Evaluation of the Atmospheric Transport Model in the MACCS2 Code and its Impact on Decision Making at Department of Energy Sites

John E. Till and Arthur S. Rood

June 5, 2012
RAC Historical Dose Reconstruction Projects

Hanford
- Washington State
- Dept. of Energy
- CDC

Idaho National Engineering Lab
- CDC

Nevada Test Site
- University of Utah/NCL

Uravan
- Dow Chemical

Rocky Flats
- CDPE
- RFCAB

Los Alamos
- US DOJ
- New Mexico Environment Dept.
- CSU

Fernald
- CDC

Savannah River Site
- CDC

Map Copyright 1995 by Ray Sterner, Johns Hopkins University Applied Physics Laboratory
“Understanding and communicating the movement of radionuclides and chemicals released to the environment, resulting exposure to humans, and the subsequent dose or risk from exposure.”
Types of Dose/Risk

- Medical
- Occupational
- Public
Dose/Risk Can Be Estimated for

- Real people
- Hypothetical people
Purpose of Assessments

- Compliance
- Decision making
- Epidemiology
- Emergency response
Approaches to Estimating Risk

- In certain situations, and depending upon the decisions to be made, if the results of relatively conservative screening assessments demonstrate that doses are well below the dose criteria (e.g., a factor of three or more), there may be no need for further detailed assessment.

- The deterministic approach multiplies single values for parameters chosen to be deliberately conservative to take account of uncertainty.

- The probabilistic approach incorporates distributions for parameter values.

- Combination of deterministic and probabilistic
<table>
<thead>
<tr>
<th>Situation</th>
<th>Type of Assessment</th>
<th>Type of Assessment</th>
<th>Type of Assessment</th>
<th>Type of Assessment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Normal</td>
<td>Past operation</td>
<td>Present</td>
<td>Future</td>
<td>Design of new</td>
</tr>
<tr>
<td></td>
<td></td>
<td>operation</td>
<td>exposures</td>
<td>facility</td>
</tr>
<tr>
<td>Existing</td>
<td>Earlier exposures</td>
<td>Present</td>
<td>Future</td>
<td>Future prolonged</td>
</tr>
<tr>
<td></td>
<td></td>
<td>exposure</td>
<td>exposures</td>
<td>(e.g., after</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>remediation)</td>
</tr>
<tr>
<td>Emergency</td>
<td>Actual impacts after</td>
<td>Actual</td>
<td>Emergency</td>
<td>Emergency</td>
</tr>
<tr>
<td></td>
<td>emergency</td>
<td>emergency</td>
<td>planning</td>
<td></td>
</tr>
</tbody>
</table>
Risk Assessment

Risk = \((S \cdot T \cdot E \cdot D \cdot R)_{uvcp}\)

where
S = source term
T = environmental transport
E = exposure
D = dose coefficient
R = risk coefficient
u = uncertainty
v = validation
c = communication of results
p = participation of stakeholders
RAC Dose Assessment for MACCS2 Evaluation

Dose = \((S \cdot \partial T \cdot E \cdot D)_{vcp}\)

where

\(S\) = source term (deterministic)

\(\partial T\) = environmental transport (partial transport limited to atmospheric dispersion — deterministic but based on distribution of meteorological data)

\(E\) = exposure (deterministic)

\(D\) = dose coefficient (deterministic)

\(v\) = validation

\(c\) = communication of results

\(p\) = participation of stakeholders
MACCS2 Was Designed to Have Built-In Conservatism

Qualitative Effect of the Codes on Safety Analysis

The gross effect of the use of computer codes can be evaluated by examining their effect on the final MOI dose values calculated as part of the accident analysis. The values chosen or calculated for each parameter in the dose equation are near the conservative tail of any distribution that would be assigned to the individual parameter. Therefore, when each parameter is multiplied using the five-factor formula to obtain the dose, the conservatism in the calculation grows. If applied consistently in each phase of the process and in a reasonably bounding manner, this large conservatism in the calculation has always provided the DOE safety analysis process with sufficient margin when the doses are used to make decisions regarding safety. Even if a single value in the dose calculation were off by an order of magnitude, the resulting value would still not approach the mean value of dose if a cumulative distribution of dose also were calculated.
MACCS2

