For perspective, a spill of 6.9E+4 lb of 55% hydrofluoric acid translates to about 7E+3 gal for a density around 74 lb/ft^3.

To exceed High MOI consequences at 1 km, Equation 9-102 applies with the following inputs:

PAC/TEEL-2 = 20 mg/m^3 [PAC, 2016]

χ/Q (site boundary) = 6.73E-4 s/m^3

MAR = [PAC/TEEL-2 × ρ × h]/[Q''/A × χ/Q (site boundary)] × [900/minimum (t_{evap}, 900)]

MAR = [(20 mg/m^3)(1.184 g/cm^3)(92.7 cm)]/[(3.6E-5 g/s/cm^2)(6.73E-4 s/m^3)] × [1] × (lb/453.6 g) × (g/1,000 mg)

Conclusion: MAR = 2.0E+5 lb or greater of 55% hydrofluoric acid, needs to be spilled to exceed PAC/TEEL-2 at a 1 km site boundary distance.

10 HAZARD CONTROL SELECTION AND CLASSIFICATION

Hazard controls are those engineered and administrative measures that act to prevent or mitigate hazards to workers, the public, or the environment. The primary purpose of the hazard and accident analysis is to select appropriate hazard controls and classify their importance to safety.

The initial identification of selection of hazard controls typically occurs as part of the HA process and is captured in the hazard evaluation table where potential means for preventing or mitigating the hazardous conditions (or hazard scenarios as described in Chapter 2) are listed. Identification of hazard controls should start during the hazard identification phase and carry through the end of the hazard evaluation or into the accident analysis phase.

Depending on the scope of the HA, hazard controls may be selected from existing controls or proposed as new controls. For design of a planned facility or major modification to an existing facility, the HA may be used to propose controls for the facility. For an existing facility, the HA may be used to evaluate the existing controls for the facility or recommended controls that may be needed.

In DSAs prepared for DOE HC-2 and -3 nuclear facilities, control selection is based on the unmitigated evaluation of hazardous conditions and accidents scenarios[110]. An unmitigated consequence potential above a predetermined level identifies events for which SS or SC controls may be needed. The mitigated evaluation involves the functioning of designated preventive and/or mitigative hazard controls that reduce consequence, likelihood, or both.

The control selection methodology depends in part on the 10 CFR Part 830 Subpart B "safe harbor" methodology being applied for the development of the DSA or other safety basis document. There are differences between the guidance from DOE-STD-3009-94 CN3, and its successor document, DOE-STD-3009-2014, and these also are different from other safe harbor methods such as the DOE-STD-1120-2016. Also, DOE-STD-5506-2007 identifies preferred and alternate controls for a range of hazardous conditions or DBA/EBAs that exist in many types of facilities that handle or dispose of TRU waste. Nonetheless, the guidance herein is general enough to apply to most control selection applications; where specific guidance from a safe harbor method is invoked, the appropriate reference is provided.

10.1 HAZARD CONTROL SELECTION

10.1.1 HAZARD CONTROL SELECTION PROCESS

The control selection process facilitates selection of those hazard controls that are relied on to prevent or mitigate a potential hazardous condition or accident, based on formal hazards and accident analyses. The process organizes and evaluates the initial identification of hazard controls from the hazard evaluation portion of the HA then provides supplemental or specific controls that are effective in preventing or mitigating postulated accidents from the formal accident analysis. The output is a compilation of controls that are essential for protection of the public, for CWs and facility workers, and for defense in depth.

10.1.1.1 HAZARD AND ACCIDENT ANALYSIS INPUT TO CONTROL SELECTION

The hazard evaluation includes the initial identification of hazard controls that is an integral element of most hazards evaluation techniques (see Section 2.8). There are several types of hazard controls (engineered, administrative) that may be designated as part of the hazard evaluation process and various ways to organize the information.

The potential severity of each hazard or hazardous condition identified in the hazard evaluation is estimated as part of the process. Control selection as described in this section is not necessary for accident scenarios that do not meet the criteria requiring SC or SS controls (i.e., are of low consequence and/or likelihood). For such low-risk events, it is sufficient to confirm that the hazard is adequately addressed by an implemented Safety Management Program, applicable regulatory requirements, and engineering features. After attributing controls to low-risk events, the controls should be reviewed and provided consideration as defense-in-depth or as a major contributor to defense-in-depth.

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[110] The term "accident" as used in this chapter may include "hazardous conditions" and "hazard scenarios" unless it is specifically referring to DBA/EBA scenarios.

Once the hazard scenarios are identified, the HA team identifies potential controls that are available for these events and to identify candidate controls that are available to prevent or mitigate the postulated accident scenarios. The list below details common practices for organizing information:

- A typical approach is to organize information into the bounding and/or representative hazardous conditions such that a common set of controls may be effective for the conditions defined. The bounding conditions facilitate the level of importance of the control set (e.g., SC); the representative conditions provide a basis for selecting the minimum set of controls that will address a common set of hazardous conditions.
- It is usual that unique conditions exist that are not completely represented by a common hazardous condition. This means that the candidate control set may be inadequate as well. In that case, those unique conditions should be evaluated as single events for which hazard controls will be determined.
- For a broad type of hazardous condition (e.g., fire events), it may be useful to represent different magnitude conditions as separate events. In this case, smaller-scale conditions may be bounding in frequency space, while larger-scale events may be bounding in consequence, or magnitude space. It is appropriate to represent both events, as the candidate controls may be different for each. For example, the smaller event may rely on preventive measures (e.g., ignition source control) to preclude ignition of combustibles, while the larger event may rely on mitigative measures (e.g., fire-rated barriers) to reduce the consequences of a major fire.

From the initial identification of hazard controls and throughout the process, the focus is to determine those controls that are most effective and practicable in controlling a particular hazard in the conditions analyzed. The HA team makes a final selection of controls that are relied on to perform or maintain a safety function, including controls required to protect assumptions. Effective control sets generally follow the recommended hierarchy[111] from DOE-STD-3009-2014, Appendix A:

1. Engineered controls[112] that are preventive and passive;
2. Engineered controls that are preventive and active;
3. Engineered controls that are mitigative and passive;
4. Engineered controls that are mitigative and active;
5. Administrative controls that are preventive; and
6. Administrative controls that are mitigative.

While this hierarchy is preferred, it may be determined that a hazard control lower in the hierarchy is more effective, reliable, or appropriate for the facility in question and for a given scenario. In such cases, a supporting basis should be developed for the selected hazard control.

The identification of hazard controls incorporates a defense-in-depth approach that builds layers of defense against a significant release of radioactive or other hazardous materials such that no single layer of defense is completely relied upon. This does not mean that all identified Safety Management Program or other hazard controls are part of the selected set of hazard controls. The control selection process evaluates the available pool of candidate controls from the hazard and accident analyses by considering the hierarchy of controls described above. Other control selection considerations are further discussed in Section 10.1.2, such as whether they are effective, efficient, reliable, and implementable.

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[111] According to DOE-STD-3009-2014, Section A.8, an exception to this hierarchy is confinement of radioactive materials. In such cases, active confinement ventilation is preferred over passive confinement systems.

[112] Engineered controls are described as “structures, systems, and components (SSCs)” in DOE-STD-3009.

Bounding, representative and unique hazardous conditions are candidates for formal accident analysis (see Chapter 3, *Accident Analysis*). The accident analysis evaluates phenomenology associated with the various accident types as they apply to the specific facility or operations being analyzed. Hazard controls from the hazard evaluation are further evaluated in the accident analysis (based on the insights from the quantitative evaluation of accident conditions) to determine their safety classifications, as discussed later in this chapter.

10.1.1.2 HAZARD CONTROL TYPES

Controls selected are passive or active, preventive or mitigative, can be engineered or administrative, or serve to protect initial conditions or crucial assumptions in the analysis. Each is discussed below.

Preventive Control: Prevents an accident scenario or accident from happening or decreases its likelihood (frequency of occurrence). Preventative control approaches may act to prevent the initiation of an accident scenario or to interrupt an accident scenario before it leads to a hazardous condition. Prevention may also involve actions by an operator to shut down a process, close a valve, or take some other protective action. Operator actions should be sparingly relied on as a control strategy, due to inherent risk of inaction or error and overall less reliability than an engineered control. Preventive controls are functional prior to the initiation of an event, but are not required to survive the event provided the preventive function has been performed. The identification of such features is made without regard to any possible pedigree of the feature, such as procurement level or existing safety classification. Note that the elimination of a hazard (e.g., through substitution of a non-hazardous material) is not typically considered a “preventive” measure, but such action falls within the definition of a hazard control, and so should be documented when performed.

Mitigative Control: Decreases the potential consequences of the hazard scenario. It acts to reduce the severity of the hazard scenario or accident by providing barriers to an uncontrolled release of radioactive and other hazardous material or energy, such as confinement or shielding. Mitigation may also involve action by facility workers to self-protect from hazardous conditions by evacuation or sheltering, even though the accident sequence may continue uninterrupted (see Section 2.5.1, Qualitative Consequences, for determination of unmitigated consequences). Note that some hazardous conditions may not provide enough time to permit self-protective actions by workers, even if detection or monitoring capability exists.

