DOE-EH-4.2.1.3-EPIcode Code Guidance

EPIcode Computer Code Application Guidance for Documented Safety Analysis

Final Report

U.S. Department of Energy
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FOREWORD

This document provides guidance to Department of Energy (DOE) facility analysts in the use of the EPIcode computer code for supporting Documented Safety Analysis applications. Information is provided herein that supplements information found in the EPIcode documentation provided by the code developer. EPIcode is one of six computer codes designated by the DOE Office of Environmental, Safety and Health as a toolbox code for safety analysis.

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EXECUTIVE SUMMARY

The Defense Nuclear Facilities Safety Board issued Recommendation 2002-1 on *Quality Assurance for Safety-Related Software* in September 2002. The Recommendation identified a number of quality assurance issues for software used in the Department of Energy (DOE) facilities for analyzing hazards, and designing and operating controls that prevent or mitigate potential accidents. The development and maintenance of a collection, or "toolbox," of high-use, Software Quality Assurance (SQA)-compliant safety analysis codes is one of the major commitments contained in *Implementation Plan for Recommendation 2002-1 on Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*. In time, the DOE safety analysis toolbox will contain a set of appropriately quality-assured, configuration-controlled, safety analysis codes, managed and maintained for DOE-broad safety basis applications. The Emergency Prediction Information Code (EPIcode) is designated as one of the toolbox codes (EPIcode® is a registered trademark of Homann Associates, Inc.).

EPIcode may require completion of quality assurance improvement measures before meeting current SQA standards. In the interim period before these changes are completed, EPIcode is still considered a useful asset in the support of safety basis calculations. To ensure appropriate application of the designated toolbox software, the Implementation Plan has committed to sponsoring a set of code-specific documents to guide informed use of the software, and supplement the available user's manual information.

The EPIcode guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

Use of the information contained here, although not ensuring correct use of EPIcode in each analytical context will minimize potential user errors and further standardize the use of EPIcode in appropriate regimes of applicability.

1.0 INTRODUCTION

In January 2000, the Defense Nuclear Facilities Safety Board (DNFSB) issued Technical Report 25, (TECH-25), *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2000). TECH-25 identified issues regarding the state of software quality assurance (SQA) in the Department of Energy (DOE) Complex for software used to make safety analysis decisions and to control safety-related systems. Instances were noted in which computer codes were either inappropriately applied or were executed with incorrect input data. Of particular concern were inconsistencies in the exercise of SQA from site to site, and from facility to facility, and in the variability of guidance and training in the appropriate use of accident analysis software.

During the subsequent 2000 to 2002 period, survey information on SQA programs, processes, and procedures was collected as well as the initial elements to a response plan. However, to expedite implementation of corrective actions in this area, the DNFSB issued Recommendation 2002-1, *Quality Assurance for Safety-Related Software at Department of Energy Defense Nuclear Facilities* (DNFSB, 2002). As part of its Recommendation to DOE, the DNFSB enumerated many of the points noted earlier in TECH-25, but noted specific concerns regarding the quality of the software used to analyze and guide safety-related decisions, the quality of the software used to design or develop safety-related controls, and the proficiency of personnel using the software.

DOE has developed a series of actions that address the Board's concerns, contained in the Implementation Plan for the DNFSB Recommendation, *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1.* Two of the actions include:

(i) identification of a suite of accident analysis software that is widely used in the DOE Complex, and

(ii) issuance of code-specific guidance reports on the use of the "toolbox" codes for DOE facility accident analysis, identifying applicable regime in accident analysis, default inputs, and special conditions for use.

Last year, safety analysis software for the DOE "toolbox" status was designated by the DOE Office of Environment, Safety and Health (DOE/EH, 2003). The supporting basis for this designation was provided by a DOE-chartered Safety Analysis Software Group in a technical report entitled, *Selection of Computer Codes for DOE Safety Analysis Applications*, (https://www.hss.doe.gov/deprep/archive/rec/2002-1/NNSACCodes1.pdf), and includes Version 6.0 of the Emergency Prediction Information Code (EPIcode® is a registered trademark of Homann Associates, Inc.). Subsequently, Version 7.0 of EPIcode was released in September of 2003.

It is believed that each code designated for the toolbox can be applied to accident analysis under the precautions and recommended input parameter ranges documented in the body of this report. This code-specific document will be maintained and updated until a minimum qualification software package is completed.

The contents of this report are applicable in the interim period until measures are completed to bring EPIcode into compliance with defined SQA standards. The primary objective of the guidance report is to provide information on the use of EPIcode for supporting DOE safety basis accident analysis. Specifically, the report contains:

- Applicability guidance for Documented Safety Analysis (DSA)-type analysis, specifically tailored for DOE safety analysis
- Appropriate regimes, recommended configurations
- Overcoming known vulnerabilities and avoiding code errors
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications
- Default input value recommendations for site-independent parameters, and
- Citations of currently available SQA documentation.

Thus, this report is intended to complement existing EPIcode user's documentation. The latter tends to be much broader in coverage of the full range of capabilities of EPIcode and the spectrum of inputs that might be needed depending upon the application, but lack cohesive and targeted guidance for particular applications such as DSA accident analyses. Furthermore, the goal of this document is to identify limitations and vulnerabilities not readily found in documentation from the code developer or published elsewhere.

The EPIcode guidance document is written using the following format. The first section contains an introduction and background providing an overview of toolbox software in the context of 10 CFR 830 (CFR, 2001). More information follows on the scope and purpose of this document. The next major section is a summary description of EPIcode. A third section discusses applicable regimes for using EPIcode in performing accident analysis. A large section on default inputs and recommendations, emphasizing appropriate inputs for DOE applications, succeeds this section. Following this discussion are sections on special conditions for use of the software and software limitations. A sample case is then provided, followed by acronyms and definitions, references, and appendices.

1.1 Background: Overview Of Toolbox Software In Context Of 10 CFR 830

In the context of 10 CFR 830, the Nuclear Safety Management rule, the six computer codes designated by DOE/EH as toolbox software will in time be of appropriate pedigree for support of safety basis documentation. After completion of the minimum required SQA upgrade measures for a toolbox code, the safety analyst would still need to justify the specific application with the code of interest, input parameters, and user assumptions, but many SQA burdens would be reduced from current requirements. The user would need to reference the toolbox code and version, identify compliance with their organization's SQA requirements and demonstrate that the code is being applied in the proper accident analysis context using appropriate inputs. The SQA pedigree would be sufficiently established for technical review purposes since the code is recognized as toolbox-supported.

Only six codes out of more than one hundred software packages applied in the DOE Complex for accident analysis purpose have been designated as “toolbox” codes. Other non-toolbox, dispersion and consequence software can still be applied in the context of support safety basis applications. However, each organization applying this category of software will need to demonstrate compliance with applicable SQA criteria, such as those applied to the toolbox software.

1.2 Scope

The EPIcode guidance report includes the following:

- Applicability information for DSA-type analysis, specifically tailored for DOE safety analysis
- Code development information and SQA background
- Appropriate regimes and code limitations
- Valid ranges of input parameters consistent with code capability and DOE safety basis applications, and
- Default input value recommendations for site-independent parameters.

1.3 Purpose

The EPIcode, while part of the toolbox collection of software, may still require SQA upgrades prior to meeting current established standards for software. However, until these EPIcode upgrades are completed so that EPIcode meets current established standards for software, EPIcode can be applied safely by following the guidance contained in this report is followed. Once SQA upgrades are finalized with EPIcode, it will be brought under configuration control and placed in the toolbox.

Use of the information contained here, although not ensuring correct use of EPIcode in all analytical contexts, will minimize potential user errors and the likelihood of use outside regimes of applicability.

1.4 Applicability

Even though EPIcode was developed as a tool for emergency response and emergency preparedness/planning, it is also widely used throughout the DOE complex to support 10 CFR 830 safety analysis. Note that this guidance document does not specifically address application issues related to emergency response or emergency preparedness/planning.

It is recognized that other computer codes besides EPIcode exist that perform similar source term and downwind concentration calculations. Moreover, manual or electronic spreadsheet calculations can be a viable alternative to using a computer code for many accident analysis applications that involve chemical spills. The relative merits of using a different computer program or using a hand calculation for a given application is a judgment that must be made by the analyst on a case-by-case basis.

The U.S. Department of Energy (DOE) has provided guidance and general recommendations in this area through the Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program. As part of this program, the Chemical Dispersion and Consequence Assessment (CDCA) Working Group (WG) was established to address issues and evaluate methodologies in the CDCA domain. Other WGs were also established for other domains of safety analysis (i.e., fire analysis, explosion analysis, spill source term analysis, in-facility transport analysis, and radiological dispersion and consequence assessment). The CDCA WG (also referred to as WG 6) issued a report that identifies and evaluates methodologies and computer codes to support CDCA applications (Lazaro, 1997). Also of interest is the WG 3 report, which performed a similar function for source term analysis of spills (Brereton, 1997). In addition to code recommendations, both the Spills WG 3 report and the CDCA WG 6 report also provide a broad set of recommended "best practices" for modeling chemical releases to the atmosphere for safety analysis applications.

This report complements the WG 3 and WG 6 work to provide guidance and recommendations that are targeted to the use of the EPIcode to calculate source terms and downwind concentrations for safety analysis applications.[1]

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[1] The spills and CDCA working group reports did not specifically evaluate EPIcode as it limited its scope to public domain codes and thus did not consider proprietary codes such as EPIcode (Brereton, 1997; Lazaro, 1997). Since the EPIcode uses similar types of input data as other codes evaluated by the working groups to calculate chemical source term and downwind concentrations, much of the input guidance in the WG 3 and WG 6 reports can be applied to EPIcode as well.

2.0 SUMMARY DESCRIPTION OF EPICODE

This section provides a summary form description of the EPIcode. A brief overview is given with additional information to follow in other sections and appendices of the report to provide more in-depth coverage of topics such as the principles of source term development for analysis of accidents that involve chemical inventories, the interface with dispersion conditions in the atmosphere, and the overall assessment of toxicological exposure to receptors.

2.1 EPIcode Development

The version of EPIcode that is addressed by this report is Version 7.0 (released in September 2003). EPIcode was developed by Homann Associates, Inc., which maintains and upgrades the code. The code is commercially available from Homann Associates, Inc. The technical contact for EPIcode is the code author, Steven Homann (www.epicode.com or epicode@aol.com).

A history of its development is shown below (Mazzola, 1995; EPIcode, 2003):

- Version 3.0 (1988): First release beta test complete.
- Version 3.5 (1989): Incorporation of user input sampling time.
- Version 4.0 (1990): Incorporation of liquid spill model.
- Version 5.0 (1993): Incorporation of high-resolution graphics
- Version 6.0 (1996): Incorporation of fire and explosion models
- Version 7.0 (2003): Revised evaporation model[2] and fuel fire model

EPIcode Version 7.0 is a full 32-bit Microsoft™ Windows software package that will run on an IBM PC or compatible. Operating systems supported are Windows 95/98/00/NT and XP.

2.2 EPIcode Summary Description

EPIcode performs calculations for chemical source terms and resulting downwind concentrations. Source term calculations determine the rate at which the chemical material is released to the atmosphere, release height, release duration, and the form and properties of the chemical upon release. The term cloud is used in this document to refer to the volume that encompasses the chemical emission. In general, the released chemical may be a gas, a vapor, or

[2] EPIcode has revised the spill model per EPA document "Risk Management Program Guidance for Offsite Consequence Analysis," United States Environmental Protection Agency, EPA 550-B-99-009, April 1999. Appendix D – Technical Background, pg. D-2 (EPA, 1999). The mass transfer coefficient of water is now assumed to be 0.67; the value of the factor that includes conversion factors, mass coefficient for water, and the molecular weight of water to the one-third power, originally 0.106, is now 0.284. The net result is an evaporation rate that is 2.68 times greater than previous versions of EPIcode.

an aerosol. The aerosol release may consist of either solid (e.g., fume, dust) or liquid (e.g., fog, mist, spray) particles that are suspended in a gas or vapor medium. Liquid particles are also referred to as droplets.

The analyst specifies the chemical and then either specifies the chemical source term rate or provides EPIcode with the necessary information and data to calculate a steady evaporation rate when the scenario involves a spill of a chemical liquid. Releases may be elevated either through discharge from a stack or as a result of plume rise from buoyancy or momentum effects.

Evolution of the mean concentration field of the chemical cloud is calculated through algorithms that model turbulent flow phenomena of the atmosphere. The prevailing wind flows and associated atmospheric turbulence serve to transport, disperse[3], and dilute the chemical cloud that initially forms at the source. For an instantaneous release or release of short duration, the chemical cloud will travel downwind as a puff. In contrast, a plume will form for a sustained or continuous release.

The wind velocity is a vector term defined by a direction and magnitude (i.e., wind speed). The wind direction and wind speed determine where the puff or plume will go and how long it will take to reach a given downwind location. For sustained or continuous releases, the wind speed has the additional effect of stretching out the plume and establishing the initial dilution of the plume (i.e., determines the relative proportion of ambient air that initially mixes with the chemical source emission). Atmospheric turbulence causes the puff or plume to increasingly mix with ambient air and grow (disperse) in the lateral and vertical direction as it travels downwind. Longitudinal expansion also occurs for a puff. These dispersion effects further enhance the dilution of the puff or plume. The two sources of atmospheric turbulence are mechanical turbulence and buoyant turbulence. Mechanical turbulence is generated from shear forces that result when adjacent parcels of air move at different velocities (i.e., either at different speeds or directions)[4]. Fixed objects on the ground such as trees or buildings increase the ground roughness and enhance mechanical turbulence in proportion to their size. Buoyant turbulence arises from vertical convection and is greatly enhanced by the formation of thermal updrafts that are generated from solar heating of the ground.

[3] The term dispersion is sometimes used in the literature to describe the combined effects of advection (transport by the bulk motion of the wind flow) and turbulent diffusion (spreading) and other times, particularly in meteorological publications, to describe only the turbulent diffusion component. The latter, narrower sense is used in this document.

[4] Atmospheric flows experience a change in speed with height due to the friction of the earth's surface in slowing down the wind adjacent to it.

EPIcode considers the chemical cloud emission to be neutrally buoyant[5] and applies standard Gaussian puff and plume models as appropriate. A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow. Appendix A contains additional discussion on the role of atmospheric turbulence, wind speed, and other parameters on downwind puff or plume concentrations, especially as these parameters relate to the Gaussian transport and dispersion models.