- Built-in conservatisms in the model and methodology
  - Straight-line Gaussian Plume Model
  - Conservative Source term
  - Meteorology (e.g., no buoyancy, no plume meander, no wet deposition, 95\textsuperscript{th} percentile concentration from 1 year of data)
  - Exposure scenario (e.g., boundary exposure, duration of the accident)
Assessment Question

Does the predicted dose from MACCS2 code as prescribed in the DOE Guidance Manual (DOE-EH-4.2.1.4-MACCS2-Code Guidance) meet the target dose criteria?
Comparison of the Atmospheric Transport Model in MACCS with Lagrangian Puff Models

Arthur S. Rood
June 5, 2012
Evaluation of (T) in MACCS2 Model

- Compare the MACCS2 dispersion model with state-of-the-art Lagrangian Puff Dispersion models, CALPUFF and RATCHET.
- CALPUFF is EPA approved complex terrain model.
- RATCHET was developed for the Hanford Environmental Dose Reconstruction Project and is incorporated into the GENII and RASCAL dose assessment models.
Objective

- Review Gaussian plume and Lagrangian puff atmospheric dispersion models as implemented in MACCS, CALPUFF and RATCHET models
- Provide a comparison of model results for the WTP accident analysis at Hanford
Types of Air Dispersion Models

- **Classic Gaussian Plume Model**
  - Relatively simple analytical model for temporally and spatially constant wind field and steady-state release that forms the basis of most old-generation regulatory compliance modeling.

- **Augmented Gaussian Plume Model**
  - Based on the classic Gaussian Plume model, but includes mixing lid reflection and dry and wet deposition processes. (MACCS2)
Types of Air Dispersion Models (continued)

- **Steady-State Plume Model**
  - Similar to Augmented Gaussian Plume model, but incorporates recent understanding of the stable and convective boundary layer, vertical inhomogeneity, and terrain effects (AERMOD)

- **Puff (Lagrangian) Dispersion Model**
  - More complex model for evaluation of non-steady-state releases in temporally and spatially variable wind fields (CALPUFF, RATCHET)
Overview of MACCS
CALPUFF/RATCHET

- **MACCS**
  - Augmented Gaussian plume model
  - Diffusion coefficients a function of downwind distance and stability class
  - Fixed deposition velocity

- **RATCHET/CALPUFF**
  - Lagrangian puff model
  - Turbulence-based /similarity theory diffusion coefficients
  - Calculated deposition velocity
  - Terrain effects (CALPUFF)
Lagrangian Puff Model
Classical GP models use a classification scheme for atmospheric stability. Six classes (termed Pasquill-Gifford Stability Categories) are generally recognized:

- Stability Class A (extremely unstable)
- Stability Class B (moderately unstable)
- Stability Class C (slightly unstable)
- Stability Class D (neutral)
- Stability Class E (slightly stable)
- Stability Class F (moderately stable)
- Stability Class G (extremely stable) OPTIONAL
State-of-the-Art Schemes for Characterizing Turbulence

- **Direct measurements of turbulence** ($\sigma_v$ and $\sigma_w$)
  - Not very practical – airports do not routinely measure turbulence directly
    - $\sigma_v$ – standard deviation of the horizontal cross wind component of the wind (m/s)
    - $\sigma_w$ – standard deviation of the vertical component of the wind (m/s)

- **Estimate** $\sigma_v$ and $\sigma_w$ from micrometeorological parameters (Hanna et al. 1982; Scire et al. 2000)
  - $u^*$ – friction velocity
  - $w^*$ – convective velocity scale
  - $h$ – mixing height
  - $L$ – Monin-Obukhov Length
The micrometeorological parameters ($u^*$, $w^*$, $L$, and $h$) can be estimated from:

- Routine meteorological data collected at airports (temperature, cloud cover, ceiling height, surface pressure, relative humidity, wind speed and direction)
- Estimates of the surface roughness height ($z_o$)
- Time-of-day and solar elevation angle
- Land use (i.e., urban, rural, desert, forest, etc.)
Representative Equations for Micrometeorological Parameters