Some controls are purely mitigative, others are purely preventative, and still others are both mitigative and preventative. Examples include:

- HEPA filtration is purely mitigative.
- The administrative control of preventing the entry of explosives into a nuclear facility is purely preventive.
- Fire suppression sprinklers can be both preventive and mitigative, but not for the same scenario (unless both functions are evaluated in an event tree analysis):
    - Suppression of the size of the fire and associated radiological or hazardous material reduces the consequence of the event (mitigative);
    - Failure of the sprinkler system may be credited to reduce the likelihood of a large fire (preventive) that has a larger radiological or hazardous material consequence than if it were credited to suppress or control the fire; or
    - Success of the sprinkler system may be credited to prevent any radiological or hazardous material release (preventive).

In practice, sprinklers are often considered preventive, that is, the controls are based on the preventive feature of sprinklers, not the mitigative, and are credited to reduce the scenario likelihood due to the failure of sprinklers, however, this is a site- or facility-specific decision.

In some cases, systems or features can serve different safety functions to different receptors. For example, shield walls are mitigative for the CW but may be preventive to facility workers by keeping them out of a high radiation area.

Engineered Control: SSCs that perform a safety function by preventing or mitigating a postulated hazardous condition or accident sequence. Engineered controls may be active or passive systems designed to function in the postulated accident environment. Active engineered controls may require one or more support systems or utilities to assure performance of their safety function. Failure mechanisms of active controls should be evaluated to identify support systems whose failure could defeat the safety function of the control. If an active control is found to not fail in a safe condition upon the loss of a support system, that support system also becomes a hazard control. Passive design features are generally more reliable than active systems when their design can withstand imposed loads or other environmental conditions postulated by the hazardous condition or accident.

When developing an engineered system, the analyst should be aware of limitations of the system and components taking into account the possibility that the event scenario may disable the functionality of the candidate control. For example, consider the limitations of a detection system. A detection system may be credited to lower a likelihood or consequence under some conditions, such as response to an alarm may be credited to reduce the potential that a small fire may become a large one and thus limit the total inventory involved. The analyst should take into account the possibility that the event scenario may disable the functionality of the candidate detection system. Necessary protective measures to prevent the loss of an engineered control due to the specific accident scenario progression will may also need to be credited as part of the hazard control.

Administrative Controls (ACs): Controls that are dependent on human actions. These controls are identified from the hazard evaluation and are designated as SACs, ACs, or are encompassed in safety management programs as committed to by a general TSR AC requirement. ACs also include (a) site/facility programs such as configuration management, (b) program elements such as control of combustible materials, and (c) safety requirements such as criticality safety limits.

DOE-STD-3009 provides a listing of safety management programs for consideration. SMPs are designed to ensure a facility is operated in a manner that adequately protects workers, the public, and the environment. By definition (10 CFR §830.3), SMPs are programs that cover topics such as quality assurance, maintenance of safety systems, personnel training, conduct of operations, criticality safety, emergency preparedness, fire protection, waste management, and radiological protection of workers, the public, and the environment. Where SMPs are selected as controls, the HA team should identify the most important elements of the program being relied upon (see DOE-STD-3009-2014, Section 4 [7.X.3]). The HA team should also determine if additional safety management programs are required based on the specific hazards present (e.g., explosives).

Depending on the situation, some ACs that perform specific preventive or mitigative functions for accident scenarios may be credited in the hazards evaluation or accident analysis. These are more specific functions than implied by general commitments to SMPs, and they may need to be raised to a higher importance level. Some of these ACs may have critical importance similar to or the same as those that would be classified as SC or SS, if the safety functions or objectives were performed by engineered safety systems. These are called SACs. SACs are selected to provide a preventive or mitigative function for specific accident scenarios, and having a safety importance equivalent to a safety SSC. A SAC may replace or augment a safety SSC when an engineered feature is not available or not practicable. SACs may also provide a limit or boundary condition for the hazard or accident analysis, such as a radioactive material inventory limit. Refer to DOE-STD-1186-2016, *Specific Administrative Controls*, for discussion of SAC types and examples, and to DOE-STD-3009-2014 discussions in Sections A.11 and A.12 regarding SMPs and SACs, respectively.

ACs and SACs may also protect initial conditions or assumptions made that provide the bounding conditions in which hazard or accident scenarios are evaluated. Initial conditions and assumptions should be explicitly identified in the event one or more of them constitute a hazard control to be further evaluated for safety classification (see Chapters 2 and 3). Controls that protect assumptions are not credited for either frequency or consequence reductions but need to be protected for basic assumptions used in the analysis (e.g., MAR) to remain valid.

10.1.1.3 USE OF RISK MATRICES FOR CONTROL SELECTION

A method to supplement control selection uses a "risk matrix" approach, encouraged by DOE-STD-3009 and DOE-STD-5506-2007. This approach begins with unmitigated risk estimates (frequency and consequences) and follows a risk ranking process to identify higher risk hazardous events and provide a qualitative tool for enhancing the selection of hazard controls. The degree to which a given hazard control is judged to be effective in performing its preventive or mitigative safety function is illustrated in the risk matrix by the movement to lower frequency and/or consequence bins as controls are applied. Although these estimates are judgment-based, consistent application provides a sound basis for comparison.

The risk ranking process bins the results of unmitigated hazard and accident analysis for the public (via the MOI receptor), CWs onsite, and optionally, for the facility workers. Table 10-1 (an adaptation of Table 2-10 from Chapter 2) establishes risk ranking bins that consider the consequence rankings from Chapter 2 Table 2-8 together with the postulated accident likelihoods defined in Table 2-9. Based on these factors, an accident is ranked as Risk Class I through IV.

Table 10-1. Typical Risk Class Matrix.

Consequence Bins

	Beyond Extremely Unlikely	**Extremely Unlikely**	**Unlikely**	**Anticipated**
High	III	II	I	I
Moderate	IV	III	II	II
Low	IV	IV	III	III

Likelihood Bins

I = Combination of conclusions from risk analysis that identify situations of major concern
II = Combination of conclusions from risk analysis that identify situations of concern
III = Combination of conclusions from risk analysis that identify situations of minor concern
IV = Combination of conclusions from risk analysis that identify situations of minimal concern

Risk Class I events for the public are addressed by hazard controls that are designated as SC SSCs or SACs, and by associated TSRs (see Section 10.2, Safety Classification of Controls) for radiological consequences or SS SSCs or SACs for chemical exposures.[113] Operational accidents resulting in high offsite radiological consequences from the hazard evaluation are moved forward into accident analysis for determination of safety classification, without consideration of likelihood. High consequence NPH DBAs as defined by DOE-STD-1020 and external events with likelihood greater than 1E-6/yr are also moved forward into accident analysis for determination of safety classification. SS controls may also be warranted for protection of the public as discussed in Section 10.2.2.

Risk Class I events for the CW are addressed by hazard controls that are designated as SS, SSCs, SACs, and by associated TSRs. Risk Class II events for all receptors, are addressed by hazard controls for which consideration as SS SSCs, SACs, and by associated TSRs should be made. The consideration of a SS hazard control is based on the effectiveness and feasibility of the controls along with the identified features and layers of defense in depth. Risk Class II events resulting in high offsite radiological consequence are included in subsequent accident analysis for determination of safety classification, without consideration of likelihood.

In essence, controls are considered for any unmitigated Risk Class I/II events. Preventive controls applied to the initial unmitigated Risk Class I/II event may suffice to prevent the event. Mitigative controls applied to the initial unmitigated Risk Class I/II event should reduce the event consequence to an acceptable value below the EG. In some cases, more than one control may be required to reduce the consequence and/or likelihood from Risk Class I/II to Risk Class III or IV depending on its reliability or efficiency.

Risk Class III – Consider defense in depth hazard controls or safety management programs to reduce risk to Risk Class IV. Risk Class III events are generally addressed by SMPs or other Administrative Controls. However, they may require further evaluation of the need for SS controls for high-consequence operational events judged to be beyond extremely unlikely. Use of qualitative risk binning does not negate the need to designate safety SSCs and/or SACs for plausible operational accidents using the consequence thresholds established in DOE-STD-3009. These events may also be considered for defense-in-depth SSCs in unique cases.

Risk Class IV – No additional hazard control measures apply that are explicitly credited with a SC/SS designation as identified in the DSA, but may still be identified in a hazard evaluation table.

As stated above, facility workers may or may not be evaluated for control selection purposes using the risk matrix approach. If included, the above risk guidelines for protection of the CW are applied for selection of controls to protect the facility worker. If the facility worker is not evaluated using the risk matrix approach, facility workers exposed to a high consequence event (as defined on Table 2-8, Consequence Thresholds) may require an SS SSC or SAC. Consequences below high generally are dealt with using an SMP or other administrative control.

When the risk matrix approach is *not* used, the designation of hazard controls as SC, SS, or SACs follow the guidance provided in Section 10.2 without the enhancement of a risk ranking to demonstrate control effectiveness.

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[113] Per DOE-STD-3009-2014 Sections 3.3.1 and 3.3.1, SC SSCs, SACs, and TSRs are established for radiological events that exceed or challenge the 25 rem Evaluation Guideline (regardless of frequency).

10.1.2 HAZARD CONTROL SELECTION CONSIDERATIONS

The hazard controls compiled from the hazards and accident analyses form the basis for control selection. Candidate hazard controls should receive specific considerations from operations, engineering, maintenance, and safety basis staff. These considerations should include the following matters.