In addition to the source term and downwind concentration calculations, EPIcode supports the use of concentration limits for the purpose of consequence assessment (e.g., assessment of human health risks from contaminant plume exposure). When available, data for Immediately Dangerous to Life or Health (IDLH), Emergency Response Planning Guidelines (ERPGs), Temporary Emergency Exposure Limits (TEELs), and Acute Exposure Guideline Limits (AEGLs) have been incorporated into the chemical library of EPIcode as discussed in Section 4.1.

[5] In the strictest sense, neutrally buoyant conditions exist when the density difference between the released chemical cloud and ambient air is small. A positively buoyant cloud is produced when the cloud density is significantly less than that of the ambient air. The positive buoyancy induces puff or plume rise that results in an effective elevated release that EPIcode can calculate with the necessary user-supplied inputs as discussed in Section 4.3.4. The Gaussian puff and plume models are used for both neutrally buoyant and positively buoyant releases.

3.0 APPLICABLE REGIMES

The objective of this section is to present a discussion of EPIcode applicability from two perspectives: (1) in terms of its overall function as a key step in accident analysis; and (2) noting the phenomenological regimes in which it provides an approximate model of dispersion in the environment and the resulting toxicological exposure to downwind individuals (receptors).

3.1 Overall Application in Safety Analysis

The EPIcode is in the toolbox under the area of applicability of chemical release and dispersion and consequence assessment. A code of this type of is used primarily to calculate the release rate to the atmosphere of a chemical involved in an accident scenario and the resulting instantaneous or time-averaged concentration of a chemical downwind from the accident. Because the DOE does not have an evaluation guideline for chemicals, the chemical concentration calculated is not used to distinguish safety-class designation for systems, structures, and components. A typical use of chemical consequence results is to confirm the selection of safety significant systems, structures, and components for worker protection.

Occasionally, chemical concentrations are used to help set limits on chemical inventory, and this may present more of a safety implication. When these code calculations are used to help set inventory limits, they have a direct effect on values used in technical safety requirements, and the quality of the calculation may be very important. Again, it is important to note that a hand calculation can often be used to verify this value.

In this context of setting limits on chemical inventory, analysts have generally applied the American Industrial Hygiene Association (AIHA) ERPGs[6] and TEELs[7] for the purpose of

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[6] The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The ERPGs are estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

> ***ERPG-1***: *The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*
>
> ***ERPG-2***: *The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*
>
> ***ERPG-3***: *The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

assessing human health effects for both facility workers and the general public (Craig, 2001). Recently, another alternative has become available to analysts. The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) has been developing acute exposure guideline levels (AEGLs) to assist federal and state agencies and private sector organizations with their need for short-term hazardous chemical exposure information in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h).[8]

Since the DOE has not provided definitive evaluation guidelines for chemical exposures for use in DSAs, the specific use of ERPGs, TEELs, and AEGLs in accident analysis remains largely an open issue. It is recommended that guidance from subject-matter experts be followed (Craig, 2001). In some cases, surrogate values for inventory limits, such as Environmental Protection Agency (EPA) or Occupational Safety and Health Administration (OSHA) limits can also be used.

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[7] The temporary emergency exposure limits (TEELs) are another set of chemical-specific concentrations that correspond to varying levels of health effects (Craig, 2001). TEELs have been developed since ERPGs are available only for a limited number of chemicals. The TEELs consist of (a) ERPG values for all chemicals for which ERPGs have been published and surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values), and (b) Permissible Exposure Limit - TWA (PEL-TWA) values for all chemicals for which PEL-TWA values have been published and surrogate PEL-TWA values for additional chemicals (i.e., the TEEL-0 values) (Craig, 2001). PEL-TWA values are developed by the Occupational Safety & Health Administration (OSHA) for use in limiting worker exposures to airborne chemicals (CFR, 1999). Most people are not expected to experience any adverse health effects to accident exposures at the TEEL-0 level (Craig, 2001).

[8] The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) is developing AEGLs in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h) and three severity levels as defined below:

AEGL-1: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL-2: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL-3: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

3.2 Phenomenological Regimes of Applicability

The atmospheric transport and dispersion algorithms of EPIcode are based on the Gaussian models for puffs and plumes. These models are best suited for specific types of conditions. The chief phenomenological regimes for applying EPIcode include:

- Temporal regime – These models are best suited for "short" duration plumes, ranging from approximately several minutes to several hours.
- Spatial regime - The class of code also does not model dispersion close to the source (less than 100 meters from the source), especially where the influence of structures or other obstacles is still significant. Dispersion influenced by several, collocated facilities, within several hundred meters of each other should be modeled with care. Similarly, EPIcode should be applied with caution at distances greater than ten to fifteen miles, especially if meteorological conditions are likely to be different from those at the source of the release, or are likely to change in time during the release or during transport. Long-range projections of toxicological exposures are better calculated with mesoscale, regional models that are able to account for multiple weather observations.
- Terrain variability – Gaussian models are inherently flat-earth models, and perform best over regions of transport where there is minimal variation in terrain.
- Extreme weather – Gaussian models do not apply to extreme weather conditions such as tornadoes.
- Atmospheric transport and dispersion basis – The Gaussian models for atmospheric transport and dispersion, as used in EPIcode, were developed for and are directly applicable to neutrally buoyant releases in which the initial chemical cloud density is approximately equal to that of the ambient air. A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow.

  If the density of the initial chemical cloud is greater than that of the ambient air, however, then the possibility exists for dense-gas type of atmospheric transport and dispersion. As atmospheric air mixes with the cloud, dilution occurs that causes dense gas transport effects to essentially become negligible as the density of the plume mixture approaches that of the ambient air. All dense gas releases, therefore, eventually transition to transport and dispersion that is characteristic of a neutrally buoyant plume. So, the Gaussian models are frequently used when the receptors of interest are far from the source, even when the released cloud is likely to exhibit dense-gas behavior near the source.

  With dense-gas type of releases, the released cloud resists the influences of the hydraulic pressure field associated with the atmospheric wind and alters the atmospheric wind field in its vicinity. Dense-gas behavior can potentially occur for gases with densities greater than air or with a chemical cloud with sufficient aerosol content such that the bulk cloud density is greater than that of the ambient air. Dense-gas behavior is more likely to occur with higher release rates and lower wind speeds.

The basis for identifying the potential for dense-gas effects is the Richardson (Ri) number. The Ri number represents a relative measure of the potential energy of the cloud with respect to the mechanical turbulent energy of the atmosphere. The source Ri (Ri_o) number, above which dense gas transport effects are assumed important, is typically considered about 50 (Hanna, 1996).

- $Ri_o \leq 50$ For neutrally buoyant atmospheric transport and dispersion
- $Ri_o > 50$ For dense-gas atmospheric transport and dispersion

It should be noted that an absolute threshold value does not actually exist. Dense-gas effects may begin to appear for Ri_o values as low as one and become more pronounced as Ri_o is increased.

For an instantaneous release, the Ri_o is defined as follows (Hanna, 1996):

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_i}{\rho_a \times D_o^2 \times u_*^2} \qquad \text{(Equation 3-1)}$$

Where,
$\rho_a \equiv$ Ambient air density
$\rho_o \equiv$ Released chemical density at source
$Q_i \equiv$ Instantaneous volumetric release
$D_o \equiv$ Scale dimension of the source
$u_* \equiv$ Friction velocity

For a continuous release, the Ri_o is defined as follows (Hanna, 1996):

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_c}{\rho_a \times D_o \times u_*^3} \qquad \text{(Equation 3-2)}$$

Where, $Q_c \equiv$ Continuous volumetric release rate

The friction velocity is equal to about 5% to 10% of the mean wind speed at the height of 10 m (Hanna, 1996). For a ground level release, the length scale parameter D_o represents the initial width or diameter of the cloud or plume before mixing with and transport by ambient air. For a release out of a stack, D_o represents the diameter of the stack (neglecting any boundary layer effects that would reduce the effective diameter of the jet or plume leaving the stack). For releases from evaporative or boiling pools, D_o is set equal to the pool diameter.

Note that alternative definitions of Ri_o and corresponding dense-gas dispersion criteria are found in published literature and used in atmospheric transport and dispersion codes.[9]

[9] For example, the Areal Locations of Hazardous Atmospheres (ALOHA) code substitutes "$u_{10} \times u_*^2$" for "u_*^3" in Equation 3-2, where u_{10} is the mean wind speed at a height of ten meters, and uses a critical Ri_o value of one (Reynolds, 1992).

4.0 INPUTS AND RECOMMENDATIONS

Input data on chemical properties, source configuration, and meteorological conditions in general factor into EPIcode calculations of downwind concentrations of released chemicals as a function of downwind distance. For a liquid spill of chemicals with a known vapor pressure, EPIcode algorithms calculate the evaporative release rate of the chemical into the atmosphere. For other release types, the user specifies the airborne release rate or equivalently the combination of the quantity released airborne and the release duration.

This section discusses and recommends input parameters needed to execute EPIcode. While emergency management applications can be supported with EPIcode, the emphasis here shall be on the type of inputs for supporting accident analysis in a DSA.

4.1 EPIcode Overview

The basic output that is produced by EPIcode is a table or graphical representation of downwind concentrations of released chemicals as a function of downwind distances. Example output including the concentration isopleth, tabular data, and X-Y plot, is shown in Figures 4.1 through 4.3, respectively, for a chlorine release.

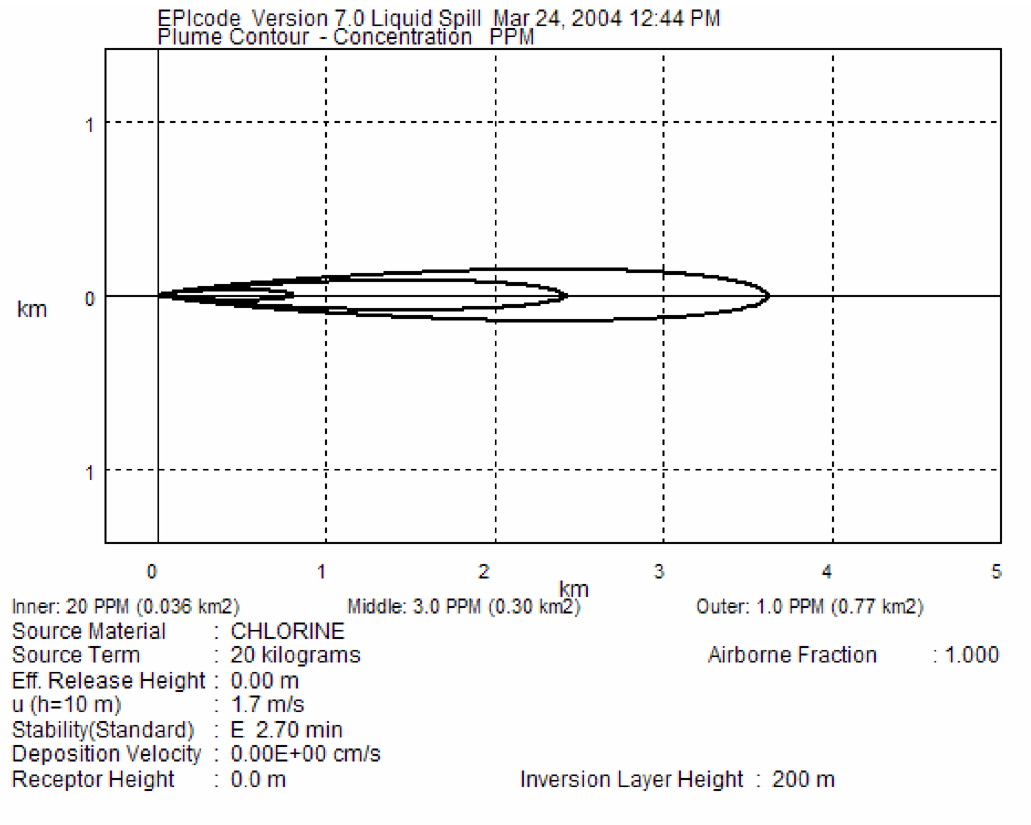

Figure 4-1. EPIcode Graphical Output – Contour Plot.