- **Friction velocity for neutral and unstable conditions (Scire et al. 2000)**
  - \( k = \) von Karman constant (0.4)
  - \( z_o = \) roughness height (m)
  - \( \psi_m = \) stability correction factor
  - \( u = \) wind speed (m/s)

  \[
  u^* = \frac{k u}{\ln\left(\frac{z}{z_o}\right) - \psi_m\left(\frac{z}{L}\right) + \psi_m\left(\frac{z_o}{L}\right)}
  \]

- **Convective velocity scale (Scire et al. 2000)**
  - \( Q_h = \) sensible heat flux (W/m2)
  - \( c_p = \) specific heat of air (996 m²/s² K)
  - \( T = \) air temperature
  - \( h = \) convective mixing height

  \[
  w^* = \left(\frac{q Q_h h}{T \rho c_p}\right)^{1/3}
  \]
Representative Equations for Micrometeorological Parameters

- **Monin-Obukhov Length (Scire et al. 2000)**
  - Positive for stable conditions
  - Negative for unstable conditions
  - Infinite for neutral conditions
  - The absolute value of $L$ can be thought of as the depth of the mechanically mixed layer near the surface
  - $u^*$ and $L$ are calculated by iteration

\[
L = \frac{\rho c_p T u^*^3}{kg Q_h}
\]

- **Mixing height for neutral and unstable conditions (Ramsdell et al. 1994)**
  - $\beta = \text{constant, } f = \text{coriolis parameter (\sim 10^{-4} \text{ s}^{-1})}$

\[
h = \frac{\beta u^*}{f}
\]
Relationship between Monin-Obukhov Length and Stability Class

Fig. 5. $1/L$ as a function of Turner classes and $z_0$. 
Representative Equations for $\sigma_v$ and $\sigma_w$

- **Stable**
  \[
  \sigma_v = c_1 u_* \left(1 - \frac{z}{H}\right), \quad \sigma_w = c_2 u_* \left(1 - \frac{z}{H}\right)
  \]

  $c_1 \sim 2$, $c_2 = 1.3$, $z$ = puff transport height

- **Neutral**
  \[
  \sigma_v = c_1 u_* \exp\left(\frac{-2f}{u_*}\right), \quad \sigma_w = c_2 u_* \exp\left(\frac{-2f}{u_*}\right)
  \]

  $f$ = coriolis parameter ($\sim 10^{-4}$ s$^{-1}$)

- **Unstable**
  \[
  \sigma_v = u_* \left(12 \frac{H}{2L}\right)^{1/3}, \quad \sigma_w = 1.3u_* \left(1 - \frac{3z}{L}\right)^{1/3}
  \]

(from Hanna et al., 1982, Ramsdell et al., 1994)
Turbulence-Based $\sigma$’s

- **Plume growth** is proportional to
  - Travel time ($t$)
  - The horizontal and vertical components of the standard deviation of the wind vector ($\sigma_w$ and $\sigma_v$)
  - The functions $f_y$ and $f_z$

- **The functional form of $f_y$ and $f_z$** depends on the Monin Obukhov Length

$$\sigma_{yt} = \sigma_v t \ f_y \left( \frac{t}{t_{ly}} \right) \quad \sigma_{zt} = \sigma_w t \ f_z \left( \frac{t}{t_{lz}} \right)$$
Diffusion Coefficients

- MACCS2 diffusion coefficients ($\sigma_y$ and $\sigma_z$) use the P-G stability classes where diffusion coefficients are based on downwind distance for a steady-state plume.
- Turbulence-based diffusion coefficients use similarity theory are based on travel time. These diffusion coefficients are used in the RATCHET and CALPUFF models.
- In general, the turbulence-based $\sigma_y$ and $\sigma_z$ are higher than P-G $\sigma_y$ and $\sigma_z$, but depend on the wind speed which in turn affects travel time.
Comparison of Diffusion Coefficients ($\sigma_y$)

Sigma-Y (m)

Distance (km)

Sigma Y
(RATCHET sigmas based on 2 m/s windspeed)