Effectiveness

- Does the control function in the accident environment postulated? Are specific qualifications needed?
- Is the control most effective in reducing risk?
- How far from the hazard are the controls located? [114]?
- Where is the control on the control hierarchy? Is the selection justified?

Efficiency

- Is the control effective for several accidents or hazardous conditions? Does it provide defense in depth or worker safety for multiple events?
- Is the control dependent on support systems or utilities? Are these also qualified for their environment?
- Does the control minimize the number of active or supporting safety features?
- Does the control provide functional diversity or redundancy?
- Is the control cost-effective?

Implementation & Reliability

- Does the control preclude the need for compensating measures or features?
- Is the control simple or straightforward to establish, surveil, and maintain?
- Is the control insensitive to random failure or false indication?
- Does the control provide advance notification of trouble (accident does not initiate upon failure)?
- Does the control incorporate human factors to ensure reliable performance or to facilitate surveillance and maintenance?
- Is implementation of the control practicable in terms of impact on the primary process and the cost of installation and operation?

Functional and environmental requirements should be defined with due consideration of the hazard analysis, accident analysis, and design engineering processes. To develop the performance specifications for equipment relied upon in mitigating or preventing the accident under conditions existing during and following the accident scenario, consider the following.

- The time-dependent temperature and pressure at the location of the equipment during the most severe DBA/EBA.
- The humidity during the accident scenario.
- Chemical effects especially if the composition of the chemicals can be affected by equipment malfunctions.
- The radiation environment associated with the DBA/EBA during which the equipment is required to remain functional.
- Aging of equipment could cause degradation which can have an effect on the functional capability of the equipment.

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[114] In some scenarios, the closest controls may be more effective.

- Synergistic effects are to be considered when these effects are believed to have a significant effect on equipment performance.
- Interactions of the system with other environmental stresses of the accident environment, such as filter loading or water spray from fire sprinkler activation.

Selected hazard controls should reflect a robust, defense in depth approach to postulated accident scenarios. Redundancy and overlap are encouraged.

10.2 SAFETY CLASSIFICATIONS OF CONTROLS

10.2.1 SAFETY CLASS DESIGNATION

DOE-STD-3009 defines an EG of 25 rem TED to the public and requires designation of SC SSC to mitigate the dose to below the EG. The dose estimates to be compared to it are those received by a hypothetical MOI or public receptor at the site boundary from a DBA or EBA causing an unmitigated release of radioactive material that challenge the EG (see DOE-STD-3009-2014, Section 3.3.1 regarding MOI unmitigated doses exceeding 5 rem TED that may challenge the EG). The control selection process of DOE-STD-3009-2014, Section 8.1 will result in the identification of hazard controls that will prevent or mitigate DBA/EBA consequences to less than the EG. Additional controls to further reduce consequences to well below the EG or to provide defense in depth may be candidates for SS designation as discussed in DOE-STD-3009-2014, Section 8.2.2.

10.2.2 SAFETY SIGNIFICANT DESIGNATION

The designation of SS SSC is based on the criteria from Section 3.3 of DOE-STD-3009-2014 for selecting SS controls are based on four criteria: (1) protecting CWs at 100m that receive an unmitigated dose of 100 rem TED; (2) protection of the public from releases of hazardous chemicals; (3) protecting facility workers from significant injury or fatality, or from exposure to radioactive or hazardous material (not including standard industrial hazards, see Section 2.2.4); or (4) determined to be a major contributor to defense in depth that provides additional protection of the public and the environment. These four criteria are more specific than the criteria of DOE-STD-3009-94, CN3.

10.2.3 CLASSIFICATION OF OTHER HAZARD CONTROLS

The hazard evaluation process could identify preventive or mitigative controls that do not rise to the level of SC or SS controls but still enhance the safety of the facility. These controls are identified in the hazard evaluation table and may be determined to be important to defense in depth or worker safety, but not explicitly credited with a SC or SS designation. See guidance on defense in depth in DOE-STD-3009-2014, and in the DOE Guide DOE G 420.1-1A, *Nonreactor Nuclear Safety Design Guide for Use with DOE O 420.1C, Facility Safety*. Such controls are maintained in accordance with SMPs or other ACs and the Unreviewed Safety Question process (which includes consideration of equipment important to safety as described in the DOE G 424.1B, *Implementation Guide for Use in Addressing Unreviewed Safety Question Requirements*).

Specific controls may be required by DOE in its Safety Evaluation Report. (See DOE-STD-1104-2016, *Review and Approval of Nuclear Facility Safety Basis and Safety Design Basis Documents*, for further guidance.) These controls will be designated SC or SS if so directed in the SER.

10.3 EVALUATION OF EXISTING FACILITIES WITH MITIGATED OFFSITE CONSEQUENCE ESTIMATES OVER THE EVALUATION GUIDELINE

There is a special case if the MOI consequences cannot be prevented or effectively reduced to below the EG. This “Over the EG” evaluation is required for all existing DOE facilities with mitigated offsite consequence estimates over the EG, regardless of the safe harbor used. This “Over the EG” evaluation is expected to be rarely applied. The following additional guidance and methods are provided for effective implementation, when used.

DOE-STD-3009-2014, Section 3.3.1, establishes requirements for existing facilities with mitigated offsite consequence estimates over the EG where the EBA is not prevented. In addition, the DOE review and approval of the DSA includes DOE requirements and guidance for this situation, as described in the DOE-STD-1104-2016, *Review and Approval of Nuclear Facility Safety Basis and Safety Design Basis Documents*, Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG. The requirements and guidance from both standards are summarized on Table 10-2, along with additional clarifications and guidance.

Table 10-2. Over the EG Evaluation.

DOE-STD-3009-2014 Section 3.3.1, SC Controls	**DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG**	**Additional Clarifications and Guidance**
In circumstances where no viable control strategy exists in an existing facility to prevent or mitigate the consequence of one or more of the accident scenarios from exceeding the EG, the following information shall be provided in the DSA, or an attachment to the DSA:	This section provides specific approval bases for rare situations where safety class controls are not provided to prevent or mitigate offsite doses below the EG. For proposed changes to an existing facility safety basis where no viable control strategy exists in an existing facility to prevent or mitigate the consequence of one or more of the accident scenarios from exceeding the EG, DOE shall verify that information is included in the proposed safety basis change that addresses the requirements described in Section 3.3.1 of DOE-STD-3009-2014. The following criteria should be used to judge technical adequacy of DSA information:	The DSA Section [3.4.3.X.5], Summary of SC and SS SSCs, SACs, and TSR Controls, may be an appropriate location to document the “Over the EG” evaluation, or depending on its complexity, an appendix may be more suitable that is referenced in this section of the EBA evaluation. An executive summary of this evaluation should be included in the DSA Section [E.6], Safety Analysis Conclusions.
• Identification of the accidents that cannot be mitigated or prevented, including the likelihood of the events and the mitigated consequences associated with the events, based on	• Accidents that cannot be mitigated below the EG or prevented, are explicitly identified, including the likelihood of the event and the mitigated consequences associated with the event.	Accidents that cannot be mitigated below the EG or prevented, are explicitly identified in the DSA accident analysis of the EBA and further evaluated. An example of an EBA that cannot be prevented or mitigated below the EG could be a collapse of the structure from a DOE Order O 420.1C design basis earthquake that has a greater magnitude due to a 10-year

DOE-STD-3009-2014 Section 3.3.1, SC Controls	DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG	Additional Clarifications and Guidance
calculations following the methodology described in this Standard.	• Accidents likelihood and consequences are determined in accordance with the DSA safe harbor methodology (e.g., Section 3.2 of DOE-STD-3009-2014). This includes source term estimates, dispersion analysis methodology, and dose consequence assumptions.	updated assessment of seismic hazards that is being evaluated for an existing facility. Accident likelihood and consequences are summarized from information that is already part of the DSA accident analysis for the EBA such as Sections [3.4.3.X.1] Scenario Development, [3.4.3.X.2] Source Term Analysis, and [3.4.3.X.3] Consequence Analysis
• A discussion of the credited controls, including their reliability and adequacy, and an analysis ….	• The reliability and adequacy of credited controls is addressed consistent with DOE-STD-3009-2014 system evaluation requirements for SC SSCs.	This should include identifying the safety function of the credited control to prevent or mitigate the EBA as described in the DSA Chapter 4 along with a description on how they prevent the event, or reduce its likelihood or consequences. The reliability and adequacy of credited controls should be described, along with discussions of potential failure modes of these credited controls, and any compensatory measures established. This information is already part of the DSA Chapter 4 and is summarized in the “Over the EG” evaluation. Significant contributors to uncertainty in both the likelihood and consequence evaluations associated with the credited controls should be identified and characterized.
• A discussion of the available controls[60] that could reduce the likelihood and/or consequences of the associated accidents, including their potential failure modes, their potential impact on accident mitigation, any relevant cost/benefit results, and the reasons why they are not selected as credited controls to reduce the consequences to below the EG. ——— [60] Controls considered but not identified as SC controls include existing controls that were not elevated to SC status, as	• Controls considered (SSCs and SACs) but not identified as SC that could further reduce the likelihood and/or consequences of the associated accidents are described in the DSA. The impact of these controls on accident mitigation, as well as the rationale for not classifying these controls as SC should be presented. Discussions of potential failure modes of SSCs and any relevant cost/benefit results are included.	Footnote 60 clarifies other available or new controls that were considered, which could include additional MAR restriction, operational restrictions, and/or additional compensatory measures. Those existing controls (SSCs and ACs) considered but not identified as SC are identified and described, including their impact on accident mitigation or further reduction in the likelihood. The rationale for not crediting and classifying these controls as SC should be provided. Some examples include lack of reliability of the SSC that cannot be augmented with compensatory measures to provide a SC safety function, effectiveness of the control, human factors considerations to implement the AC as a SAC, and feasibility of implementing a new control. Discussions of potential failure modes of these potentially available controls and any relevant cost/benefit results should be included in the discussion. This section addresses controls that were consider that can be readily