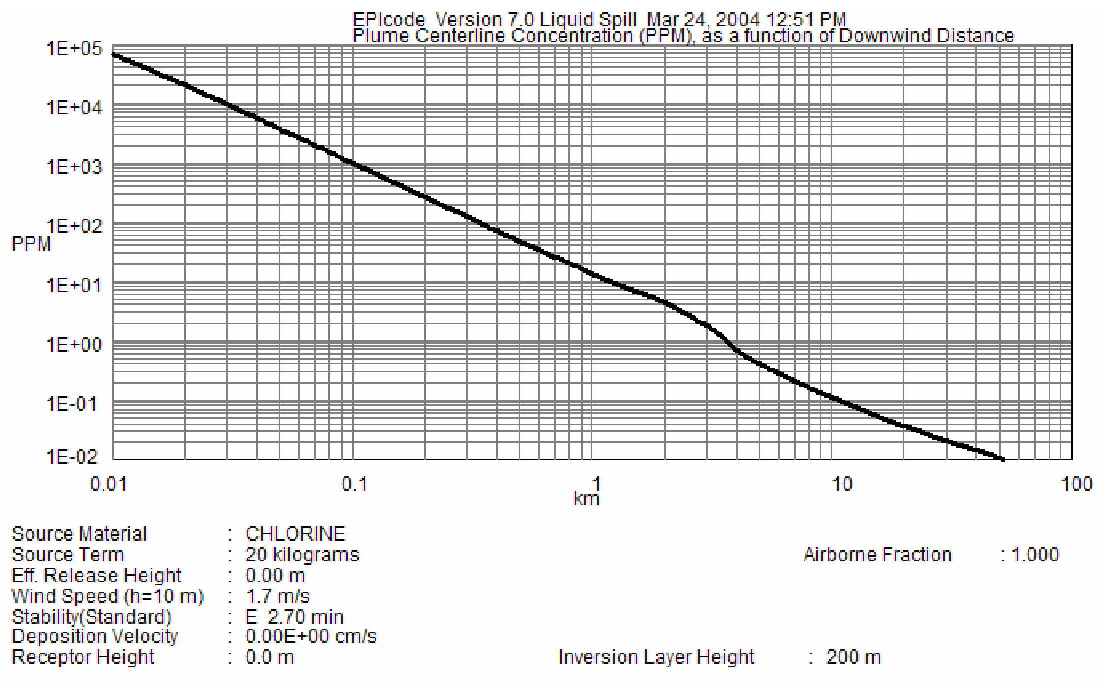

Figure 4-2. EPIcode Graphical Output – X-Y Plot.

```
EPIcode  Version 7.0 Liquid Spill
Mar 24, 2004 12:52 PM

Source Material            : CHLORINE
CAS Number                 : 7782-50-5
Source Term                : 20 kilograms
Spill Area                 : 1.36 m2
Spill Temperature          :25.0 deg C
Spill Vapor Pressure       : 5.74E+03 torr
Airborne Fraction          : 1.000
Evaporation Rate           : 124 gram/sec
Total Evaporation Time     : 2.7 minute
Physical Height of Spill   : 0 m
Wind Speed (h=10 m)        : 1.7 m/s
Distance Coordinates       : All distances are on the Plume Centerline
Stability Class (Standard) : E
Deposition Velocity        : 0.00E+00 cm/s
Receptor Height            : 0.0 m
Inversion Layer Height     : 200 m
Sample Time                :  2.70 min
Maximum Concentration      :  66,000   PPM
Max Concentration Distance : 0.010 km
ERPG-1                     : 1.000 PPM
ERPG-2                     : 3.000 PPM
ERPG-3                     : 20.00 PPM
Exceeds ERPG-1 Out To      : 3.60 km
Exceeds ERPG-2 Out To      : 2.40 km
Exceeds ERPG-3 Out To      : 0.80 km
```

DISTANCE km	MAXIMUM CONCENTRATION (mg/m3)	(PPM)	ARRIVAL TIME (hour:min)
0.030	28,000	9,600	<00:01
0.100	2,900	990	00:01
0.200	770	260	00:03
0.300	350	120	00:05
0.400	210	71	00:06
0.500	140	47	00:08
0.600	98	34	00:10
0.700	74	26	00:12
0.800	59	20	00:13
0.900	48	16	00:15
1.000	40	14	00:17
2.000	13	4.3	00:34
4.000	1.9	0.66	01:08
6.000	0.82	0.28	01:43
8.000	0.47	0.16	02:17
10.000	0.32	0.11	02:52
20.000	0.10	0.036	05:44
40.000	0.040	0.014	11:28
60.000	0.024	0.0084	17:13
80.000	0.017	0.0060	22:57

Figure 4-3. EPIcode Tabular Output.

The first step in using EPIcode for chemical consequence analysis is to select the chemical. EPIcode 7.0 contains a library of over 2,000 toxic substances along with the associated exposure levels accepted by various professional organizations and regulatory agencies. These include the AIHA ERPGs, TEELs, and AEGLs. Typical units are milligram per cubic meter (mg/m^3) or parts per million (ppm). The DOE has not provided definitive evaluation guidelines for chemical exposures, so the specific use of exposure limits in accident analysis remains an open issue. It is recommended that guidance from subject-matter experts be followed (Craig, 2001).

The EPIcode library also contains information on substances that are listed in the Threshold Limit Values (TLVs) for Chemical Substances and Physical Agents and Biological Exposure Indices published by the American Conference of Governmental Industrial Hygienists (ACGIH).[10] IDLH data are also included when available.

Substance information is retrieved from the library by selecting the substance name or common synonym, U.S. Department of Transportation (DOT) Number, or Chemical Abstract Service (CAS) Number. Chemical property data in the library include molecular weight, specific gravity, boiling point, melting point and vapor pressure.

The user may add new chemicals to a user-defined chemical library and supply associated property, identification, and exposure limit data. Data in the EPIcode-supplied chemical library, however, cannot be altered. This prevents unintended corruption by the user of the EPIcode library, but a disadvantage of this setup is that data cannot be updated. For example, the user cannot readily update ERPG data when the ERPG data for a chemical is revised, as occasionally happens. A way to circumvent this limitation is to add the particular chemical to the user chemical library with the same information as in the EPIcode-supplied library, but with the updated ERPG data.

4.2 Input Recommendations for Source Term Parameters

EPIcode models five types of releases to the atmosphere:

- Term Release

---

[10] The time-weighted average TLV (TLV-TWA), the short-term exposure limit TLV (TLV-STEL), and ceiling TLV (TLV-C) are defined as follows.

> ***TLV-TWA****: The time-weighted average concentration for a normal 8-hour workday and 40-hour workweek, to which nearly all workers may be repeatedly exposed, day after day, without adverse effect.*
>
> ***TLV-STEL****: The concentration to which workers can be exposed continuously for a short period of time without suffering from 1) irritation, 2) chronic or irreversible tissue damage, or 3) narcosis of sufficient degree to increase the likelihood of accidental injury, impair self-rescue or materially reduce work efficiency, provided that the daily TW is not exceeded.*
>
> ***TLV-C****: The concentration that should not be exceeded during any part of the working exposure.*

  - Surface Line Source
  - Elevated Line Source
  - Surface Area Source
  - Elevated Area Source
  - Point Source
- Continuous Release
  - Surface Line Source
  - Elevated Line Source
  - Surface Area Source
  - Elevated Area Source
  - Point Source
- Liquid Spill Release
- Fire Release
- Explosive Release

With the first two release types, the source may be modeled as a point, a line, or an area. With the line and areas source models, the cloud at the source location has a finite dimension in either one or two directions. The EPIcode algorithms translate each source dimension into a virtual source that is upwind of the actual source. Thus, credit is taken for initial distribution of the cloud in the form of an initial effective dispersion that lowers predicted cloud centerline concentrations particularly at short distances from the source (in comparison to modeling the release with a point source at the actual source location). This effect becomes increasing less significant as the plume travels further away from the source. The liquid spill release, fire release, and explosive release all employ area source models.

A term release differs from a continuous release in that it is of finite duration. As the release duration increases, the results from the term-release model approach that from the continuous-release model for equivalent specifications of release rates and other input variables. At the other end of the spectrum for term releases (i.e., releases of very short duration) is the instantaneous release. When the user specifies an instantaneous term release, EPIcode uses the puff model. For other term releases (i.e., non-instantaneous), EPIcode automatically selects the puff or plume equation at each downwind location based on the relative dimension of the cloud width with respect to the cloud length. When the cloud length is less than the cloud width, the puff equation is considered to be a more accurate model of the dispersion. Continuous releases are always modeled as plumes.

The airborne release rate to the atmosphere is established in one of three ways for the various types of releases:

- Specify source term rate directly – applicable to continuous release type

- Specify source term quantity and release duration – applicable to term release type; for fire and explosive release types, the quantity is specified by the user and EPIcode determines the release duration
- Let EPIcode calculate an evaporative release rate – applicable to liquid spill type release (when vapor pressure for chemical is known).

For specification of the source term rate or source term quantity, EPIcode accepts the input on a mass or volume basis (usually with a choice of units) at the preference of the user.

4.2.1 Source Term Rate

The user specifies this input signifying the rate at which the chemical substance is made airborne for continuous releases. The basis for the input can be measurement, but for DSA applications will likely be an external calculation. The latter can be the result of either a manual calculation or the output from another code. Note that for the liquid spill release, EPIcode internally calculates the airborne release rate and the release duration corresponds to the total time for all the liquid to evaporate.

Recommendation: Calculated downwind concentrations are proportional to the release rate. So, the release rate should be conservatively estimated on the high side if there is some uncertainty or variability with its value. In some scenarios, variability results from an unsteady source term rate. The use of a time-weighted average (TWA) is typically used in these situations. For example a peak 15-minute TWA is recommended for some situations as discussed in Section 4.4.2 (Craig, 2001).[11] Note that the analyst should normally specify the sample time input that is discussed later in Section 4.4.2 in a manner that is consistent with or conservative with respect to the release duration.

4.2.2 Source Term Quantity and Release Duration

The user specifies this input combination for term releases and fire releases. For these releases, the combination of source term quantity and release duration is used to establish the airborne release rate to the atmosphere. Note that for explosive releases, the user inputs the quantity released and EPIcode internally calculates the release duration.

The release duration also is used by EPIcode to determine whether the released cloud is best modeled as a puff or a plume. Recall that continuous releases are modeled as plumes and that the results from the term-release model approach that for the continuous-release model as the release duration increases. The basis for this input combination of source term quantity and release duration can be measurement, but for DSA applications will likely be an external calculation.

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[11] The peak 15-minute TWA is the highest rolling average over any 15-minute segment of the release period.

A zero value input for time duration signifies an instantaneous release (EPIcode automatically sets the release duration to 1 second). With an instantaneous release, EPIcode uses the puff model.

Recommendation: For plume releases, the source term quantity divided by the release duration defines the release rate, the recommendations above in Section 4.2.1 apply. Calculated downwind concentrations are proportional to the release rate for plumes (i.e., the same downwind concentrations will be calculated for various combinations of source term quantity and release duration that result in the same release rate). So, the release rate (through the input combination of source term quantity and release duration) should be conservatively estimated on the high side if there is some uncertainty or variability with its value.

Generally, the possibility of puff dispersion behavior exists for release durations of 10 minutes or less. For puff releases, the calculated downwind concentrations are proportional to the total quantity released and not to the release rate. For puff releases, it is important that the source term quantity be conservatively estimated on the high side if there is some uncertainty or variability with its value and the release duration then set accordingly. Generally for DSA applications, a duration of one minute is specified if the duration is less than one minute (Craig, 2001).

In many situations it may be difficult for the user to know apriori, whether EPIcode will model the release as a puff or plume. If this uncertainty exists, it may be practical for parametric runs to be performed to guide specifying the source term quantity and duration in a manner that maintains reasonable conservatism.

Note that the analyst should normally specify the sample time input that is discussed later in Section 4.4.2 in a manner that is consistent with or conservative with respect to the release duration.

4.2.3 Release Height

This input can reflect a physical stack height or the effective plume rise, from source momentum or buoyancy, or the combination of the two. The basis for the effective plume rise can be measurement, but for DSA applications will likely be an external calculation. Alternatively, the user has the option of supplying additional inputs and choosing to have EPIcode calculate the effective plume rise. The input specifications for the EPIcode plume rise option are discussed in Section 4.3.5.

Recommendation: With elevated plumes either from a stack or as a result of plume rise mechanisms, the separation of the plume centerline from the ground lowers the plume concentration that is observed at ground level. Thus, the most conservative approach generally is to assume a ground-level release. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures. Releases from a stack can be drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs.

NRC Regulatory Guides 1.111 and 1.145 define a true "stack" release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977; NRC, 1983). It is recommended that the analyst enter the stack height only when this criterion is met of 2.5 times the height of adjacent structures. Otherwise, the release should be treated as ground level, or alternatively, a reduced effective release height can be determined (Hanna, 1982).

The identification of adjacent structures must take into account the extent of influence that the building has on the flow field in its vicinity. The wind flow that is directly over the top of the building is entrained downward into the wake cavity. The extent of the wake cavity downwind, as measured from the lee face of the building, can range from 2.5 times as great as the building height (H_b) to approximately 10 H_b for buildings that have large width-to-height ratios (Hanna, 1982). The wake cavity is marked by increased turbulence levels that decay progressively as a function of distance from the building. For releases from stacks not meeting the criterion of 2.5 times the height of adjacent solid structures, the effects of downward-directed entrainment into the wake cavity serve to increase ground-level concentrations above what would be observed in the absence of the building. The term downwash is frequently used to collectively describe these effects. An accepted practice by the EPA is to assume that downwash effects can influence plumes that are released from stacks that are located in the range of 2 L upwind to 5 L downwind of building, where L is the lesser of the building height or projected width (EPA, 1995).

The release height should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

4.2.4 Source Dimensions

For source configurations other than the point source and explosive release, EPIcode prompts the user for one or more source dimensions as indicated below.

- Line Source – horizontal dimension
- Area Source – horizontal dimension and vertical dimension
- Liquid Spill Source – spill area
- Fire Source – release radius

These input specifications are used to calculate upwind virtual point sources. For the fire source, the single input of the release radius is used to establish virtual sources for both the horizontal and vertical directions. Thus, credit is taken for the effective initial dispersion of a realistic source that has finite dimensions in comparison with the often-used conservative assumption of a point-source release at the source location. Note that for the explosive release, the input of explosive strength (see Section 4.2.6) is used to model initial vertical and horizontal dispersion and thus establish the virtual sources.

Also note that if the release is from a stack and the user desires to calculate the plume rise from momentum or buoyancy effects, the user is prompted to input the stack radius. This input is discussed separately in Section 4.3.5.

Recommendation: A source dimension should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

4.2.5 Fire Heat Emission Rate

For fires scenarios, the user may specify the effect release height from buoyancy effects or choose to have EPIcode calculate buoyant plume rise based upon the heat emission rate. The heat emission rate, in turn, may be directly specified by the user or calculated by EPIcode from user-supplied inputs of volume of fuel, fuel heat of combustion and burn duration.

Recommendation: In plumes arising from fire-related source terms, the user should exercise caution with codes such as EPIcode that use the Briggs model (Briggs, 1975). The Briggs model for accounting for sensible energy in a plume is valid for "open-field" releases. That is, the Briggs model is not applicable to situations in which the plume transport and dispersion can be influenced by buildings (and other obstacles). The presence of a building wake can inhibit plume rise, keeping the plume closer to the ground resulting in higher ground-level concentrations.

The most conservative assumption is generally not to credit plume rise from the sensible energy of fires and therefore to assume a non-buoyant release from ground level. In this situation, the release may be modeled as a term release with a surface-area or surface-line source or most conservatively with a point source. If the fire is well defined and sufficiently distance from buildings or similar obstructions such that the source term analysis can defend the amount of sensible energy, the temporal history, and the spatial distribution, then the fire release model may be used as part of the accident and consequence analysis. If the user chooses to input the heat emission rate, then it should be conservatively estimated on the low side if there is some uncertainty or variability with its value. Similarly, if the user alternatively inputs the combination of the volume of fuel, fuel heat of combustion and burn duration, then the volume of fuel and heat of combustion should be estimated conservatively on the low side and the burn duration on the high side in order to account for some uncertainties or variability with these specifications. Note that the burn duration is specified independently of the source term release duration, which is covered in Section 4.2.2.[12]

[12] The source term release may not occur uniformly throughout the duration of the fire, with the possibility that the majority of the release occurs during a period that is a fraction of the total burn duration.