MACCS-Stab A
MACCS-Stab C
MACCS-Stab F
RATCHET-Stab A
RATCHET-Stab C
RATCHET-Stab F
Comparison of Diffusion Coefficients ($\sigma_z$)
Comparison of Diffusion Coefficients ($\sigma_y$), 2 m/s and 4 m/s
Assumptions Specific to the Gaussian Plume Model

- Homogeneity of turbulence
- Stationary turbulence conditions and steady-state pollutant release
- Sufficiently long diffusion times (averaging times)
- Spatially constant, non-zero wind speed
- Material continuity (no sources or sinks) while being transported
- Total reflection of the plume on the ground
Puff Dispersion Models

- Typically composed of two modules
  - Wind field interpolation module
  - Pollutant transport model
- Allows variable/curved plume trajectories\(^1\)
- Spatially-variable meteorological conditions\(^1\)
- Non steady-state releases
- Retains spatial distribution of concentrations from the previous meteorological sampling period

\(^1\)Not all puff dispersion models incorporate this feature
Benchmark – RATCHET Gaussian Plume,

Conservative Tracer (no decay or deposition)
4 m/s windspeed, Stability Class D

- RATCHET
- Gaussian Plume using RATCHET Sigmas
- Gaussian Plume using PG Sigmas

Average Concentration at 24-hours (Ci m⁻³)

Downwind Distance (km)
Deposition Velocity

- In MACCS, deposition velocity is specified by the user.
- Modern atmospheric transport models (CALPUFF, AERMOD, RATCHET) calculate deposition velocity based on:
  - Wind speed
  - Friction velocity (turbulence level, roughness height)
  - Brownian diffusion (CALPUFF and AERMOD)
  - Gravitational settling
Deposition Velocity Models

- **Resistance model for particles**
  \[ v_d = \frac{1}{r_a + r_d + r_a r_d v_g} + v_g \]

- **Resistance model for gases**
  \[ v_d = \frac{1}{r_a + r_d + r_c} \]

- **Deposition velocity is a function of the friction velocity, viscosity of air, Brownian diffusivity, particle density and diameter, roughness length, and vegetation type**

- \( r_a = \) aerodynamic resistance (s/m)
- \( r_d = \) deposition layer resistance (s/m)
- \( r_c = \) canopy layer resistance (s/m)
- \( v_g = \) gravitational settling (m/s)
Deposition Velocity as a Function of Particle Size for two Different Resistance Models
## Measured Deposition Velocity ($v_d$) Values

<table>
<thead>
<tr>
<th>Effluent</th>
<th>Value (cm/s)</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reactive gases</td>
<td>1</td>
<td>Brenk et al. 1983</td>
</tr>
<tr>
<td>Reactive gases</td>
<td>0.73</td>
<td>Geometric mean of measured values given in Hoffman et al 1984</td>
</tr>
<tr>
<td>Aerosols (1 $\mu$m in diameter)</td>
<td>0.1</td>
<td>Brenk et al. 1983</td>
</tr>
<tr>
<td>Particulates</td>
<td>0.33</td>
<td>Geometric mean of measured values given in Hoffman et al 1984</td>
</tr>
<tr>
<td>Un-reactive gases</td>
<td>0.01</td>
<td>Brenk et al. 1983</td>
</tr>
</tbody>
</table>
How does RATCHET Compare with Measurements at Hanford?