DOE-STD-3009-2014 Section 3.3.1, SC Controls	**DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG**	**Additional Clarifications and Guidance**
well as new controls that could have been established through changes to the facility or to its operations. This includes controls to reduce the radiological source term. Controls can include SSCs and ACs.		implemented rather than those additional controls that are being committed to and identified in the next section on planned operational or safety improvements.
• A discussion of any planned operational or safety improvements, including potential facility modifications, reductions in MAR, and/or additional compensatory measures, and associated schedules, to further reduce the likelihood and/or mitigate consequences of an accident. Note: Where DOE has accepted a path forward, the path forward may be used to support this discussion.	• Planned operational or safety improvements are presented and include potential facility modifications, removal of MAR, packaging of MAR into containers, operational restrictions, and/or additional compensatory measures, and associated schedules, to further reduce the likelihood and/or mitigate consequences of an accident.	This section addresses additional measures that are being committed to, including new preventive or mitigative controls that can't be readily implemented, and are identified as planned operational or safety improvements. The STD-1104 guidance identifies some of the potential improvements, and discussion of associated schedules. Where compensatory measures that are not readily implementable will be provided, these should be clearly identified and summarized.
• A discussion of … an analysis of the expected likelihood and mitigated offsite consequence estimates of the associated accidents. The analysis should include a discussion of the significant contributors to uncertainties in both the likelihood and consequence evaluations. The analysis should compare the risk (i.e., likelihood and consequences) based on calculations performed per Section 3.2 of this Standard to the risk calculated using	• Mean or best estimate values used for source-term and dispersion input parameters that are part of comparative analyses (as described in DOE-STD-3009-2014, Section 3.3.1, bullet #2) have a valid technical basis that includes logical assumptions that are based on experiments, tests, or sound engineering judgment. The analysis describes the significant contributors to uncertainties in both the likelihood and consequence evaluations. The mean or best estimate calculation is used to provide perspective regarding the degree of conservatism that is imbedded in the consequence calculation.	A more realistic risk assessment of the EBA provides an important perspective for the contractor and DOE acceptance of risk associated with not preventing or mitigating the EBA to below the EG. This section should present any quantitative or qualitative evaluations of the risks and document the basis for risk acceptance. DOE Policy 420.1, *Nuclear Safety Policy*, establishes two goals (not requirements) for public protection: 1) The risk to an average individual in the vicinity of a DOE nuclear facility for prompt fatalities that might result from accidents should not exceed one-tenth of one percent (0.1%) of the sum of prompt fatality risks resulting from other accidents to which members of the population are generally exposed. For evaluation purposes, individuals are assumed to be

DOE-STD-3009-2014 Section 3.3.1, SC Controls	DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG	Additional Clarifications and Guidance
mean or best estimate values for source-term and dispersion input parameters (with supporting technical basis). - A qualitative or semi-quantitative comparison of the facility risk from the identified scenarios and total facility risk (i.e., cumulative risk estimate for facility accidents) with the quantitative safety objectives provided in DOE Policy 420.1. Discuss the level of risk and the basis why this risk is acceptable, taking into account an evaluation of available alternatives, the benefits to the public of the alternatives, and the costs to the public of the alternatives.	- A qualitative or semi-quantitative comparison of the facility risk from identified scenarios and cumulative facility risk (for all facility operations) estimate for facility accidents (including the results in response to the second bullet) is presented along with a comparison to the quantitative safety objectives provided in DOE Policy 420.1. A discussion of the level of risk and the basis why this risk is acceptable is provided, taking into account an evaluation of available alternatives, the benefits to the public of the alternatives, and the costs to the public of the alternatives.	located within one mile of the site boundary. 2) The risk to the population in the area of a DOE nuclear facility for cancer fatalities that might result from operations should not exceed one-tenth of one percent (0.1%) of the sum of all cancer fatality risks resulting from all other causes. For evaluation purposes, individuals are assumed to be located within 10 miles of the site boundary Site-specific or locality-specific quantitative data should be used whenever available. For the DOE Policy 420.1 risk perspectives, the risk from the facility includes the full-spectrum of operations, including normal operations, operational accidents, external events, and NPH events. Other accidents/events could be presented for perspective, such as risk of a prompt fatality or latent cancer fatalities from aircraft crashes, dam failures, fires, explosions, chlorine releases, and natural phenomena events as previously evaluated for the nuclear reactor industry.
The level of detail for the analysis above may be implemented on a graded approach that considers the remaining operating life of the facility and the extent of deviation from the EG. For example, where the remaining lifetime of the facility is less than five years, a detailed analysis using mean values and making comparisons to the DOE Policy 420.1 safety goals is not necessary, but a discussion of available controls considered and planned safety improvements and associated schedules is expected.	The level of detail for the analysis above may be graded based on the remaining operating life of the facility and the extent of deviation from the EG. The DOE review should consider the best available mission statements related to facility operations and determine whether there is a high likelihood that projected estimates of remaining operational life are supported and commensurate with details provided in the DSA. Likewise, the extent of deviation from the EG for mitigated consequences estimates should be explicitly addressed by the DOE review team and discussed in the SER as part of the approval basis. Planned operational or safety improvements, including compensatory measures, should be pursued where the deviation	

DOE-STD-3009-2014 Section 3.3.1, SC Controls	DOE-STD-1104-2016 Section 4.9, Existing Facilities with Mitigated Offsite Consequence Estimates over the EG	Additional Clarifications and Guidance
	from the EG is significant (such as where the mitigated offsite dose estimate is more than two to three times greater than the EG), the remaining life is significant (such as more than 1-3 years), and the likelihood is significant (such as more often than 1 in 10^6 years). Compensatory measures should be commensurate with the significance of the deviation from the EG, the likelihood of accidents, and the length of time needed to resolve the condition.	

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APPENDIX A: HAZARD ANALYSIS TABLE DEVELOPMENT

This appendix provides examples of the documentation of hazard analysis (HA) results to support development of a safety design basis document. Although other formats may be used to capture this information, a table format has been selected to capture the requirements. This table is prepared with columns or sections corresponding to the headings of sections A.1 through A.10 of this appendix. Those sections describe the content of the corresponding column of the table for each HA hazard scenario. This format can be used to document the Preliminary Hazard Analysis (PHA) developed during the conceptual design, or the hazard evaluation at the process level developed during the preliminary or final design. It should be updated as the design matures through final design and transition to operations.

As this documentation is a central element of the safety basis, it is maintained after project transition to operations as a basis document for the final Documented Safety Analysis (DSA) or a supporting document for the DSA. Although alternate formats such as a database may be used to capture and retrieve this information, the material identified in this appendix is required to be developed for projects subject to DOE-STD-1189-2016, *Integration of Safety into the Design Process* or its predecessor, DOE-STD-1189-2008. The appropriate HA technique is selected that will be sufficiently detailed to provide a comprehensive examination of the hazards associated with the facility given the complexity of the operation and degree of design maturity and develop the information required by this appendix. See Chapter 2, “Hazard Analysis,” for further discussion of the hazard evaluations.

A.1 SCENARIO DESCRIPTION

Describe each postulated hazard scenario that could lead to the release of radioactive and hazardous materials or energy. The description should appropriately describe the mechanisms that lead to the release. Examples include spills, over-pressurization, deflagration, fire, and similar mechanisms. This description should be as complete as possible for the current design stage to facilitate use in developing controls and their functional and design requirements, as well as support unreviewed safety question determinations during operation.

The description should also include an explicit description or reference to the Material at Risk (MAR), chemical or radiological, as appropriate, involved with or potentially affected in the scenario. As appropriate, describe the effect that the initiating event has on the major facility structures, systems, and components (SSCs), primarily those that could release energy or radioactive/hazardous material.

Scenarios identified during the PHA process for conceptual design will be facility-level or major MAR location events for the facility. The objective in conceptual design is to review the release mechanisms for the major MAR inventory locations sufficiently to ensure that high-cost safety functions have been identified and included in the project design and cost estimates.

A.2 INITIATING EVENT FREQUENCY

Provide the conservatively assigned likelihood or frequency of the initiating event of the hazard scenario, where a series of events contribute to a release of material, such as fire events or a natural phenomena hazard (NPH) followed by spill or fire. The goal is to qualitatively bin the event likelihood (Anticipated, Unlikely, Extremely Unlikely, and Beyond Extremely Unlikely) sufficiently to aid in event prevention and mitigation strategy selection. The initiating event frequency should be consistently applied as the initiator frequency.