4.2.6 Explosion Strength

For explosion scenarios, the user is given the option of specifying the trinitrotoluene (TNT) equivalent of the explosion for the purpose of letting EPIcode approximate the initial effective plume rise and dispersion of the hazardous chemicals that are involved in the explosion.

Recommendation: Like the fire model, the explosion model was developed for "open-field" releases. The presence of buildings or other obstruction can inhibit plume rise with explosions (in a similar manner as with fires), keeping the plume closer to the ground resulting in higher ground-level concentrations. The most conservative assumption is not to credit plume rise from the explosion and therefore to assume a non-buoyant release from ground level. The burden is on the analyst to justify that the EPIcode explosion model is applicable for the scenario that is being analyzed and assign an appropriate TNT-equivalent value. If the analyst chooses to make use of the EPIcode explosion model and inputs the TNT-equivalent value to characterize the explosion strength, then it should be conservatively estimated on the low side to account for uncertainty or variability with its value.

4.2.7 Liquid Spill Release

For liquid spill scenarios, EPIcode prompts the analyst for inputs of total quantity of liquid that is spilled, surface area of pool that forms from the spill, the chemical vapor pressure and the liquid temperature. From these inputs, EPIcode calculates the evaporative release rate to the atmosphere and the duration of the release.

The evaporation rate is directly proportional to the vapor pressure and the surface area of the pool that forms from the spill. The depth determines the duration. For a pool that forms from an unconstrained spill,[13] one usually considers the total volume spilled and assumes spreading occurs to some minimum depth. The basic equations are given below that relate the puddle diameter (d), surface area (A), volume (V) and depth (Δh).

$$A = V/\Delta h \qquad \text{(Equation 4-1)}$$

$$d = (4/\pi \times A)^{0.5} \qquad \text{(Equation 4-2)}$$

Recommendation: The recommendation is given in multiple parts in order to account for the various component inputs that are needed to characterize the airborne release rate from the pool of a spilled chemical.

<u>Total quantity spilled</u> – A reasonably conservative estimate of the chemical inventory that is involved in the spill scenario should be specified. The specification of the quantity spilled

[13] An unconstrained spill is analyzed when no barriers are present or have assumed to fail or when an unmitigated analysis is being performed in which no credit is being taken for the barriers that are present.

should be conservatively estimated on the high side if there is some uncertainty or variability with its value. Based on this input, EPIcode provides three recommended values for the surface area input that follows. These three surface-area recommended values are based on Equation 4-1 and pool depths of 1 cm, 1 mm, and 1 inch.

Surface area of the spill – For an unmitigated analysis, the surface area of the spill is to be consistent with the total quantity spilled and a spreading of the spill to some minimum depth. It is recommended that a minimum depth of one centimeter (10 mm) be conservatively specified for an unmitigated spill analysis (EPA, 1987; Brereton, 1997).[14] As discussed above, the analyst should consider the maximum inventory in determining the volume spilled to form the pool. That is, the specification of the volume spilled should be conservatively estimated on the high side if there is some uncertainty or variability with its value. This volume together with the one-centimeter depth should be used with Equation 4-1 to calculate the pool surface area.

For a mitigated analysis, the analyst may consider crediting the presence of a dike or similar structure to constrain the spill and specify the surface area accordingly. Topography can also play a similar role in confining the extent of liquid spreading.

Chemical vapor pressure and liquid temperature – The evaporation rate is directly proportional to the chemical vapor pressure, and the vapor pressure of the chemical constituent is a strong function of its temperature in the liquid state. The vapor pressure therefore should be conservatively estimated on the high side if there is some uncertainty or variability with its value. The specification of the liquid temperature should be consistent with the specification of the vapor pressure. In practice, the analyst will probably first consider the range of possible liquid temperatures, consistent with the storage/operating temperature or the environment temperature (see discussion in Section 4.3.5), and then specify the liquid temperature and its corresponding vapor pressure at that temperature.

4.3 Input Recommendations for Meteorological and Environmental Parameters

Once the source term is quantified, the next step is to characterize the meteorological and environmental conditions that will control the atmospheric transport and dispersion of the cloud of released material as it is carried by the wind away from the source. A comprehensive treatment of atmospheric dispersion is so complex that many approximations are needed to make it tractable. Since turbulence is random and chaotic, it cannot be parameterized and one must resort to empirical formulations. One early attempt to simplify the treatment of turbulence was to define atmospheric stability classes and associate a rate of lateral and vertical dispersion with each class as a function of downwind distance only. For continuous releases, the mean wind speed dilutes the chemical concentration but the longitudinal dispersion is negligible. As the

[14] The 1-cm puddle depth is commonly used and suggested by EPA guidance (Brereton, 1997; EPA, 1987). Brereton (1997) notes that the 1-cm depth is somewhat arbitrary and recommends future development of an approach with more technical basis, such as one that would consider liquid physical properties (e.g., surface tension, viscosity) and ground surface properties (e.g., surface roughness).

plume moves downwind it gets progressively larger due to lateral and vertical dispersion, and hence becomes less concentrated. If the release is of short duration (i.e., puff), the mean wind speed only acts as a transport agent and the turbulence in the longitudinal direction becomes more important.

Appendix A contains additional discussion on the role of atmospheric stability class, wind speed, and other parameters on downwind puff or plume concentrations, especially as these parameters relate to the Gaussian transport and dispersion models for neutrally buoyant releases. Input guidance on specifying these parameters for use in EPIcode is given below.

4.3.1 Terrain Factor (Dispersion Coefficient Set)

Different set of dispersion coefficient curves have been established for rural environments and urban environments to account for the additional mechanical turbulence that is generated in urban settings by increased ground roughness due to building structures being taller and spaced closer together. Also, the heat-retention capabilities of urban surfaces (e.g., concrete structures) can drive buoyant flows that increase dispersion.

Two sets of atmospheric dispersion coefficients are included in EPIcode that correspond to standard (rural) terrain or city (urban) terrain. The increased dispersion that is associated with city terrain generally leads to lower concentrations. In guidance for the Risk Management Program (RMP), EPA considers the term rural to refer to terrain that is generally flat with few buildings or other obstructions (e.g., hills, trees) (EPA, 1999). The EPA guidance recommends assuming urban conditions for a site area with many obstructions “even if it is in a remote location that would not usually be considered urban” (EPA, 1999).

Recommendation: It is generally conservative to choose the standard terrain dispersion coefficients. It is recommended, however, that the analyst uses judgment based on site observation and published guidance to take credit for surface roughness effects in increasing puff and plume dispersion where appropriate. Ideally, consultation with the laboratory or site meteorology organization responsible for recording and maintaining site meteorological data is available to the analyst to assist in specifying this input and defending its use.

4.3.2 Atmospheric Stability Class

In calculating puff or plume concentrations, both “unfavorable” and “typical” dispersion conditions are of special interest in accident analyses. For accident analysis consideration of the offsite receptor, unfavorable meteorology is ideally based on site data. In defining unfavorable meteorological conditions for chemical releases, it seems reasonable to follow the practices that are used for radiological consequence analysis. Unfavorable meteorology refers to the meteorology that coupled with the source term would lead to doses (or concentration exposures for chemicals) that are exceeded less than five percent of the time. The method should be conservative or consistent to the discussion in the NRC Regulatory Guide 1.145 (Position 3) (NRC, 1983) as summarized in Appendix A to DOE-STD-3009-94, CN2 (DOE, 2002a). The 95th percentile result of the distribution of doses (or concentration exposures for chemicals) to the offsite receptor, accounting for variation in distance to the site boundary as a function of direction, is generally the consequence result of interest. The median or the 50th percentile result of the consequence distribution is usually the basis for typical meteorological conditions. The determination of the meteorological conditions that correspond to 50th and 95th percentile consequence results will require the simultaneous consideration of both atmospheric stability class and wind speed (the effect of ambient temperature on chemical vapor pressure may also be considered for scenarios that involve pool evaporation).

Meteorological variables such as wind speed and solar radiation affect both the evaporation rate and the amount of dilution of the puff or plume during atmospheric transport. Generally, these variables affect the evaporation rate and atmospheric dilution in opposite ways with regard to the effect produced on downwind concentrations. For example, higher wind speeds increase the evaporation rates, but also support greater dilution of the plume. Similarly, higher solar radiative influx and warmer temperatures also increase the evaporation rates, but typically support atmospheric conditions that are less stable and more dispersive. Meteorologists at Savannah River Site (SRS) studied these effects and concluded that the dominant influence of the meteorological variables generally occurs with atmospheric dispersion and dilution (Hunter, 1993). Higher downwind concentrations are associated with stable atmospheric conditions and low wind speeds (Hunter, 1993).

The size of the data set used in the meteorological assessments should be sufficiently large that it is representative of long-term meteorological trends at most sites. Meteorological data, qualified and meeting requirements of Regulatory Guide 1.23 (NRC 1972), available at most DOE sites should be applied that is representative of long-term trends. A five-year data set is desirable, but a one-year data set can be applied under the right circumstances.[15]

In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations. For example, F stability class and 1.5 m/s wind speed is recommended by the EPA for analysis of ground-level releases of neutrally buoyant plumes for unfavorable dispersion conditions (EPA, 1999). As mentioned above, accident analysis calculations under typical meteorological conditions may sometimes be performed. Atmospheric stability class D is the most common stability class for many DOE sites. This is due to the large number of combinations that can result in stability class D. For example, high-wind conditions and/or cloudy conditions during the day or at night are normally associated with stability class D. A wind speed of 4.5 m/s together with atmospheric stability D has been suggested to represent typical meteorological conditions (FEMA, 1989). This set of conditions is also consistent with a basis by chemical process industry for determining limits on chemical inventories, and is representative of most U.S. regions (CFR, 1992) and for radiological hazard categorization of DOE facilities (DOE, 1997).

[15] In Regulatory Guide 1.194, this subject is discussed as follows: “The NRC staff considers five years of hourly observations to be representative of long-term trends at most sites. With sufficient justification of its representativeness, the minimum meteorological data set is one complete year (including all four seasons) of hourly observations.” (NRC, 2003)

For elevated releases, the lofted plume must travel further downwind with stable atmospheric conditions before reaching the ground and exposing receptors to the hazardous contaminant. Therefore, neutral or even unstable stability conditions may produce the most unfavorable meteorological conditions for receptors close to the elevated release. In general, the atmospheric stability class associated with unfavorable meteorological conditions will be dependent upon the distance of the receptor from the source. At very close distances, the ground level concentration may be zero for stable conditions as the puff or plume simply passes overhead. Unstable atmospheric stability will result in the highest ground-level concentrations at close distances as high levels of turbulence will promote rapid dispersion of the puff or plume to the ground from its elevated release position. At receptor locations further downwind, neutral atmospheric buoyant conditions produce the highest ground-level concentrations with the Gaussian plume model. Even further downwind, the highest ground-level concentrations occur with stable atmospheric conditions as the puff or plume has traveled far enough downwind for the puff or plume to disperse enough so that the ground is exposed to higher-concentration regions of the puff or plume.

It should be noted that in the long run, site data is normally preferable over the default conditions for accident analysis. Meteorologists evaluated SRS data and found the specific meteorological conditions (i.e., atmospheric stability class and wind speed) that were associated with the 95th percentile results varied with release height and receptor distance (Hunter, 1993). For most facility distances to the offsite boundary, it was determined that E stability and the following wind speeds were associated with 95th percentile consequence results for neutrally buoyant plumes.[16]

- 1.7 m/s wind speed (release height 0 m – 10 m)
- 2.1 m/s wind speed (20-m release height), and
- 3.0 m/s wind speed (60-m release height).

For mitigated hazard analysis, DOE has not established guidance for evaluating the mitigative benefit of safety structures, systems, and components (SSCs). Both median statistical basis (i.e., 50th percentile) and 95th percentile bases have been applied to determine onsite receptor doses.

Recommendation: As discussed above, the preferred approach for specifying the atmospheric stability class and wind speed is statistical analysis of site-specific meteorological data. In absence of such data, the accident analysis may use generally accepted, default stability and wind speed combinations (e.g., F stability class and 1.5 m/s wind speed applied to a ground level release to represent unfavorable meteorological conditions). Guidance is complicated with elevated releases. With elevated releases of neutrally buoyant gases, it is recommended that a parametric study be performed among the various combinations of wind speed and atmospheric stability classes to determine unfavorable meteorological conditions for the receptor locations of interest. EPIcode has a useful feature that can aid in this process. When viewing the plume

[16] The cited wind speeds reflect the value at the release height (at 10 m for the 0 m – 10 m release height range).

centerline concentrations graphically, the user has the option of requesting that EPIcode display results for each of the six stability classes simultaneously.

It should be noted that the specification of the deposition velocity and its effect on plume depletion also plays an important role in the consequence calculations and establishing unfavorable meteorological conditions. For example, if the deposition velocity is set to zero, the F stability class will always result in the maximum ground-level concentration for a ground level release. If the deposition velocity is set to 1.0 cm/s, however, the maximum ground level concentration at a given downwind location may be associated with another stability class, such as E stability class. The deposition velocity is discussed in Section 4.4.3.

4.3.3 Wind Speed

EPIcode accepts wind speeds in the range of 0.5 m/s through 50 m/s at a reference height of 2 m through 100 m. The height input parameter for the wind speed is discussed separately in the next section.

Recommendation: As discussed above, statistical analysis of site-specific, wind speed measurements is the preferred approach for specifying wind speed. The determination of the meteorological conditions that are associated with 50th and 95th percentile consequences will require the simultaneous consideration of both atmospheric stability class and wind speed (ambient temperature may also be considered for scenarios that involve pool evaporation).

In general, higher downwind concentrations (i.e., unfavorable meteorological conditions) are associated with lower wind speeds. In lieu of site-specific meteorological data, the following default wind speeds may be considered for each atmospheric stability class (Lazaro, 1997). It is recommended that a parametric study among the various combinations of wind speed and atmospheric stability classes be performed to gain useful insights about the role of wind speed and atmospheric stability class in determining unfavorable meteorological conditions.

	Atmospheric Stability Class					
	A	B	C	D	E	F
Default Wind Speed [m/s]	2.0	*	*	4.5	1.5	1.5

* Lazaro (1997) does not specify default wind speeds for B and C stability classes. The 2.0 m/s default wind speed value that is specified for A stability class would seem to be a reasonably conservative choice based on information presented in Appendix A.