<table>
<thead>
<tr>
<th>Monitoring Location</th>
<th>Monitoring Period</th>
<th>Number of Samples</th>
<th>Median P/O Ratios</th>
<th>Full Meteorological Data</th>
<th>Limited Meteorological Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>300 Area trench</td>
<td>1983–1987</td>
<td>42</td>
<td>1.12</td>
<td>2.06</td>
<td></td>
</tr>
<tr>
<td>300 Area trench</td>
<td>1983–1987</td>
<td>25</td>
<td>1.24</td>
<td>1.82</td>
<td></td>
</tr>
<tr>
<td>Fir Road</td>
<td>1984–1987</td>
<td>34</td>
<td>1.28</td>
<td>2.44</td>
<td></td>
</tr>
<tr>
<td>Prosser barricade</td>
<td>1984–1987</td>
<td>28</td>
<td>1.62</td>
<td>1.43</td>
<td></td>
</tr>
<tr>
<td>Ringold</td>
<td>1983–1987</td>
<td>41</td>
<td>2.31</td>
<td>2.36</td>
<td></td>
</tr>
<tr>
<td>Sagehill</td>
<td>1984–1987</td>
<td>32</td>
<td>1.72</td>
<td>1.59</td>
<td></td>
</tr>
<tr>
<td>Pasco</td>
<td>1986–1987</td>
<td>22</td>
<td>1.16</td>
<td>1.23</td>
<td></td>
</tr>
<tr>
<td>Eltopia</td>
<td>1986–1987</td>
<td>15</td>
<td>1.62</td>
<td>3.31</td>
<td></td>
</tr>
<tr>
<td>Sunnyside</td>
<td>1984–1987</td>
<td>41</td>
<td>1.09</td>
<td>0.82</td>
<td></td>
</tr>
<tr>
<td>Yakima</td>
<td>1986–1987</td>
<td>18</td>
<td>1.13</td>
<td>0.89</td>
<td></td>
</tr>
<tr>
<td>All stations</td>
<td>1983–1987</td>
<td>316</td>
<td>1.45</td>
<td>1.85</td>
<td></td>
</tr>
</tbody>
</table>

Overall RACTHET over predicts Kr-85 concentrations at Hanford by about a factor of 1.45 using full meteorology and 1.85 using limited meteorology

Ramsdell et al. 1994
How Does the Gaussian Plume and Lagrangian Puff Model Compare with Measurements?

<table>
<thead>
<tr>
<th></th>
<th>Gaussian Plume</th>
<th>Lagrangian Puff Models</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ISC</td>
<td>TRAC</td>
</tr>
<tr>
<td><strong>8 km data</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Geometric Mean P/O ratio</td>
<td>1.9</td>
<td>1.0</td>
</tr>
<tr>
<td>Geometric Std P/O ratio</td>
<td>2.2</td>
<td>2.3</td>
</tr>
<tr>
<td><strong>16 km data</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Geometric Mean P/O ratio</td>
<td>2.7</td>
<td>1.9</td>
</tr>
<tr>
<td>Geometric Std P/O ratio</td>
<td>2.2</td>
<td>3.9</td>
</tr>
</tbody>
</table>

From Rood 1999, Rood et al, 1999, 1-hr maximum concentration in 8-hr period
Model Comparison of MACCS, CALPUFF, and RATCHET for Hanford WTS

- Compare overall dispersion patterns
- 1-year of meteorological data (1994)
- \( V_d \) of 0, 0.1, 0.3, and 1.0 applied for MACCS
- \( V_d \) internally calculated for CALPUFF and RATCHET
- Compared the 95% highest X/Q at various distances
Hour 3 of a 14-hour Simulation using CALPUFF
Hour 3 of a 14 hour Simulation using Gaussian Plume Model
95% X/Q, No Deposition
($V_d=0$)

$V_d = 0.0 \text{ m s}^{-1}$

- MACCS2
  - 3.75x10^4
  - 9.08x10^6

- CALPUFF, PG DFs
  - 4.13x10^4
  - 9.52x10^6

- CALPUFF, Similarity DFs
  - 4.99x10^4
  - 7.01x10^6

- RATCHET
  - 2.09x10^6
95% X/Q, No Deposition ($V_d=0$)
95% X/Q, MACCS $V_d = 0.1$ cm/s

CALPUFF and RATCHET $V_d$ calculated internally

![Graph showing 95% X/Q values for different models and distances.](image)
95% X/Q, MACCS \( V_d = 0.3 \text{ cm/s} \)

CALPUFF and RATCHET \( V_d \) calculated internally.
95% X/Q, MACCS $V_d = 1.0 \text{ cm/s}$

CALPUFF and RATCHET $V_d$ calculated internally

$V_d = 1.0 \text{ cm s}^{-1}$

- 1 km
- 5 km
- 9.3 km

95% X/Q Value (s m$^{-3}$)