A.3 UNMITIGATED CONSEQUENCE EVALUATION

Describe the radioactive and hazardous material or energy release with respect to facility workers in each unique location, co-located workers, and offsite public that are affected.

Identify the consequence to each receptor for the event. Although detailed knowledge may not be available, qualitative conservative determinations of dose consequences are needed so that the safety control selection is also conservative. When available, quantitative information should be used as a guide for consequences due to chemical or radioactive material releases based on bounding assumptions. However, binning into defined ranges is preferred and specific values are not required. This is especially true for facility worker consequences, which are intended to be qualitative, but also applies to qualitative estimates of co-located worker and public consequences.

Assumptions established as a part of the consequence determination should be identified, in order to provide the technical basis for parameters of interest. Particularly, the radioactive or hazardous material inventory, airborne release fraction (ARF), and damage ratio (DR) and their bases should be described. Reference appropriate calculations that support the identified consequence, when they have been performed.

While an assessment of the level of hazard scenario consequences is necessary to determine the need and safety classification of SSCs providing protection of facility workers, these assessments should be, at most, “back of the envelope” calculations, to give a sense of the order of magnitude of the doses. In the case of facility worker consequences, especially immediately involved workers, the assumptions that could be made in the course of any more definitive calculations could easily affect the results by orders of magnitude. Thus, such calculations, if used to apply a numerical criterion, would divert attention from good safety decisions to arguments about the calculations and assumptions during the review.

A.4 SAFETY FUNCTIONS

Within an operating facility, or during the preliminary and final design phases of a new facility, controls (SSCs or ACs) are already identified to perform a generic preventive or mitigative safety function. However, during the conceptual design phase of a new facility, generic safety functions are first defined instead of the controls themselves. The next entry in the hazard analysis table is a list of these generic safety functions needed to prevent or mitigate any release event. The safety function is a qualitative statement of a function that prevents an initiating event or release, or that mitigates the outcome. The safety function is the desired result from an SSC or administrative action and should be stated in a general way, while still describing the preventative or mitigative action.

For conceptual design, the safety function in this entry should not specify a SSC or otherwise state how the safety function is satisfied. This has two purposes: (1) it provides flexibility in SSC selections; and (2) it ensures that the specific functional and design attributes for a selected SSC fulfill the defined higher-level safety function identified for the event. Additional considerations in defining safety functions are as follows:

- The safety function statement during the conceptual design phase serves as a link between the HA and the safety SSCs that are later identified to fulfill safety functions, thus defining the overall objective and top-level functional requirements for the SSC. The top-level functional requirements are those performance parameters of special importance because they are specifically relied upon in the safety analysis.

- Safety functions should not be predicated on the SSCs or Specific Administrative Controls (SACs) that may be chosen to provide the function. The opportunity for novel and improved solutions is reduced when the solution drives the requirement.
- The generic safety function statement at this stage should be sufficiently specific to enable assigning appropriate supporting SSCs or SACs to fulfill the needed safety function completely.
- Safety functions should include the following:
    - situations and any general hazard scenario or accident types during which the function is required to be met;
    - specific functional needs that prevent, detect, or mitigate an event; and
    - sufficient description to enable clear functional requirements and later, design requirements and performance criteria for those SSCs ultimately chosen to meet the top-tier safety function described.

A.5 PREVENTIVE FEATURES (DESIGN AND ADMINISTRATIVE)

List all SSCs and administrative controls (ACs) that have the potential to prevent the release or the event initiator, or reduce the frequency of accident progression. This should be consistent with the approach used to determine the likelihood (see Section A.2 above). In the early stages of the conceptual design process, this listing may include SSCs that are currently not part of the conceptual design; but, if selected, would be added to the conceptual design. Initiating events that cannot be prevented, such as NPH events that lead to a release, should be listed as not applicable (N/A).

This listing will be used to select the suite of safety systems, important to safety systems, and/or defense in depth SSCs for the release events. When complete at Critical Decision-1, only SSCs actually present in the conceptual design should be included.

A.6 METHOD OF DETECTION

Identify all SSCs and administrative functions that could detect the event. This would include SSCs that may or may not be selected, as well as direct observation by the operators. In the early stages of the conceptual design process, this listing may include SSCs that are currently not part of the conceptual design.

A.7 MITIGATIVE FEATURES (DESIGN AND ADMINISTRATIVE)

List all SSCs and ACs that potentially could mitigate the event by limiting the consequences after the event has happened. In early stages of the conceptual design process, this listing may include SSCs that are not currently part of the conceptual design. Consideration of the following mitigative systems and design features should be included:

- Fire suppression/detection;
- Confinement ventilation;
- Emergency power;
- Nuclear criticality design features and/or alarms, consistent with DOE-STD-3007-2017;[116]
- Seismic design, including addressing level of confinement for primary confinement system (building structure); and

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[116] If the facility is expected to contain a critical mass of fissionable material.

- Flammable gas controls.

A.8 SSC SAFETY CONTROL SUITE AND SAFETY FUNCTIONS

Summarize the suite of hazard controls, including safety SSCs that will be relied upon to detect, prevent, or mitigate each event. The requirements in DOE O 420.1C, *Facility Safety*, are essential inputs to the identification of the safety control suite selected, the functional classification of selected SSCs, and the NPH requirements.

The hazard controls identified in the conceptual design PHA are preliminary until later safety analysis confirms their need and validates that they are the correct and adequate controls for the event. The identification of the hazard controls should be conservative to establish an appropriate cost and schedule basis for the project. The selection of hazard controls is iterative. If, after selecting one or more of the available controls, the mitigated consequence still exceeds the applicable threshold criteria, additional controls are selected or identified and classified accordingly. In some cases, it may be prudent to use multiple controls where only one may be required to effectively prevent or mitigate the event. Where SACs are included in lieu of an SSC, an explanation should be provided. The final list of selected controls should be provided in the PHA tables.

A.9 MITIGATED CONSEQUENCES

Estimate the consequences for the identified receptor after crediting the hazard controls. During conceptual design, the quantitative results for the unmitigated events may not be known. In this case, the mitigated results are qualitatively estimated based on a reduction factor on the unmitigated consequences. Once the design basis accident (DBA) analysis is performed, this section will be updated with the results of this quantitative analysis. If the preventive controls eliminate the hazard or terminate the hazard or accident scenario and prevent a release of radioactive or other hazardous materials, this result is reported in the mitigated consequence column as “prevented.” The result is input to the overall control suite of the safety design basis.

A.10 PLANNED ANALYSES, ASSUMPTIONS AND RISK/OPPORTUNITY IDENTIFICATION

List remaining analysis or assumption validations and risk/opportunities associated with the selected strategies. The bounding events that require further analysis are identified in the PHA. The events selected are grouped into DBAs that are representative of the hazardous conditions and accident categories. The DBAs are defined in such a way as to predict the consequences so as to be bounding for all similar events with the same control suite. Other events, for which the need for hazard controls (or the functional classification or NPH criteria) was not obvious, should also be evaluated in more detail (potentially quantitatively) later in the preliminary design phase. This will ensure that the selection for each safety control has a firm basis and that the assigned functional classifications and design criteria are also based on objective determinations.

Assumptions used in the PHA process need to be verified as the design matures. As an example, the facility MAR used in the hazards analysis may have been based on a highly conservative assessment of tank volumes and concentrations. When the final documents and process and instrumentation drawings are issued in preliminary design, the actual tank volumes should be used in the DBA analyses. Other assumptions concerning the event progression, such as impact to SSCs, are also verified. Remaining evaluations to be performed are identified.

Potential risks and opportunities should be fed into the Risk and Opportunity Assessment as the safety control suite is constructed. The presentation of risks and opportunities associated with the strategies are essential elements of risk-informed decision-making in the authorization for the project to proceed to preliminary design.

A.11 HAZARDS EVALUATION TABLE

Construct the final hazard evaluation table. This table includes the items discussed above and portrays the hazard scenarios associated with the facility and the safety systems that will detect, mitigate, or prevent unacceptable MAR and energetic releases. The table should present the logical binning of events evaluated. In essence, these scenarios are those from which the DBAs for the facility are selected. The table provides valuable information to be included in the risk and opportunities analysis and needed studies to validate fundamental assumptions. This table portrays the functional safety attributes for the facility safety systems that are to be incorporated into the conceptual design and cost estimates. The final table will be used as the foundation for development of the safety basis design documents, which will describe the events evaluated and the safety control suite in a format that can be used as the foundation for a final DSA for the facility.

APPENDIX B: CRITICALITY ACCIDENTS

B.1 INTRODUCTION

The purpose of this appendix is to provide guidance for the quantitative estimate of radiological doses to support the qualitative assignments of consequences for the DSA hazard evaluation as discussed in Section 2.3.2, Nuclear Criticality Hazard Evaluation, of this Handbook. As discussed in Section 2.3.2, criticality hazards are those associated with process operations, not nuclear reactors or sub-categories of nuclear reactors, such as critical experiments. The general approach to evaluate a dose from a criticality accident is:

1. Determine the fission yield (i.e., power history).
2. Determine the direct (prompt) dose at the appropriate distance.
3. Determine fission product quantities.
4. Determine the source term for inhalation dose. This includes the determination of nuclides present in the released cloud at the time of exposure, including the effects of decay during transport.
5. Determine external beta and gamma doses from the cloudshine and groundshine.