4.3.4 Wind Speed Height

EPIcode accepts at a reference height from 2 m through 100 m. EPIcode algorithms, however, use the wind speed at the effective release height (2 m if the effective release height is 2 m or less). EPIcode accounts for the variation of wind speed with distance from the earth's surface as caused by friction using the basic power-law formula that is represented by Equation A-3 in

Appendix A. Therefore, EPIcode needs the height that is associated with the wind speed that is entered.

Recommendation: The input for this parameter must be consistent with the wind speed input (that was discussed above). If the value for wind speed that is input into EPIcode is based on site measurements at a known height, then that height should be input. Typically, the National Weather Service (NWS) measures and reports wind speeds at 10 meters. When using the generally accepted, default combination of F stability class and 1.5 m/s wind speed or the equivalent for analysis of ground-level releases of neutrally buoyant plumes, specifying a 10-meter measurement height is expected to yield a more conservative result than that obtained from specifying a 2-meter measurement height. With a 10-meter measurement height specification, EPIcode will calculate a wind speed at 2 meters that is less than 1.5 m/s for use in the Gaussian plume model, and the Gaussian plume model predicts downwind concentrations that are inversely proportional to wind speed as shown in Appendix A.

4.3.5 Stack Height / Effective Plume Rise

If the release is from a stack and additional information is available on the stack diameter, effluent temperature, and discharge velocity, EPIcode can calculate an effective release height that takes into account plume rise mechanisms. Plume rise can occur from either momentum effects or buoyancy effects (Briggs, 1969; Briggs, 1975). EPIcode calculates plume rise from each effect separately and chooses the larger of the two results.

Recommendation: With elevated plumes either from a stack or as a result of plume rise mechanisms, the separation of the plume centerline from the ground lowers the plume concentration that is observed at ground level. Thus, the most conservative approach generally is to assume a ground-level release. It is recommended, however, that the analyst use judgment based on site observation and published guidance to take credit for lower ground-level concentrations that can occur with elevated releases. Site observation is necessary since the elevated release from a stack can be negated by nearby structures. Releases from a stack can be drawn downward and entrained behind a building into its cavity due to the aerodynamic effect of the building on the wind field in which the release occurs.

NRC Regulatory Guides 1.111 and 1.145 define a true “stack” release condition as one in which release occurs at or above 2.5 times the height of adjacent solid structures (NRC, 1977; NRC, 1983). It is recommended that the analyst model an elevated release only when this stack-height criterion is met of 2.5 times the height of adjacent structures. Otherwise, the release should be treated as ground level, or alternatively, a reduced effective release height can be determined (Hanna, 1982). Issues related to the identification of adjacent structures were discussed in Section 4.2.3 and should be followed. Also, the stack height should be conservatively estimated on the low side if there is some uncertainty or variability with its value, consistent with the recommendation given in Section 4.2.3.

Additional recommendations are given in multiple parts in order to account for the various component inputs that are needed to characterize the plume rise from buoyancy or momentum effects.

<u>Stack exit velocity</u> – The basis for the input can be measurement, but for DSA applications will likely be an external calculation. The latter can be the result of either a manual calculation or the output from another code. Plume rise from momentum effects increase with increasing stack exit velocity. The stack exit velocity should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

<u>Effluent temperature</u> – The basis for the input can be measurement or external calculation. Plume rise from buoyancy effects increase with increasing effluent temperature. The effluent temperature should be conservatively estimated on the low side if there is some uncertainty or variability with its value.

<u>Environment temperature</u> – Statistical analysis of site-specific, meteorological measurements is the preferred approach for specifying meteorological conditions, including the ambient air temperature. Plume rise from buoyancy effects decrease with increasing ambient air temperature. The ambient air temperature should be conservatively estimated on the high side in order to address variability with its value. For air temperature, a reasonably bounding high temperature is recommended based on analysis of the site data. For example, Lazaro suggests the 95th percentile value of a five-year record of daily high temperatures for the warmest month of the year (Lazaro, 1997).

<u>Stack diameter</u> – Plume rise from both buoyancy effects and momentum effects increase with increasing stack diameter. The stack diameter should be conservatively estimated on the low side if there is some uncertainty with its value.

4.4 Input Recommendations for Additional Parameters

The parameters that were discussed above in Section 4.2 (source term parameters) and in Section 4.3 (meteorological and environment parameters) are treated by EPIcode as scenario-specific parameters in the sense that there are no default values for these parameters (in the earlier Version 6.0 of EPIcode, EPIcode would prompt the user to input data for most of the parameters covered in Sections 4.2 and 4.3 as needed for a scenario). The parameters that are discussed in this section have preset default values that may be overwritten by user input: inversion layer height (5000 meters)[17], sample time (10 minutes), deposition velocity (0 cm/s for gases and vapors and 0.3 cm/s for solid particulates), and receptor height (1.5 meters).

[17] A 5000-m inversion layer height effectively translates to the specification of no inversion layer.

4.4.1 Inversion Layer (or Mixing Layer) Height

The inversion layer is a region of air in which the temperature increases with increasing distance from the ground (i.e., inverted temperature gradient). The elevation where this layer begins is referred to as the inversion layer height or the mixing layer height (as the layer of air between the earth's surface and the inversion layer is generally referred to as the mixed or mixing layer). In atmospheric transport and dispersion modeling, the inversion layer is assumed to act as a barrier to rising thermals of air from below and thus limit the extent of vertical mixing. The inversion layer height varies throughout the day and throughout the seasons. During clear nights or early mornings when inversions are present, the inversion layer is relatively low, while during sunny days the inversion layer is much higher. The magnitude of these heights can be obtained from balloon soundings or from remote sensing techniques, such as acoustic or radar soundings. In the absence of such data, regional tables can be consulted.

The default value in EPIcode is 5000 m.

Recommendation: The analyst should base mixing layer height on seasonal averages and day/night time of day through application of archived site or laboratory meteorological data. If this is not available, the analyst use regional data as default input values, such as those of Holzworth (1972).[18] Since lower inversion heights can lead to higher downwind concentrations, it is appropriate for conservatism to specify an inversion height value that is reasonable, but skewed more towards the lower end of the observed or expected range.

4.4.2 Sample (or Averaging) Time

Even with a steady, source-term release rate, downwind instantaneous concentrations of the hazardous chemical will vary with time due to the turbulent nature of atmospheric conditions. Moreover, the time-average concentration at a given downwind location will depend on the time interval over which the concentrations are averaged. This time interval is referred to as the sample or averaging time. The horizontal and vertical dispersion coefficients that are used by EPIcode are based on field measurements of puff and plume releases.[19] The sample time over which measurements were taken to establish these horizontal and vertical dispersion coefficients determines the averaging time for the time-averaged concentrations that are predicted by EPIcode through the Gaussian dispersion equations that make use of these dispersion coefficients.

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[18] The mean mixing heights for mornings in the continental United States range between approximately 200 m and 1200 m depending upon season and location (Holzworth, 1972). The mean mixing heights are higher for afternoons, ranging between 500 m and 4000 m (Holzworth, 1972).

[19] For releases other than continuous releases, EPIcode automatically selects the puff or plume equation at each downwind location based on the relative dimension of the cloud width with respect to the cloud length.

Averaging time is important because greater apparent dispersion resulting in lower centerline plume concentrations occurs with larger averaging time due to plume meander. Accounting for plume meander effects is typically done for radiological dose analysis, which can be concerned with radiological exposures that are integrated over times that may exceed the reference time for the set of dispersion coefficients for which the Gaussian dispersion model is based.

For chemical consequence analysis, toxic effect on human health can be immediate upon short-duration exposures, and the severity of the toxic effect may correlate more closely to concentration than to dose. Thus, an ideal chemical consequence analysis may, in some instances, be concerned with the peak concentrations that may last only a minute or so. In these cases, the use of a shorter averaging time allows for better characterization of these higher concentrations that may only span a short period of time.

In the Gaussian dispersion model, the effect of averaging time is typically addressed through a correction factor to the horizontal dispersion coefficient. A fuller discussion of this phenomenon and an empirical correction factor that has been developed to quantify its effect are found in Appendix A.

The default sample time, which is labeled “Max Sample Time”, for a continuous release in EPIcode is 10 minutes, which corresponds to the experimental basis for the plume dispersion coefficients. For other release types (term, liquid spill, fire, and explosive releases), the sample time is also set to the “Max Sample Time” value if the “Override” box is checked on the “Setup” page. If the “Override” box is unchecked, the sample time is set to the lesser of the two values between the release duration and the “Max Sample Time” value. Recall that the release duration is specified by the user for term and fire releases and internally determined by EPIcode for liquid spill and explosive releases.

Recommendation: The sample or averaging time should reflect the exposure time that is associated with the toxic exposure guideline of interest and should generally be equal to or less than the release duration (EPA, 1999). For example, if the toxic exposure guideline is the 10-minute Acute Exposure Guideline Level (AEGL), then an averaging time of 10 minutes is appropriate when the release duration is 10 minutes or more and an averaging time equal to the release duration is appropriate when the release duration is shorter than 10 minutes.

Guidance for the use of TEELs and ERPGs in DOE applications make a distinction between chemicals that have toxic effects that are best characterized as being concentration dependent versus those that have toxic effects that are best described as being dose dependent (Craig, 2001). For dose-dependent chemicals, the toxic effects correlate to the total quantity of material to which an individual is exposed. For dose-dependent chemicals, the peak 15-minute TWA or peak 1-hour TWA may be justified with any release duration (Craig, 2001).

Concentration-dependent chemicals have fast-acting toxic effects that correlate more closely with exposure concentration than with the total quantity. Chemicals should be considered concentration dependent if it has been assigned a short-term exposure limit (STEL) or ceiling (C) value such as an OSHA PEL-STEL or PEL-C or ACGIH TLV-STEL or TLV-C (Craig, 2001). If the release duration is 15 minutes or greater, a peak 15-minute TWA of the source term rate is recommended for use with TEEL or ERPG values for these chemicals (Craig, 2001). For release duration less than 15 minutes, the TWA should generally correspond to the release duration, with the minimum time basis for the TWA being one minute (Craig, 2001).

4.4.3 Deposition Velocity

Larger solid particles released in a puff or plume will fall to the ground due to gravitational settling. Smaller particles and even gases will deposit on ground surface elements (e.g., ground vegetation) through a variety of processes that can include chemical, biological, and physical interactions between the contaminant (particle or gas) in the puff or plume and the ground surface elements. Depletion of the contaminant in plume occurs as a result.

The EPIcode default value for deposition velocity is 0 cm/s for gases and vapors and 0.3 cm/s for solids.

Recommendation: The most conservative results are generally obtained with the deposition velocity set to zero. This assumption could lead to unrealistically large concentration predictions for particles, particularly at large distances downwind. The EPIcode default values of 0 cm/s for gases and vapors and 0.3 cm/s for solids are therefore generally recommended, although other values may be used with justification.

4.4.4 Receptor Height

The EPIcode default value is 1.5m.[20]

Recommendation: For non-buoyant, ground-level releases, a zero or near-zero specification is appropriate and generally conservative. An analyst would only want to conceivably consider a value significantly different from zero when the release is elevated (e.g., from stack or plume rise mechanism) and when a reasonable possibility exists for a receptor to be in an elevated position.

[20] Note that for a ground level release and the default receptor height, the peak plume concentration at the receptor height occurs downwind of the release location (e.g., at a distance of approximately 50 m for F atmospheric stability class).

5.0 SPECIAL CONDITIONS FOR USE

EPIcode was developed as a tool to plan for and respond to chemical emergencies. This document does not specifically address application issues related to emergency response or emergency preparedness/planning.

Even though EPIcode was not developed specifically for safety analysis applications, it is also widely used throughout the DOE complex for this purpose and has been designated for the DOE Safety Software Toolbox to support 10 CFR 830 safety basis documents. This document serves as a guide for prudent implementation of the EPIcode for the purpose of modeling chemical source terms and consequence phenomenology applicable to safety documentation. The user, however, must still demonstrate that EPIcode is being used within its domain of applicability and that site/laboratory procedures governing use of safety analysis software are being followed.

6.0 SOFTWARE LIMITATIONS

This section discusses limitations and areas of improvement of EPIcode. Section 6.1 summarizes technical limitations of Version 7.0 of EPIcode. Section 6.2 provides a summary of the outcome of the SQA gap analysis.

6.1 EPIcode Issues

The limitations of a computer code must be discussed in the context of its intended use. The limitations of EPIcode that are discussed in Table 6-1 below relate to both its use in general and specifically for safety analysis applications (recall that EPIcode was developed to plan for and respond to chemical emergencies).[21]

Table 6-1 EPIcode Limitations

EPIcode Limitation	Comment
Results are less reliable for conditions of low wind speed or very stable atmospheric conditions.	Issue of general concern to atmospheric transport and dispersion codes.
Results have high uncertainty very close to the source.	Issue of general concern to atmospheric transport and dispersion codes.
EPIcode does not model dense gas releases.	The basis for identifying the potential for dense-gas effects is the Ri number. The dense-gas effects are more pronounced near the source of the release. As atmospheric air mixes with the cloud, dilution occurs that causes dense gas transport effects to essentially become negligible as the density of the plume mixture approaches that of the ambient air. All dense gas releases, therefore, eventually transition to transport and dispersion that is characteristic of a neutrally buoyant plume. So, the Gaussian models are frequently used when the receptors of interest are far from the source, even when the

[21] Differences exist in the computational capabilities that are needed for a safety analysis calculation compared to those that are needed by people responding to a chemical accident. For example, the direction that a chemical puff or plume is traveling is of utmost importance to an emergency responder, since this information is crucial if efficient evacuation procedures are to be implemented. Thus, the inability of EPIcode to model the response of plume segments to shifts in wind direction during the course of modeling an accidental chemical release is a code limitation that affects emergency response calculations. Safety analysis calculations, however, traditionally consider exposures to a hypothetical receptor that is stationed on the centerline of a plume that is invariant with time. Thus, the inability of EPIcode to model shifts in wind direction does not constitute a limitation in the context of safety analysis calculations.