<table>
<thead>
<tr>
<th>Method</th>
<th>1 km</th>
<th>5 km</th>
<th>9.3 km</th>
</tr>
</thead>
<tbody>
<tr>
<td>MACCS2</td>
<td>7.34x10$^6$</td>
<td>2.22x10$^6$</td>
<td>1.94x10$^5$</td>
</tr>
<tr>
<td>CALPUFF, PG DFs</td>
<td>8.51x10$^6$</td>
<td>1.64x10$^6$</td>
<td>2.20x10$^5$</td>
</tr>
<tr>
<td>CALPUFF, Similarity DFs</td>
<td>6.79x10$^6$</td>
<td>6.79x10$^6$</td>
<td>6.79x10$^6$</td>
</tr>
<tr>
<td>RATCHET</td>
<td>4.58x10$^4$</td>
<td>4.58x10$^4$</td>
<td>4.58x10$^4$</td>
</tr>
</tbody>
</table>
95% X/Q, MACCS $V_d = 1.0 \text{ cm/s}$

$V_d$ calculated internally

CALPUFF and RATCHET $V_d$ calculated internally
95% X/Q vs Distance (Vd>0)
Conclusions

- **With No Deposition**
  - The Gaussian plume and Lagrangian puff models yield about the same 95% X/Q value at 1 km.
  - The Gaussian plume and Lagrangian puff models 95% X/Q values diverge with increasing distance.
  - At 9.3 km, the Gaussian plume model 95% X/Q is about 3 to 4 times higher than Lagrangian puff models.
Conclusions (continued)

- **With Deposition**
  - At 9.3 km, the Gaussian plume model 95% X/Q using a deposition velocity of 1 cm/s is about the same as the Lagrangian puff models using internally calculated deposition velocity.
Comparison of Gaussian plume and Lagrangian puff models at distances in the 8-16 km range reveal that the Gaussian plume model overpredicts concentrations for short-term (i.e. 1-hr) average concentrations.
Conclusions (continued)

- The reasons for difference results among the models are numerous and complex, but in general differences may be attributed to:
  - Conceptual differences in the Gaussian Plume and Lagrangian Puff Models
  - Differences in diffusion coefficients
  - Differences in deposition velocity
What Have We Learned?

John E. Till June 5, 2012
What We have Learned

- The MACCS2 as implemented in its documentation with a $V_d$ of 1.0 cm s$^{-1}$ results in approximately the same concentration of radionuclides at the point of exposure when compared to state of the art meteorological models using Hanford site-specific meteorological data and an internally calculated $V_d$.

- The calculated $V_d$ for WTP analyses using state of the art models and site specific meteorological conditions is in the range of 0.1-0.3 cm s$^{-1}$.
Conservatisms in MACCS2, namely the use of a conservative source term, the straight-line Gaussian Plume model for short-duration events, and exposure occurring at the 9.3 km receptor distances, result in a highly conservative estimate of atmospheric concentrations regardless of the use of a deposition velocity of 1 cm s\(^{-1}\).

But how conservative?

What level of conservatism is our goal?
We recommend a target level of conservatism be established to be used in decision making related to nuclear safety.
Conclusions (2)

Ground rules must be established for decision making using agreed upon methods and the prescribed level of conservatism.
Conclusions (3)

We conclude that the MACCS2 code as designed for generic use at DOE sites provides a useful tool for screening calculations for decision making.

When the results of screening calculations show there is no significant chance of exceeding the target dose criteria, no further action should be taken related to the assessment of dose.
Conclusions (4)

When screening fails, we recommend the use of site specific environmental transport data, state of the art meteorological models, and a more comprehensive probabilistic approach to make decisions related to nuclear safety.

A tiered approach to decision making should be considered, applying codes such as MACCS2 (v. 2.5) or GENII prior to implementing robust site-specific analyses that incorporate comprehensive probabilistic calculations.
Conclusions (5)

The comprehensive probabilistic methodology should consider the following deterministic and probabilistic components:

- Probabilistic source term with a 100% chance of occurring
- Probabilistic transport calculations including pathway analysis to clearly show key pathways of exposure
- Deterministic exposure scenario parameters using ICRP 101 guidelines
- Deterministic dose coefficients
THANK YOU!

www.racteam.com

johntill@mindspring.com
803-536-4883

asr@kspar.com
208-528-0670