Section B.2 provides a brief overview of current regulatory requirements, recommendations, and guidance. Guidance for the first two these steps is provided in Section B.3 on determining fission yields, and in Section B.4 on direct (prompt) dose. The last three steps are briefly addressed in Section B.5 on the source term analysis of fission product inventories, airborne release fractions (ARFs) and respirable fractions (RFs), and radiological dose assessments.

Criticality accident hazards are unique to nuclear facilities and even then only to a subset of these facilities. This subset has a fissile material inventory that is significant, generally defined as exceeding the single parameter subcritical mass limits given in ANSI/ANS-8.1-2014, *Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors*, and requiring specific criticality controls to reduce the likelihood of a criticality accident to an acceptable level. This acceptable level is generally one that results in the accident likelihood being judged to be incredible.

Commonly accepted terminology, as used in the criticality safety discipline, is found in report LA-11627-MS (Paxton, 1989). In particular the following two terms are important to the discussions in this Appendix:

> **Criticality Accident:** The release of energy as a result of accidentally producing a self-sustaining or divergent fission chain reaction.
>
> **Criticality Safety:** Protection from the consequences of a criticality accident, preferably by prevention of the accident. Encompasses procedures, training, and other precautions in addition to physical protection.

Criticality accidents outside of reactors (such as process criticality accidents) are the subject of this Appendix. Criticality accidents associated with reactors, including critical experiments, are considered and analyzed under the umbrella of Reactor Safety, a separate discipline.

Process criticality accidents have been few, both in the US and worldwide, 7 and 22, respectively; and fatalities have been similarly infrequent, 2 and 9, respectively (LA-13638, McLaughlin et al., 2000). The most recent US criticality accident was in 1978 and worldwide in 1999. No accidents have resulted in any significant mechanical energy release, and radiation exposure is the only significant hazard. From criticality accidents seen to date, significant doses have only been associated with nearby facility workers, with insignificant exposures to co-located workers (CWs) outside the facility, the public, or the environment.

When criticality accident likelihoods are judged to be non-trivial in a facility, then it is almost always concluded that a criticality accident alarm system is an appropriate safety system for consequence mitigation, in accordance with ANSI/ANS-8.3-1997 (R2012), *Criticality Accident Alarm System*. Competing risks associated with the response to false alarms may rarely modify the decision as to when a criticality accident alarm should be installed.

B.2 REGULATORY REQUIREMENTS, RECOMMENDATIONS AND GUIDANCE

DOE O 420.1C, *Facility Safety*, and 10 CFR Part 830, Subpart B, both address the process analysis requirement from ANSI/ANS-8.1 Section 4.1.2:

> Before a new operation with fissionable material is begun, or before an existing operation is changed, it shall be determined that the entire process will be subcritical under both normal and credible abnormal conditions.

Credible accidents, including credible criticality accidents, are analyzed in the Documented Safety Analysis (DSA). It is assumed that controls for the prevention of criticality accidents are, or will be, in place. It is also assumed that the need for criticality alarms will be determined, and alarms installed, if required by the ANSI/ANS-8.3 evaluation. This Appendix also assumes that enough fissionable material is being handled in a manner such that any potential criticality accident is identified by the hazards evaluation. If the fissionable quantities are below the minimum subcritical limits in the appropriate ANS-standard (ANSI/ANS-8.1-2014 or ANSI/ANS-8.15-2014, *Nuclear Criticality Safety Control of Selected Actinide Nuclides*) analysis of a criticality accident may not be needed, and in this instance would not be identified in the hazard evaluation.

In addition to the guidance provided in this Appendix, ANS-8 Standards that are particularly pertinent to accident analysis include ANS-8.1; ANS-8.3; ANS-8.10 and ANS-8.23. Additional DOE guidance is found in DOE-STD-3009-2014 and in DOE-HDBK-3010-94.

B.2.1 UNMITIGATED ANALYSIS

DOE-STD-3009 provides guidance on unmitigated accident analysis. In essence, unmitigated analysis means that controls intended to prevent or mitigate an accident are assumed not to function. In the case of a criticality accident, this means, in part, that the accident is assumed to happen with no mitigative features taken into account. An exception to this is that passive safety features that can be shown to survive the initiating event may be considered in the analysis. For example, if a seismic event causes a criticality accident in a shielded area (including building walls), and the shield can be shown to survive the event, then the effectiveness of the shield in mitigating worker accident doses can be accounted for in the unmitigated analysis. Passive features assumed to perform their safety functions are evaluated per DOE-STD-3009 for designation as safety class or SS SSCs and protection as TSR controls.

For the analysis of criticality accidents that have the potential for lasting longer than an initial pulse, the accident duration should be limited to two (2) hours, except for scenarios that are slow to develop and complete. In those cases, the accident duration should be limited to eight hours (based on guidance from DOE-STD-3009). These analyses should be based on bounding scenarios. If able to be estimated, the dose integration time should be based on the power history of the postulated accident scenario.

DOE-STD-3009 requires the analysis of unmitigated accidents to determine the class of needed controls, that is, safety class or SS. For purposes of this Appendix, the need for safety class controls is based on the unmitigated consequences to the public at the site boundary, and the need for SS controls is based on the unmitigated consequences to the co-located worker. The co-located worker is 100 meters from the criticality accident for direct exposure calculations. For atmospheric dispersion, the co-located worker is 100 m from the building emission point. DOE-STD-3009 also has requirements related to selecting SS controls based on other criteria; however, these criteria are not addressed in this Appendix. In general terms, if the dose to the public at the site boundary is less than 0.05 Sv (5 rem), safety class controls are not needed, and if the unmitigated dose exceeds 0.25 Sv (25 rem) then safety class controls are required. If the dose to the co-located worker at 100 meters is less than 1 Sv (100 rem), SS controls are not needed.

For the analysis of criticality accidents, Chapter 6 of DOE-HDBK-3010-94, Change Notice 1, provides values for fission yields, and is a recognized source for other accident analysis parameters. ANSI/ANS-8.23 requires evaluation of bounding, operational-specific accidents, including locations, yields, and dose determinations. Further, for solution or solution-like criticality accidents, Appendix C of ANSI/ANS-8.23 presents data directly useful for estimating bounding first-spike and time-integrated fission yields. As with any accident parameter, fission yields should be justified and shown to be applicable to the accident situation.

A bounding criticality accident that requires further evaluation in the DSA hazard evaluation is one that would be expected to have the highest unmitigated potential radiological consequences to the co-located worker or public, and is selected from similar types of criticality accidents evaluated in the criticality safety evaluations. For example, the bounding solution criticality accident would generally involve the largest volume in a hydrogenous, liquid environment coupled with making the conservative assumption that the system reaches the prompt critical state such that the information in Figure B-1 as discussed in Section B.3.1 would be applicable. This would lead to the largest number of fissions and thus be “bounding,” which is viewed as the maximum “credible or plausible” accident yield rather than the most probable yield. Rare, extenuating circumstances such as larger accidents that are more remote or in shielded areas may result in a “bounding” accident that does not coincide with the largest number of fissions.

For both existing and new facilities the DSA or safety design basis document should provide information as to planned operations and facility layouts and features such as wall compositions and thicknesses. This information should be used with the techniques discussed in Section B.3 to estimate bounding, unmitigated fission yields.

B.3 ACCIDENT FISSION YIELDS

As with many known hazards, the understanding of, and thus the control of, the criticality accident hazard has improved dramatically since this hazard was first introduced in the 1940s with the advent of the production of significant quantities of plutonium and enriched uranium. Both the causes, largely human factors, and the personnel effects, localized to within a few to several meters of the accident location, are now well understood. Nevertheless, risks will never vanish and a thorough hazards analysis (in this case, a criticality safety evaluation) should always be performed. For operations with credible criticality accident likelihoods, fission yield determination, and, as needed, follow-on consequence analysis should be conducted.

B.3.1 FISSION YIELDS OF SOLUTION AND SOLUTION-LIKE SYSTEMS

History has shown that process criticality accidents have occurred almost exclusively in (hydrogenous) liquid media. The most common medium was fissile material in nitric acid, followed by organic solutions and then suspensions/slurries. The hydrogenous nature of the medium results in relatively slow fission excursions and insignificant likelihoods of mechanical (destructive) energy releases. The liquid nature of the medium results in a combination of instantaneous bubble generation and thermal expansion as the major feedback mechanisms for limiting the first-spike yield (fissions) of the excursion. Flooded solids such as metal fines and powders also fall into this category since the water is the dominant factor in determining the fission yield (although they have not been associated with any known criticality accidents).

ANSI/ANS-8.23, Appendix C, provides a comprehensive summary of data from criticality accident simulations in controlled environments and the application of this data to estimating accident yields, both the first spike and the steady-state fission rate should the accident not immediately self-terminate. The data cover broad ranges of important parameters, most importantly the solution volume and the reactivity insertion rate.

Two figures from reference documents, reproduced in ANSI/ANS-8.23, Appendix C, are also reproduced here. Figure B-1 shows the variation in the specific yield of the first spike for prompt critical excursions from the literature data. As is shown, for all but very rapid excursions the specific, first-spike fission yield is ~1 x 10^{15} fissions/liter.