EPIcode Limitation	**Comment**
	released cloud is likely to exhibit dense-gas behavior near the source.[22] The burden is on the analyst to justify the applicability of this approach to the specific analysis.
EPIcode does not account for terrain steering effects.	A natural canyon or street canyon formed by large buildings can constrain the lateral dispersion of the puff or plume. Development of codes that are suitable for complex terrain and urban settings is a general area of ongoing research.
EPIcode does not model dispersion effects associated with building wakes.	Since wake effects near the source tend to enhance dispersion for that provides additional dilution for non-buoyant ground-level releases, it is generally believed to be conservative to neglect these effects in estimating chemical concentrations at downwind locations for these types of releases. This is not true for elevated releases (e.g., elevated either through discharge from a stack or as a result of plume rise from buoyancy or momentum effects). For an elevated release, the puff or plume can be drawn downward and 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 effects of downward-directed entrainment into the wake cavity serve to increase ground-level concentrations above what would be observed in the absence of the building. Guidance in this document recommends modeling the release as non-buoyant from ground level in this situation.

[22] For a large ammonia release, the EPIcode user's manual maintains that dense gas effects are significant when the cloud concentration is approximately 5% (50,000 ppm) or more, and that EPIcode can provide reasonable estimates when the cloud concentrations approximately below 5% (50,000 ppm). At this concentration level, passive dispersion is the dominant transport and dispersion mechanism.

EPIcode Limitation	**Comment**
EPIcode does not allow for one or more years of meteorological data to be input and processed so that statistical methods can be employed to determine the 50^{th} percentile (median) or 95^{th} percentile (unfavorable) concentration results.	EPIcode accepts a single input combination of atmospheric stability class and wind speed. The user is responsible for specifying an appropriate combination of atmospheric stability class and wind speed that will yield representative median or unfavorable concentration results. If one or more years of meteorological data are available, other atmospheric dispersions that can accept and process the meteorological data can be used to assist in these specifications. For example at SRS, meteorologists evaluated SRS data with another atmospheric and dispersion code for neutrally buoyant plumes and found that the meteorological conditions that correspond to 95^{th} percentile consequence results were associated with E stability class and 1.7-m/s wind speed for ground level releases (Hunter, 1993). Alternatively, an electronic worksheet may also be programmed to perform similar analysis. In lieu of site-specific meteorology, the accident analysis may use generally accepted, default stability and wind speed combinations. For example, F stability class and 1.5 m/s wind speed is recommended by the EPA for analysis of ground-level releases of neutrally buoyant plumes (EPA, 1999).

6.2 Outcome of Gap Analysis

A gap analysis of Version 7.0 of the EPIcode computer code has been completed (DOE, 2004). The gap analysis reviewed the program, practices, and procedures associated with development of EPIcode compared with NQA-1 based requirements as contained in U.S. Department of Energy, Software Quality Assurance Plan and Criteria for the Safety Analysis Toolbox Codes (DOE, 2003a). It was determined that the EPIcode 7.0 does meet its intended function for use in supporting documented safety analysis. However, as with all safety-related software, users should be aware of current limitations and capabilities of the software for supporting safety analysis. Informed use of the code can be assisted by appropriate use of current EPIcode documentation and this EPIcode guidance report for DOE safety analysts. Furthermore, while SQA improvement actions are recommended for EPIcode, no evidence has been found of programming, logic, or other types of software errors in EPIcode 7.0 that have led to non-conservatisms in nuclear facility operations, or in the identification of facility controls.

Of the ten SQA requirements for existing software at the Level B classification (important for safety analysis but whose output is not applied without further review), two requirements are met at an acceptable level, i.e., *Classification* (1) and *User Instructions* (7). Improvement actions are recommended for EPIcode to fully meet the remaining eight requirements and are summarized in Table 6-2. This evaluation outcome is deemed acceptable because: (1) EPIcode is used as a tool, and as such its output is applied in safety analysis only after appropriate technical review; (2) User-specified inputs are chosen at a reasonably conservative level of confidence; and (3) Use of EPIcode is limited to those analytic applications for which the software is intended.

Table 6-2 — Summary of Important Exceptions, Reasoning, and Suggested Remediation

No.	Criterion [Section refers to Gap Analysis Report for EPIcode, (DOE, 2004)]	Reason Not Met	Remedial action(s)
1.	SQA Procedures/Plans (Section 4.2)	SQA Plans and Procedures were not available for the gap analysis.	SQA Plans and Procedures should be developed and made available for review.
2.	Requirements Phase (Section 4.3)	A Software Requirements Document does not exist for review. Thus, it was necessary to infer requirements from draft model description and user guidance documents.	A Software Requirements Document should be prepared and made available for review.
3.	Design Phase (Section 4.4)	A Software Design Document does not exist for review. Thus, it was necessary to infer the intent of the design from draft model description and user guidance documents.	A Software Design Document should be prepared and made available for review.

No.	Criterion [Section refers to Gap Analysis Report for EPIcode, (DOE, 2004)]	Reason Not Met	Remedial action(s)
4	Implementation Phase (Section 4.5)	Documentation to support the implementation is lacking.	A verifiable, written set of SQA plans and procedures including implementation, test case descriptions, and associated criteria related to design should be made available.
5.	Testing Phase (Section 4.6)	A Software Testing Report Document does not exist for review.	A Software Testing Report Document should be prepared and made available for review.
6	Acceptance Test (Section 4.8)	A verifiable, written set of SQA plans and procedures, which would include acceptance-testing documentation, is lacking.	Documented acceptance testing should be developed.
7.	Configuration Control (Section 4.9)	A Configuration and Control Document does not exist for review.	A Configuration and Control Document should be prepared and made available for review.
8.	Error Notification (Section 4.10)	An Error Notification and Corrective Action Report do not exist for review.	While a Software Problem Reporting system is apparently in place, written documentation should be provided to the Central Registry for verification of its effectiveness.

By order of priority, it is recommended that EPIcode software improvement actions be taken, especially:

1. Correcting known defects in the SQA process
2. Upgrading existing SQA documentation, and
3. Revising and developing new software documentation.

A new software baseline set of documents is recommended for EPIcode to demonstrate completion of the revision to software documentation item (above). The list of revised baseline documents includes:

- Software Quality Assurance Plan
- Software Requirements Document
- Software Design Document

- Test Case Description and Report
- Software Configuration and Control
- Error Notification and Corrective Action Report Procedure, and
- Updated User's Manual.

It is estimated that a concentrated program to upgrade the SQA pedigree of EPIcode to be compliant with the ten criteria discussed important for software development would require fourteen to sixteen full-time equivalent (FTE)-months.

7.0 SAMPLE CALCULATIONS

Problem Statement: A vessel at Anytown, USA stores 210 gallons of concentrated (> 90 wt%) nitric acid (HNO_3) at ambient pressure and temperature. A scenario is postulated in which the vessel ruptures catastrophically, and the 210 gallons of HNO_3 spill on the ground. Determine the following: (1) the maximum concentration at 100 meters downwind and compare with the ERPG-3 value of 78 ppm and (2) the maximum concentration at 2500 meters downwind and compare with the ERPG-2 value of 6 ppm.

Analysis: The EPIcode chemical database contains properties for 100 wt% nitric acid since only pure chemicals, and not solutions, are part of the EPIcode chemical library. New chemicals can be added to the library. As indicated in the body of the report, a dilute acid solution can be added as a new chemical if sufficient property information is available. For evaporation calculations from chemical pools, the vapor pressure is generally the controlling parameter. The table below shows the sensitivity of HNO_3 vapor pressure to the HNO_3 wt% at 30 °C (Perry, 1997).

Table 7-1 Vapor Pressure of Nitric Acid in Solution as a Function of Concentration

HNO_3 wt%	HNO_3 Vapor Pressure [mm Hg]
40	0.1
50	0.6
60	1.7
70	5.5
80	14
90	36
100	77

In this sample problem, we have assumed concentrated HNO_3 (>90 wt%) and will conservatively analyze the spill on the basis of 100 wt% HNO_3.

The following set of inputs are entered into the EPIcode:

- Chemical - Nitric acid (The default vapor pressure of 62 mm Hg is set for 25 ºC; EPIcode will adjust the vapor pressure once the liquid temperature is enter as discussed below.)
- Type of release - Liquid spill
- Terrain factor - The terrain factor input is based on judgment taking into account site terrain characteristics. For the purposes of this sample calculation, calculations are performed first specifying rural terrain and then specifying city terrain in order to show the sensitivity of the results to this input parameter.

- Stability class - E stability (For neutrally buoyant plumes that are released at ground level, worst-case meteorological conditions are associated with stable atmosphere and low wind speed. The meteorological conditions that are associated with the 95th percentile consequence results for such releases as determined from assumed analysis of site data are taken to be E stability class and 1.7 m/s wind speed at measurement height of 10 meters for the purposes of this sample calculation.)
- Wind speed - 1.7 m/s
- Quantity spilled - 210 gallons
- Spill area - 79.5 m^2 (This area corresponds to a pool depth of 1 cm (10 mm). In the dialog box for this input, EPIcode provides recommended values of 79.5 m^2, 795 m^2 31.3 $m^2$and for pool depths of 1 cm, and 1 mm, and 1 inch respectively.)
- Liquid temperature - 29 ºC (The 95th percent highest air temperature as determined from site data is assumed to be 29 °C for the purposes of this sample calculation. Here, the liquid temperature is assumed to be the same as the air temperature.)
- Vapor pressure - 77 mm Hg (This is the value calculated by EPIcode, based on the temperature above, and presented in a dialog box for acceptance or revision. After this entry, EPIcode provides the following source term results: evaporation rate of 83 g/s and time for total evaporation of 4.0 hours.)
- Inversion height - 200 m (An inversion height of 200 m is taken as worst-case based on regional data (Holzworth, 1972). The default value of 5000 m, or effectively no inversion layer, is thus overridden.)
- Receptor height - 0 m
- Sample time - 10 minutes (This is the EPIcode default value, which is generally appropriate for predictions of the desired peak 15-minute TWA concentrations as discussed in Sections 4.2.2 and 4.4.2.)
- Deposition velocity - 0 cm/s (This is the EPIcode default value for gases and vapors.)

The following results are obtained.

- Centerline concentration at 100 m - 430 ppm (> ERPG-3 value of 78 ppm)
- Centerline concentration at 2500 m - 1.8 ppm (< ERPG-2 value of 6 ppm)

Note: To show the effect of the terrain factor, the calculations were re-run with the city terrain factor specified. The centerline concentration results were significantly lower (by a factor of three or more) yielding results of 120 ppm at 100 m and 0.6 ppm at 2500 m.

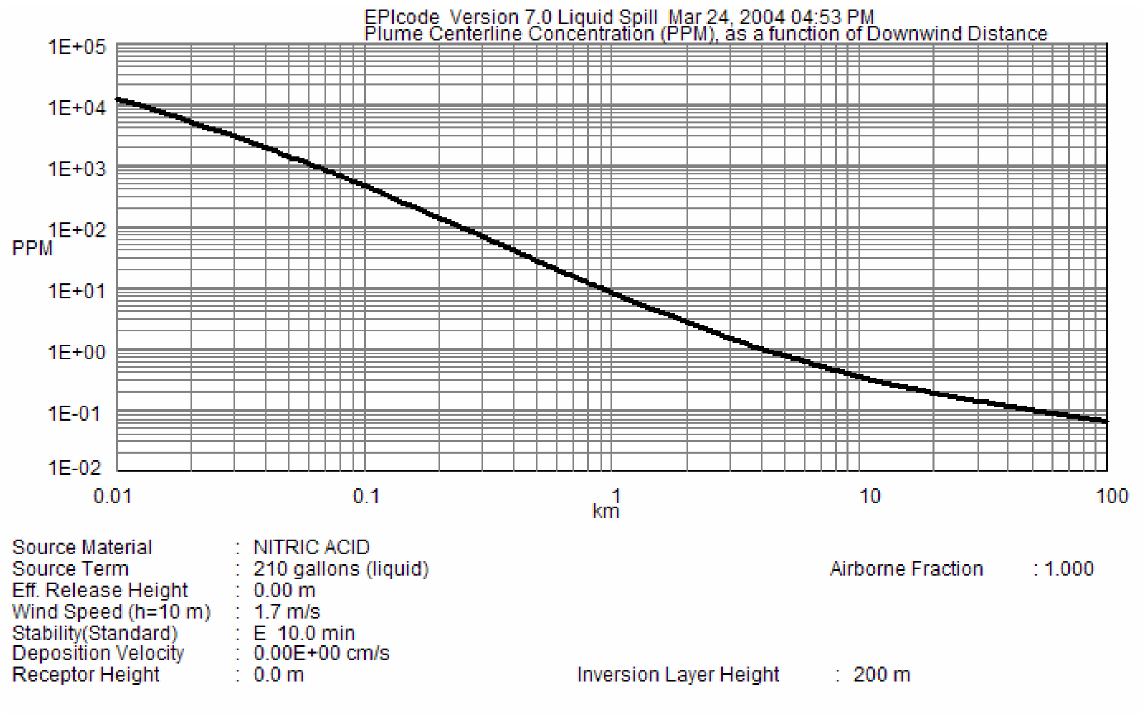

Figure 7-1. Epicode Sample Problem — Nitric Acid Concentration Versus Distance

Additional Analysis:

The maximum concentration at 100 meters downwind will now be calculated for an evaporative release from a 210-gallon puddle of 70 wt% HNO_3 in city terrain and compared with the ERPG-3 value of 78 ppm. This additional calculation will highlight the large difference in evaporation rates between pure HNO_3 and 70 wt% HNO_3. From the table of HNO_3 vapor pressure at 30 °C as a function of weight percent shown earlier in this section, the vapor pressure for HNO_3 70 wt% is 5.5 mm Hg (0.0072 atmospheres) compared to 77 mg Hg for pure the HNO_3 (Perry, 1997). Therefore, a much lower evaporation rate and 100-m concentration can be expected since the vapor pressure for 70 wt% HNO_3 is approximately 7% of that for 100 wt% HNO_3. The results will show that evaporation rate and predicted concentration at 100 meters for the 70 wt% HNO_3 case are approximately 7% of the values calculated for the 100 wt% HNO_3 case.

All inputs are the same as before except for the vapor pressure input.

Vapor pressure - 5.5 mm Hg

The following results are obtained.

- Evaporation rate - 6 g/s (compared to 83 g/s for 100 wt% HNO_3)
- Centerline concentration at 100 m - 31 ppm (< ERPG-3 value of 78 ppm and < 430 ppm calculated for 100 wt% HNO_3)

8.0 ACRONYMS & DEFINITIONS

Selected Terms and Definitions Used in Source Term, Atmospheric Transport and Dispersion, and Consequence Analysis

Acute Exposure Guideline Levels (AEGLs) – Threshold exposure limits for the general public above which acute exposure would be expected to lead to adverse effects of increasing severity for AEGL-1, AEGL-2, and AEGL-3. The National Advisory Committee for Acute Exposure Guideline Levels for Hazardous Substances (NAC/AEGL Committee) is developing AEGLs to assist Federal and State agencies and private sector organizations with their need for short-term hazardous chemical exposure information in terms of five emergency exposure periods (10 and 30 min, 1 h, 4 h, and 8 h) and the three severity levels as defined below:

AEGL-1: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience notable discomfort, irritation, or certain asymptomatic nonsensory effects. However, effects are not disabling and are transient and reversible upon cessation of exposure.

AEGL-2: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience irreversible or other serious, long-lasting adverse health effects or an impaired ability to escape.

AEGL-3: airborne concentration of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening health effects or death.

Advection – The transport of a fluid property by the bulk motion of the fluid, sometimes called convection in engineering terminology.[23]

Aerosol – Solid or liquid particles (droplets) that are suspended in a gas or vapor medium.

Atmospheric Stability Class – Characterization of the state of atmospheric turbulence.[24] The different atmospheric stability classes typically used by meteorologist range from

[23] Some of the definitions for atmospheric transport and dispersion terms are taken from the Chemical Dispersion and Consequence Assessment Working Group of the DOE-sponsored Accident Phenomenology and Consequence Methodology Evaluation Program (Lazaro, 1997).

A for very unstable conditions to F (or sometimes G) for very stable conditions and account for differing levels of buoyant turbulence. High levels of buoyant turbulence are associated with unstable conditions.

Atmospheric Transport and Dispersion – The movement and dilution of a contaminant cloud under the influence of the prevailing wind flows and associated atmospheric turbulence.

Buoyant Turbulence – Atmospheric turbulence that is generated by solar heating of the ground and the formation of thermal updrafts.

Chi-over-Q (χ/Q) – For a chemical release into the atmosphere, this parameter represents the ratio of the airborne concentration of the chemical constituent in a cloud at given downwind location to the airborne release rate. The parameter provides a measure of dilution from atmospheric transport and dispersion processes at a given downwind distance. [25]

Cloud – The volume that encompasses a chemical (contaminant) emission.

Dense Gas (Heavy Gas) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that can occur when the density of the chemical cloud at the source is greater than that of the ambient air (i.e., negatively buoyant cloud). In dense-gas atmospheric transport and dispersion, the dense-gas cloud resists the influences of the hydraulic pressure field associated with the atmospheric wind, and the cloud alters the atmospheric wind field in its vicinity. Dense-gas releases undergo what has been described in the literature as "gravitational slumping". Gravitational slumping is characterized by significantly greater lateral (crosswind) spreading and reduced vertical spreading as compared to the spreading that occurs with a neutrally buoyant release.

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[24] A comprehensive treatment of atmospheric dispersion is so complex that many approximations are needed to make it tractable. Since turbulence is random and chaotic, it cannot be parameterized and one must resort to empirical formulations. One early attempt to simplify the treatment of turbulence was to define atmospheric stability classes and associate a rate of lateral and vertical dispersion with each class as a function of downwind distance only. Although computations based on these stability classes provide only a rough approximation to reality, they have proved extremely useful and are still in use, although more accurate treatments are available. Wind direction variability and vertical temperature difference are the most common techniques that are employed.

[25] In practical terms, χ/Q values are time-averaged characterizations based generally on an average release rate over a specified time period and time-averaged dilution characterization of the atmospheric transport and dispersion effects. In the Gaussian plume model, the dispersion coefficients are empirically based on field observations over a given time period, referred to as the averaging time or sampling time. For releases of radiological material, χ/Q values are generally defined in an equivalent fashion as the ratio of the time-integrated airborne concentration in a cloud at a given downwind location to the total amount of material released.

Dilution – The reduction of the cloud concentration due to mixing with ambient air.

Dispersion – Spreading of the cloud boundaries due to atmospheric turbulence. Atmospheric, turbulent dispersion is the result of rapid and irregular fluctuations in wind components, such as velocity.

Dispersion Coefficients – A measure of the spreading of a contaminant cloud as it travels downwind. In Gaussian puff and plume formulations:

σ_x = longitudinal dispersion coefficient (function of downwind distance, x), representing the standard deviation of the concentration distribution in the downwind axis direction;

σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction; and

σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction.

Emergency Response Planning Guidelines (ERPGs) – Estimates of concentrations for specific chemicals above which acute exposure (up to 1 hour) would be expected to lead to adverse health effects of increasing severity for ERPG-1, ERPG-2, and ERPG-3. The American Industrial Hygiene Association (AIHA) has issued three levels of ERPG values based on toxic effect of the chemical for use in evaluating the effects of accidental chemical releases on the general public (AIHA, 2002). The definitions of each ERPG level in terms of toxic effects are as follows (AIHA, 2002).

ERPG-1*: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing more than mild, transient health effects or without perceiving a clearly defined objectionable odor.*

ERPG-2*: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing irreversible or serious health effects or symptoms that could impair an individual's ability to take protective action.*

ERPG-3*: The maximum airborne concentration below which it is believed nearly all individual could be exposed for up to 1 hour without experiencing or developing life-threatening health effects.*

Evaporation – Process by which molecules of a liquid come off the surface of a liquid and enter the vapor space.

Friction Velocity – A measure of the mechanical turbulence and a direct measure of the frictional forces of the wind in the boundary layer adjacent to the earth's surface. It can be thought of as the representing the consequences of Reynolds stresses, which cause velocity fluctuations to transport momentum.[23]

Gaussian Puff/Plume Model – A diffusion model for vapor or gas chemical releases to the environment in which the lateral and vertical distribution of the chemical concentration follow a normal or Gaussian distribution. Additionally in the puff model, the longitudinal distribution follows a normal or Gaussian distribution. A segmented Gaussian puff/plume model incorporates a computational approach in which the Gaussian puff/plume is spatially segmented into individual volume sources with each segment generating a concentration field.[23]

Inversion Layer – A region of air in which the temperature increases with increasing distance from the ground.[23] The stable temperature gradient in the inversion layer suppresses vertical turbulence and mixing. In addition, the inversion layer acts as a cap to rising thermals of air from below. Thus, the inversion layer restricts the range and magnitude of vertical turbulence. The vertical extent of this elevated inversion is known as the inversion layer height (z_i). The region below z_i is often referred to as the mixed or mixing layer. In Gaussian dispersion modeling, the inversion layer is generally assumed to act as barrier that contains the contaminant cloud below z_i.

Mechanical Turbulence – Atmospheric turbulence that is generated from the shear forces that result when adjacent parcels of air move at different velocities (i.e. either at different speeds or directions). Fixed objects on the ground such as buildings or trees increase the ground roughness and increase mechanical turbulence in proportion to their size.

Neutrally Buoyant (Passive) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that occurs when the density difference between the chemical cloud and the ambient air is small. A neutrally buoyant cloud does not alter the atmospheric wind field. The term passive is used to describe the phenomenological characteristics associated with atmospheric transport and dispersion of the cloud as the cloud follows the bulk movements and behavior of the atmospheric wind flow.

Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) – Chemical concentration limits that are developed by the Occupational Safety & Health Administration for use in limiting worker exposures to airborne chemicals.

Plume – Term used to describe the form of the chemical cloud for a sustained or continuous release.

Plume Meander – Variation of the location of the plume centerline (i.e., plume swings back and forth), due to turbulent velocity fluctuations. The receptor on the time-averaged centerline location is only exposed intermittently to the concentration of the instantaneous plume centerline. As a result, the time-averaged concentration decreases on the centerline and increases on the outer edges of the plume. The magnitude of the plume meander effect on the time-averaged centerline concentration is a function of averaging time.

Positively Buoyant (Passive) Atmospheric Transport and Dispersion – Type of atmospheric transport and dispersion that can occur when the density of the chemical cloud at the source is significantly less than that of the ambient air. A positively buoyant cloud behaves like a neutrally buoyant cloud with the added effect that the positive buoyancy produces upward forces that cause the puff or plume to rise.

Puff – Term used to describe the form of the chemical cloud for an instantaneous release or release of short duration.

Richardson (Ri) Number – Relative measure of the potential energy of the cloud with respect to the mechanical turbulence energy of the atmosphere. Potential energy is associated with buoyancy forces that tend to suppress turbulence. Wind shear generates mechanical turbulence energy.

Source Term – The rate of release (may be time dependent), duration, and physical and energetic characteristics of hazardous material released to the environment.

Surface Roughness Length (z_o) – Measure of the amount of atmospheric mechanical turbulence that is induced by the presence of surface roughness elements such as vegetation and man-made structures.

Temporary Emergency Exposure Limits (TEELs) – Surrogate ERPG values for chemicals for which ERPGs have not been published (i.e., the TEEL-1, -2, and -3 values) and surrogate Permissible Exposure Limit - Time-Weighted Average (PEL-TWA) values for all chemicals for which PEL-TWA values have been published (i.e., TEEL-0 values).

Vapor – The gas produced from the evaporation of a liquid.

Vapor Pressure – The equilibrium pressure of the pure component vapor over the pure component liquid. When a chemical exists in a solution or mixture, the term partial pressure is generally used.

95th Percentile Consequence – A statistical method described in the U.S. Nuclear Regulatory Commission Regulatory Guide 1.145 (February 1983) to quantify the consequences for an airborne release conservatively taking into consideration the variability of meteorological conditions that may be present at the time of the release (NRC, 1983).[26] While this method was originally established for radiological releases, the concept easily extends to hazardous chemical releases. Given site-specific data, the 95th percentile consequence is determined from the distribution of meteorologically-based χ/Q values calculated for a postulated

[26] This method is prescribed in Appendix A to DOE-STD-3009-94 for consequence assessment to quantify the radiological dose that is received by the maximally exposed offsite individual (MOI) (DOE, 2000).

release to downwind receptors at the site boundary that would result in a χ/Q values that is exceeded 5% of the time (based on hourly data over a period of one year or more).[27] Although the methods allows for variations in distance to the site boundary as a function of angular sectors to be taken into consideration in conjunction with the wind direction, assuming the minimum distance to the site boundary applies in all directions is a conservative implementation that is easily supported and that essentially makes the calculations sector independent. The site-specific meteorological data consist of (generally) hourly data of wind speed and atmospheric stability class at minimum (wind direction is also needed if sector-dependent distances to the site boundary are considered).

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[27] Terminology that is sometimes unfortunately used in this context and that should be avoided is terms such as "95th percentile meteorology." The distribution and selection of the 95th percentile value are based on consequence results (e.g., χ/Q values) that are a function of meteorological parameters and not on the meteorological parameters themselves (e.g., wind speed).

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Appendices

Appendix	Subject
A	Gaussian Models for Atmospheric Transport and Dispersion
B	Tornado Dilution Factor

APPENDIX A: GAUSSIAN MODELS FOR ATMOSPHERIC TRANSPORT AND DISPERSION

Two broad categories exist to characterize atmospheric transport and dispersion that are based upon the released chemical cloud density and how it affects the interaction of the chemical cloud with the atmospheric wind flow. For airborne releases in which the initial chemical cloud density is less than or equal to that of the ambient air, the cloud is characterized as neutrally buoyant and the atmospheric transport and dispersion as passive.[28] If the density of the initial chemical cloud is greater than that of the ambient air, then the possibility exists for either passive or dense-gas type of atmospheric transport and dispersion. Dense gas behavior at the source is determined on the basis of the source Ri number having a value greater than one.[29] This appendix discusses the atmospheric transport and dispersion of neutrally buoyant releases and the Gaussian models that are the basis for the equations used in EPIcode.

Time-averaged concentrations obtained from field studies of neutrally buoyant chemical releases are observed to follow Gaussian or bell-shaped distributions. The Gaussian plume and puff dispersion models that have been developed to predict the outcome of chemical releases that are represented by these field studies are well established and widely used. As the plume develops and moves downwind, it approximates a Gaussian distribution in both the crosswind (lateral) and vertical directions. For continuous releases, the mean wind speed dilutes the chemical concentration but the longitudinal dispersion is negligible. As the plume moves downwind it gets progressively larger due to lateral and vertical dispersion, and hence becomes less concentrated. If the release is of short duration (i.e., puff), the mean wind speed only acts as a transport agent and the turbulence in the longitudinal direction becomes more important. Accordingly, a puff is described by a three-dimension Gaussian equation.

The range of distances over which the Gaussian plume model should be used varies with conditions, but the model is considered generally applicable over the range of 100 m to 10 km and possibly beyond (Hanna, 1982). The basic form for the Gaussian plume model is given below beyond (Hanna, 1982).

$$\chi(x,y,z)=\frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \qquad \text{(Equation A-1)}$$

where:

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[28] A neutrally buoyant chemical cloud that is released to the atmosphere does not alter the atmospheric wind flow, and therefore, the term passive is used to describe the phenomenological characteristics associated with its atmospheric transport and dispersion. As a passive contaminant, the released chemical follows the bulk movements and behavior of the atmospheric wind flow.

[29] Definitions of source Ri number for continuous and instantaneous releases are given by Equation 3-1 and Equation 3-2, respectively.

χ = atmospheric concentration [mg/m^3] for chemical releases

Q = source term release rate [mg/s] for chemical releases

x = downwind distance (relative to source location) [m]

y = crosswind distance (relative to plume centerline)[m]

z = vertical axis distance (relative to ground) [m]

H = effective release height (relative to ground) [m]

σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction [m]

σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction [m]

u = average wind speed[30] [m/s]

The last term accounts for reflection of the plume at the ground surface through adding an image source at distance H beneath the ground surface.

Note that the concentration is inversely proportional to the wind speed (i.e., greater initial dilution with higher wind speeds).[31] The concentration is also inversely proportional to the horizontal and vertical dispersion coefficients (i.e., higher dispersion enhances the dilution of the puff or plume). These dispersion coefficients are a measure of the effect of atmospheric turbulence in causing the plume to increasingly disperse in the lateral and vertical direction as the plume travels downwind. The dispersion coefficients account for the two sources of atmospheric turbulence, namely, mechanical turbulence and buoyant turbulence.