Some of the process criticality accidents did not even reach the prompt critical state and thus had much smaller specific yields. However, this value of ~1 x 10^{15}/liter is judged to be a practical upper bound for a first spike yield for the purpose of accident analysis. None of the process accidents exhibited specific yields statistically greater than this value. The data in the figure for the very short period excursions, <10 ms, that do show larger specific yields resulted from reactivity insertion rates that are likely not credible during process accident conditions. During the accident analysis for postulated accidents the scenario development will necessarily include information that enables estimates of the reactivity insertion rate and the related reactor period.

Figure B-2 shows a curve judged to be a practical bounding envelope of the integrated specific fissions during the first 10 minutes subsequent to a prompt critical excursion that is neither self-terminating nor otherwise terminated. Application of the information in Figures B-1 and B-2 enables a conservative upper estimate to be made of both the first-spike and the integrated total number of fissions from a postulated process accident. It also enables the analyst to estimate the dose rate at various locations in order to make decisions as to immediate evacuation zone boundaries and appropriate muster locations. Finally, if this 10-minute time window is consistent with site emergency plans and procedures, then the fission yield curve in Figure B-2 would be appropriate for determining bounding co-located worker and public exposures prior to possible further personnel relocations/evacuations. To take credit for emergency response actions being a mitigating factor, a SAC may be required per DOE-STD-3009.

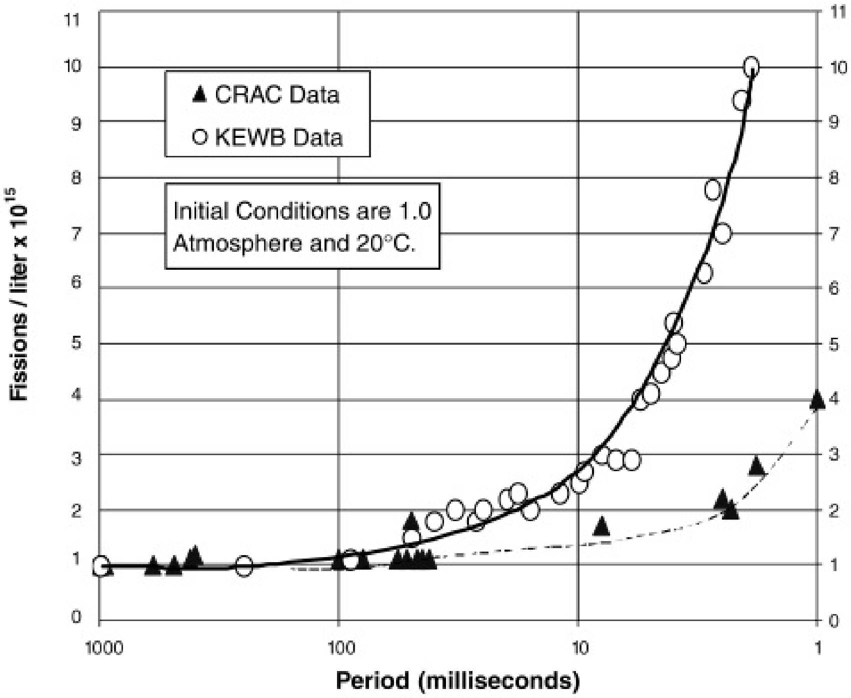

Figure B-1 – Specific fissions in first spike as a function of reactor period.
Reactor period is the time required for power to increase by Euler's number (Napier's constant)
(Extracted from Figure C.1 of American National Standard ANSI/ANS-8.23-2007 (R2012)
with permission of the publisher, the American Nuclear Society)

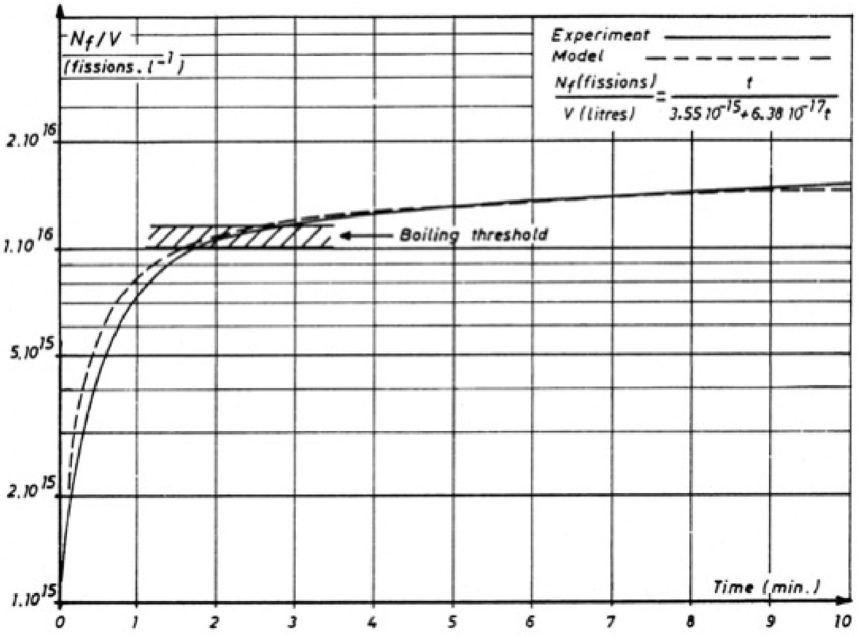

Figure B-2 – Maximum specific fission yield resulting
from criticality solution excursions in CRAC and Silene

(Extracted from Figure C.2 of American National Standard ANSI/ANS-8.23-2007 (R2012)
with permission of the publisher, the American Nuclear Society**)**

For an unmitigated accident with an 8-hour duration there is scant data upon which to base total fission/liter estimates. The Hanford (1962), Novosibirsk (1997) and Tokai-Mura (1999) accidents are the only reported process accidents to have continued fissioning for at least 8 hours. No accident simulations, such as the CRAC series, were allowed to run for more than minutes. Based on these three accidents and the reality that the fission rate is (theoretically) expected to decrease over time, and did in these three accidents, one can only estimate the ratio of the 8-hour fissions to first-spike fissions as perhaps a factor of 30.

The information contained in Figure B-2 has also been incorporated into the Nuclear Criticality Slide Rule that may also be used to estimate bounding fission yields (NUREG/CR-6504). Similar results will be attained.

B.3.2 FISSION YIELDS OF NON-SOLUTION-LIKE SYSTEMS

As the world-wide accident history shows, non-solution accidents are rare. From a review of the circumstances leading up to the one reported non-solution accident, it is apparent that this accident was enabled by a long-standing working environment that condoned significant procedural violations in the interest of expediency. It also had , as a contributing factor, a significant, negative human factors aspect. This human error situation was that the container in which the accident occurred could both accommodate a larger than critical volume/mass of metal and the contents could not be readily seen by the operator. The following should assure that similar breakdowns of operational discipline at DOE facilities be quite rare.

1. Application of DOE O 420.1C, Chg.1, *Facility Safety*, requirements;
2. A well-considered implementation of ANSI/ANS nuclear criticality safety standards; and
3. Effective oversight by both the contractor and DOE.

With well-developed Conduct of Operations programs in DOE facilities, criticality accidents in non-solution environments, be they metals, compounds/powders, or storage operations, will be rare events and may well be shown as not credible per a comprehensive application of ANSI/ANS-8.1 and DOE-STD-3007-2017, *Preparing Criticality Safety Evaluations at Department of Energy Nonreactor Nuclear Facilities*.

The non-solution fissile material types and forms discussed in the following paragraphs are those mentioned in DOE-HDBK-3010-94, Section 6.2.3, and originally documented by Woodcock, 1966. The fission yields discussed in DOE-HDBK-3010-94 are based exclusively on critical experiment experience and Woodcock's professional judgments for operations at his facility more than 50 years ago in England. In summary, the fission yields that are presented as "judged or considered to be bounding" in DOE-HDBK-3010-94, Section 6.2.3, have no technical basis when applied to process operations.

B.3.2.1 METALS/SOLIDS – ONE OR A FEW LARGE PIECES

Bounding first-spike yields with uranium or plutonium in metal/alloy form consistent with known accidents, are 1 x 10^{18} and 1 x 10^{16} fissions, respectively. For these large, judged to be bounding, first-spike yields prompt shutdown due to mechanical shock would be expected. For lesser first-spike yields a delayed-critical fission reaction is bounding and judged to produce maximum 8-hour yields of 1 x 10^{19} and 1 x 10^{18} fissions respectively. Radiation exposures from metal critical experiment accidents are known to be essentially all from direct neutrons and gamma rays with insignificant fission product releases. For fissile material operations conducted inside typical facilities with thick concrete walls that can be credited as passive design features if protected by Technical Safety Requirements (TSRs) as discussed in Section B.2.1, there would be minimal exposures to co-located workers or the MOI from these bounding fission sources.

B.3.2.2 DRY, UNMODERATED SOLIDS – NUMEROUS SMALL PIECES, AND LARGE ARRAYS

There is no accident history associated with either process or critical experiments for systems such as these (e.g., metal fines, loose oxide powders) that would be dominated by fast neutron fissions. This is judged to be primarily due to the very large critical masses that would be associated with such low-density configurations. For large arrays such as vault storage operations, Woodcock speculated on a fission yield but it is not possible to analyze such an event and relatively easy to protect against the accident by appropriate packaging of individual items. For both of these accident types the Criticality Safety Evaluations (CSEs) have been able to document no credible accident sequences.