The horizontal and vertical dispersion coefficients, σ_y and σ_z, required in the Gaussian dispersion equation are obtained either from site-specific meteorological measurements (e.g., standard deviations of wind angles) or through established curves that are based on field experiments and the concept of atmospheric stability class. The averaging time over which the σ_y and σ_z parameters were determined in the field experiments establishes the averaging time for the time-averaged concentrations predicted by the Gaussian dispersion equation. Averaging time is important because greater apparent dispersion occurs with larger averaging time due to plume meander. Plume meander refers to variation of the location of the plume centerline (i.e., plume swings back and forth), due to turbulent velocity fluctuations. The receptor on the time-averaged

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[30] Since the wind speed varies with distance above the earth's surface, the wind speed value in the Gaussian plume equation will ideally represent some average value over the plume depth, such as the wind speed at the plume centroid (center of mass). In practice, simpler specifications are made such as the wind speed at the effective release height or the wind speed at the height of 10 meters (EPIcode uses either the wind speed at the release height or at 2 meters for release heights of 2 meters or less).

[31] Calm winds below 0.5 m/s are rare and generally not considered so that evaluating the Gaussian plume equation at a wind speed of zero is not an issue.

centerline location is only exposed intermittently to the concentration of the instantaneous plume centerline. As a result, the time-averaged concentration decreases on the centerline and increases on the outer edges of the plume. The magnitude of the plume meander effect on the time-averaged centerline concentration is a function of averaging time.[32] The time-averaging effect on plume meander dispersion is generally accounted for by the following algebraic expression suggested by Gifford that relates the horizontal dispersion coefficient (σ_y) for the averaging time of interest (t_a) to a known reference horizontal dispersion coefficient ($\sigma_{y,ref}$) that is associated with a reference averaging time ($t_{a,ref}$) (Hanna, 1982).

$$\sigma_y = \sigma_{y,ref} \times \left(\frac{t_a}{t_{a,ref}} \right)^q ; \qquad \text{(Equation A-2)}$$

where, $q = 0.2$ for 3 minutes $< t_a <$ 1 hour

$q = 0.25$ to 0.3 for 1 hour $< t_a <$ 100 hours

Accounting for plume meander effects is typically done for radiological dose analysis, which can be concerned with radiological exposures that are integrated over times that may exceed the reference time for the set of $\sigma_{y,ref}$ values on which the Gaussian dispersion model is based. For chemical consequence analysis, toxic effect on human health can be immediate upon short-duration exposures and the severity of the toxic effect may correlate more closely to concentration than to dose. Thus, an ideal chemical consequence analysis may, in some instances, be concerned with the peak concentrations that may last only a minute or even less. In practice, $\sigma_{y,ref}$ values developed for Gaussian dispersion codes are generally based on averaging times that range from 3 minutes to 1 hour. If the above correlation is be used to calculate (σ_y) for ($t_a < t_{ref}$), a prescribed minimum of t_a equal to 20 seconds has been recommended (Hanna, 1996).

As the plume travels downwind, its vertical spread may be limited by the presence of an elevated temperature inversion layer. The temperature increases with increasing distance from the ground in the inversion layer. The stable temperature gradient in the inversion layer suppresses vertical turbulence and mixing. In addition, the inversion layer acts as a cap to rising thermals of air from below. Thus, the inversion layer restricts the range and magnitude of vertical turbulence. The vertical extent of this elevated inversion is known as the inversion layer height (z_i). The region below z_i is typically referred to as the mixed or mixing layer. In Gaussian dispersion modeling, the inversion layer is generally assumed to act as barrier that contains the contaminant cloud below z_i. The Gaussian dispersion equation can be modified to consider reflection from

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[32] In most engineering flow systems, the scales of turbulent motions are limited by the physical size of the system components (e.g., pipe diameter) so that time scales are on the order of seconds or minutes. For these systems, steady statistical averages can be achieved with reasonable sampling periods. Conversely, the range of spatial and time scales in the atmosphere is extremely large. As a consequence, observed statistics are not invariant with averaging time (i.e., one cannot obtain steady mean values since it is not possible to sample atmospheric parameters over a long enough time period) (Wilson, 1995).

the elevated temperature inversion layer.[33] Reflection eventually results in a uniform concentration in the vertical direction (throughout the plume depth from ground to inversion layer boundary).

Determination of σ_y and σ_z from established, empirical curves is a common and acceptable practice. Each σ_y or σ_z curve represents a different atmospheric stability condition based upon the classification scheme first developed by F. Pasquill and later modified by F. A. Gifford. The different atmospheric stability classes range from A for very unstable conditions to F (or sometimes G)[34] for very stable conditions and account for differing levels of buoyant turbulence.

The stability class is a function of both the amount of incoming solar radiation and the wind speed (Turner, 1970; Turner, 1994). High incoming solar radiation (as would occur on sunny days) and low wind speeds characterize unstable conditions (e.g. stability class A or B) and result in high levels of buoyant turbulence. With unstable conditions, the air temperature of the atmosphere near the earth's surface declines rapidly with elevation. Warm parcels of air near the surface travel a long distance upward before cooling to the temperature of the air around it. As warmer air rises, the cooler air that is displaced sinks downward. Large-scale, convective motions develop that provide substantial vertical mixing. At the other end of the spectrum, stable atmospheric conditions (e.g., stability class E, F or G) can occur on clear nights with low wind speeds. The smaller atmospheric temperature gradient that occurs with stable atmospheric conditions limits upward convection and reduces vertical mixing. Neutral stability conditions (e.g., stability class C or D) that occur with high wind speeds or with moderate wind speeds and cloud cover, represent intermediate stability conditions that produce moderate levels of buoyant turbulence.

Original descriptions and conditions of occurrence given by Pasquill for each stability class are given below (Turner, 1994).

- A: <u>Extremely Unstable (Strong superadiabatic)</u>. Normally occurs during bright sunshine with relatively low wind speed (< 3 m/s).
- B: <u>Moderately Unstable (Moderate superadiabatic)</u>. 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.

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[33] The ground and the inversion layer boundary are treated as impenetrable and totally reflecting surfaces. Some Gaussian plume models such as ALOHA treat reflection through addition of mirror image sources both below the ground and above the inversion layer boundary (Reynolds, 1992). For reflection off the inversion layer boundary, an addition term is added to Equation (A-1) that is similar to the ground-reflection term. Additional terms can be added to account for multiple reflections off the ground and inversion layer boundary. Also at some point downwind (generally where σ_z approaches z_i), the value of the vertical dispersion coefficient, σ_z, in the Gaussian dispersion equation is typically limited to approximately z_i.

[34] EPIcode does not support the input of G stability class.

- 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.
- 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). Normally occurs at night or early morning with very light to nearly zero wind speed.

Different set of dispersion coefficient curves have been established for rural environments and urban environments to account for the additional mechanical turbulence that is generated in urban settings by increased ground roughness due to building structures being taller and spaced closer together. Also, the heat-retention capabilities of urban surfaces (e.g., concrete structures) can drive buoyant flows that increase dispersion.

A forest can have a similar effect to that of buildings in increasing ground roughness. A surface roughness length (z_o) is typically used to characterize the amount of mechanical turbulence that is induced by the presence of surface roughness elements. A rule of thumb is that the surface roughness length is approximately one tenth the value of the height of the average surface roughness elements (Hanna, 2002). A surface roughness correction to σ_z is of the form $(z_o)^r$, where r is in the range of 0.1 to 0.25, with 0.2 being a commonly used value (Hanna, 1982; Hanna, 2002).

Recall that the atmospheric wind speed varies with distance from the ground (z). The wind speed (u) used in the Gaussian plume equation should ideally approximate the wind speed at the plume centroid (center of mass). Typically, the National Weather Service (NWS) measures wind speeds at 10 m (u_{10}). The following formula can be used to estimate the wind speed at other heights (Hanna, 1982).

$$u = u_{10} \times \left(\frac{z}{10}\right)^p \qquad \text{(Equation A-3)}$$

The power-law exponent parameter (p) can be estimated on the basis of atmospheric stability class and general surface roughness characterization. An urban and rural set of power-law exponents that are found in the published literature are shown below (Hanna, 1982; Irwin, 1979).

Atmospheric Stability Class

	A	B	C	D	E	F
Urban	0.15	0.15	0.20	0.25	0.40	0.60
Rural	0.07	0.07	0.10	0.15	0.35	0.55

A puff model is used for instantaneous or near-instantaneous releases (Hanna, 1996). For a puff, longitudinal dispersion also occurs.

$$\chi(x, y, z; t) = \frac{Q_T}{(2\pi)^{3/2}\,\sigma_x \sigma_y\,\sigma_z} \exp\left[-\frac{1}{2}\left(\frac{x - x_o}{\sigma_x}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] \left\{\exp\left[-\frac{1}{2}\left(\frac{z - H}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z + H}{\sigma_z}\right)^2\right]\right\} \text{(Eq. A-4)}$$

where:

Q_T = total source term [mg] for chemical releases

σ_x = longitudinal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the downwind axis direction [m]

x_o = $u \times t$; representing center of the puff in the longitudinal direction [m]

It is common practice to set σ_x equal to σ_y. The dispersion parameters for a puff release are known to be different than those for a plume release (Hanna, 1996).[35].

[35] For convenience, some dispersion models use plume dispersion parameters for both puff and plume releases. More extensive data are available for plume releases (Hanna, 1996).

APPENDIX B: TORNADO DILUTION FACTOR

Atmospheric transport and dispersion of chemical material from the facility into the environment during a tornado can be modeled with a design basis accident 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 as discussed in Appendix A. The Fujita scale is commonly used to categorize tornadoes. For most safety analysis applications, the tornado is assumed to be either Fujita - 2 (F2) or F3. Figure B-1 shows Ψ/Q values (s/m^3) as a function of downwind distance (km) for different mean translational speeds of the F2 tornado (Weber and Hunter, 1996). The consequence analysis should pick a maximum Ψ/Q for the assumed translational speed. For example, the translational speed of 7.5 m/s leads to a maximum air concentration at approximately three kilometers. The product of thus maximum Ψ/Q value with the release rate of the chemical to the atmosphere yields the ground-level air concentration at the location of interest.

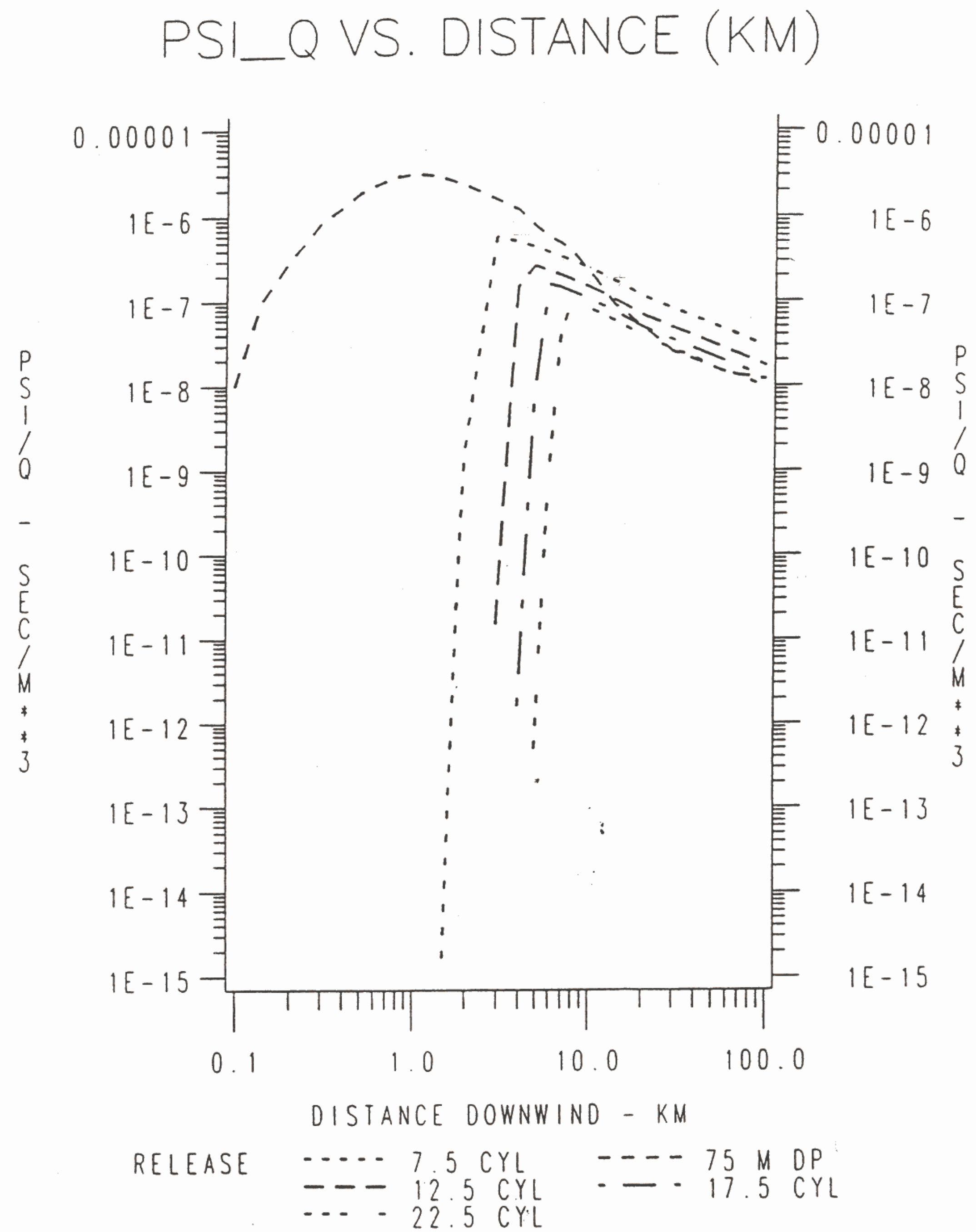

Figure B-1. The maximum time-integrated ground-level centerline air concentration (s/m^3) versus downwind distance (km). Applied for different mean translational speeds from 7.5m/s to 22.5 m/s. In this case, the downdraft speed is 10 m/s and the height of the cylindrical mesocyclone is 3500 m (from Weber and Hunter, 1996).