B.3.3 FISSION YIELDS OF AUTOCATALYTIC ACCIDENTS

This deals with a criticality accident where the reactivity initially increases as the fission reaction progresses, conceptually due to the effects of temperature and pressure causing material rearrangement within the fissioning medium. One early estimate of excursion yields in a specific facility postulated an unusual accident whose reactivity initially increased due to the initial energy release (Woodcock, 1966). This type of event has not been observed in accident history. However, if the accident being evaluated has the potential for self-propagation, this should be considered.

B.4 EVALUATION OF DIRECT RADIATION DOSES

The prompt dose depends only upon the number of fissions in the criticality accident, the distance from the accident site to the receptor, and the amount of intervening shielding material, such as self-attenuation within the fissioning medium or building walls, that can be credited as passive design features if protected by TSRs as discussed in Section B.2.1. The Nuclear Criticality Slide Rule gives curves of unshielded dose as a function of distance, number of fissions, and time after the criticality accident. There is also information on the shielding effect of typical construction materials. See discussion in Section 8.2.5, Prompt (Direct) Dose.

B.5 CRITICALITY ACCIDENT SOURCE TERMS

Chapter 5, Source Term Analysis, covers source term estimation in detail depending on the accident stress on the material. For criticality accidents, however, the source term is fundamentally defined by the number of fissions occurring. This specialized subject will therefore be covered as part of this Appendix.

There are two main contributors to the criticality accident source term: fission products generated by the excursion, and releases of neutrons and gamma rays from the fission process itself. From the fission products, the major components of concern have historically been the noble gases (i.e., isotopes of krypton and xenon) and isotopes of iodine, due to their propensity to become airborne and escape filtration. However, decay products also have to be accounted for in analyzing criticality accidents.

B.5.1 FISSION PRODUCT INVENTORIES

A criticality accident generates the same types of fission products generated in spent nuclear reactor fuel. These are the primary fission product isotopes along with the subsequent decay of the initial fission products into other radioactive isotopes that, in turn, continue the decay chain. The typical pattern for total fission product activity in a criticality accident is a decrease in activity by orders of magnitude in the first 30 seconds after the criticality accident terminates. This is due to the loss of high-energy, short half-life isotopes that decay almost immediately. The activity then continues to decrease at a slower rate, with the contributions from various elements and classes of elements changing due to the ongoing decay process.

In withdrawn Regulatory Guides 3.33, 3.34 and 3.35, the NRC provided an estimate of "the radioactivity of significant nuclides released" for fuel reprocessing solutions, uranium solutions, and plutonium solutions. The criticality accident assumed had a 1×10^{18} fissions initial burst followed by 47 bursts of 1.9×10^{17} fissions each over the next 8 hours for a cumulative total of 1×10^{19} fissions. This particular scenario has not often been justified in a technical document. The significant nuclides noted were isotopes of krypton, xenon, and iodine. Their activity levels were based on the cumulative yield for the fission energy spectrum, an assumption noted as "very conservative" since it did not consider decay schemes for these nuclides.

Historical practice for DOE DSAs has been to use the information in the withdrawn Regulatory Guides 3.33, 3.34, and 3.35 for all criticality accidents, simply scaling the results to reflect total fission yields less than 1×10^{19} fissions (and eliminating the 8-hr duration for single spike criticality accidents). With the availability of modern code systems and cross sections, it is entirely feasible to calculate the fission products from a postulated criticality accident.

B.5.2 PARTICULATE RELEASE AND HEALTH RELATED PARAMETERS

As presented in Chapter 5 of this Handbook and in Chapter 6 of Handbook 3010-94, the ARFs and RFs are major parameters in determining the amount of radioactive or other hazardous material released in an accident. These parameters are normally evaluated by comparing a given phenomenology to available experimental data such as boiling of solutions or oxidation of metal. Unfortunately, no direct criticality accident release experiments have ever been conducted. Furthermore, the fission yields assigned are intended to bound fission product formation of noble gases and radioiodines, as opposed to estimating the physical changes experienced by the fissionable/fissile material and how many particulates may become airborne.

Accordingly, criticality accident release fractions have been developed only in a general sense without attempting to extrapolate them back to detailed phenomenological modeling of different accident stresses. The majority of the effort expended in developing them has also focused on the fission product release of noble gases and radioiodines. However, as related to release of particulates due to melting of metal, boiling of a solution, heating of powders, or energetic dispersal of a powder, the recommended bounding ARFs and RFs are based on experimental data for those types of changes in the materials based on the accident stresses discussed in Chapter 5.

As presented in Chapter 8, Radiological Consequence Assessment, the dose a person might receive from the fission products released by a criticality accident depends on many factors such as half lives and dose conversion factors. The primary pathways of interest from a criticality accident to receptors outside the facility are inhalation, cloudshine, and groundshine; prompt (direct) radiation may be significant for the 100 m CW, but generally not for the offsite public (MOI) due to the longer site boundary distance. These pathways are discussed in Chapter 8. Dose conversion factors for these pathways are discussed in ICRP-68, *Dose Coefficients for Intakes of Radionuclides by Workers,* and in ICRP-72, *Age-Dependent Doses to Members of the Public from Intake of Radionuclides, Part 5.*

Release estimates for solution criticality accidents derive from the now withdrawn NRC Regulatory Guides 3.33, 3.34, and 3.35 (see Chapter 6 of Handbook 3010-94). In these guides, the NRC established three assumptions. First, all noble gases are assumed to be released from solution and subsequently leave the facility. Second, it assumed that 25 percent of radioiodine ultimately escapes from the facility, either because only that much escapes from solution or because only that much of this element does not react with physical surfaces within the facility. Third, it was generically assumed that the criticality accident terminates when 25 percent of the available solution evaporates. The bounding ARF for boiling liquid is 2×10^{-3} (see Chapter 5). Applying the 25 percent factor to this ARF yields an effective release fraction of 5×10^{-4}, which the NRC originally applied to the base matrix of fissile plutonium in solution in Regulatory Guide 3.35.

However, the numerous experiments associated with the data in Figures B-1 and B-2 and 20 of the 21 known solution criticality accidents produced negligible evaporation since the boiling temperature was not reached. For those that did not shut down quickly, but fissioned for many hours, such as Tokai-Mura, the fission energy deposition was easily removed by convection cooling from the exterior of the vessel at temperatures well below the boiling point, such that no measurable evaporation occurred. Therefore, the 2×10^{-3} ARF/RF assumption of particulate releases from vigorous boiling (which was based on 90% evaporation of the solution) and its 25% reduction factor (effective 5×10^{-4} ARF/RF) may be an over-estimate, and a 3×10^{-5} ARF/RF for heating of solution in flowing air without surface rupture of bubbles (i.e., no visible surface disruption) from DOE-HDBK-3010-94 Section 3.2.1.1, Heating of Shallow Pools, may be an appropriate conservative estimate. This heating value bounds the experimental data from two experiments reported in DOE-HDBK-3010-94 Section 3.2.1.2, Heating of Pools, which exhibited simmering of the solution and a maximum ARF of 4.5×10^{-6} was measured.

The values cited above have been reiterated in NUREG/CR-6410, which also formally extended the 5×10^{-4} release fraction to the seven significant isotopes (Sr-91, Sr-92, Ru-106, Cs-137, Ba-139, Ba-140, and Ce-143). That document further noted that the 5×10^{-4} value is considered “applicable to all non-volatile compounds in the liquid.” The portion of the actinides released is assumed to be proportional to the mass of actinides in the solution as the actinides are released through the spray caused by the bursting bubbles that reach the surface of the solution. The mass of the actinides depends upon their concentration in the solution. A more detailed discussion of this phenomenology and estimating particulate source terms is provided in DOE-HDBK-3010-94, Section 6.3.1, Solutions.

B.6 CRITICALITY ACCIDENT EXAMPLE

This example assumes that there is a fissile solution that inadvertently and very rapidly accumulates in a 150-liter vessel/volume and that the system just reaches the prompt critical state as the vessel becomes full. Thus, conservatively assuming that the prompt critical state is reached and that the system remains critical, and then applying the information from Figure B-2, the first spike, 10-minute, and 2- and 8-hour fissions can be calculated as:

First spike yield = 150 liters x 1×10^{15} fissions/liter = 1.5×10^{17} fissions.
10-minute yield = 150 liters x 1.5×10^{16} fissions/liter = 2.25×10^{18} fissions.
2-hour yield = $1.5 \times 10^{17} \times 20 = 3.0 \times 10^{18}$ fissions
8-hour yield = $1.5 \times 10^{17} \times 30 = 4.5 \times 10^{18}$ fissions.

Once the total fission yield is known, a fission product inventory is determined as discussed in Section B.5.1, and estimates of particulate releases are determined as discussed in Section B.5.2. With these criticality source terms, a DOE Toolbox dispersion and radiological dose assessment code can be used to calculate the doses to the CW at 100 m and the offsite public (MOI) at the site boundary. If important, the prompt (direct) dose can be calculated as discussed in Section B.4.