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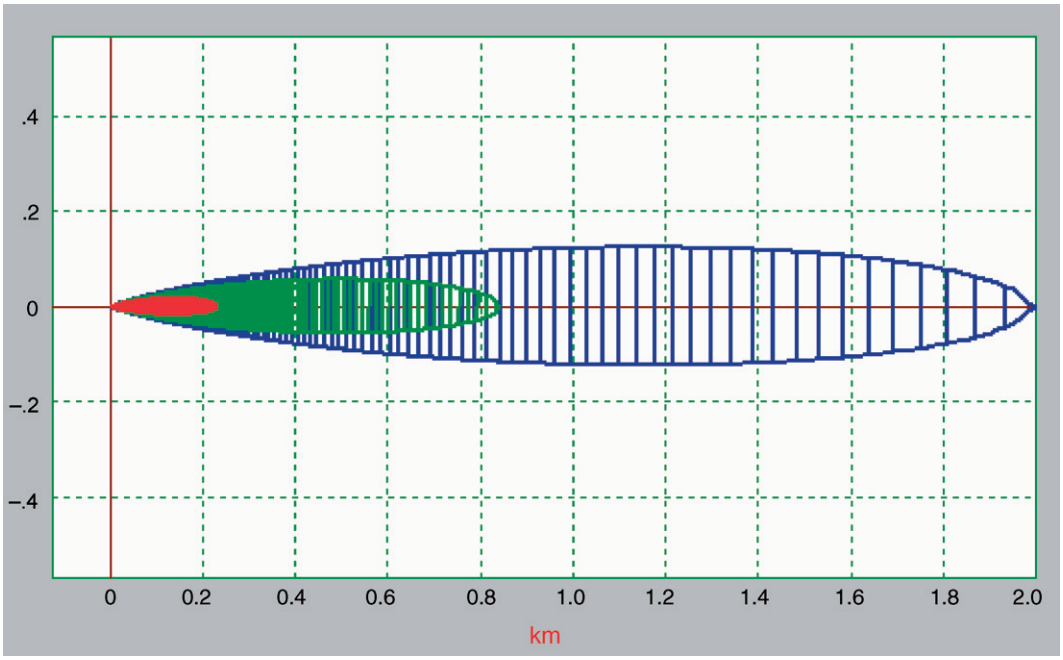
Industrial respirator use

Airborne release fractions in particulate releases

Pesticide residues in "organic" and conventional foods in India



Dispersion model comparisons, p. 20

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FEATURE

Comparison of ALOHA and EPIcode for Safety Analysis Applications

EPIcode (version 7.0) and ALOHA (version 5.2.3) are two of the designated toolbox codes identified in the Department of Energy's Implementation Plan for DNFSB Recommendation 2002-1 on Software Quality Assurance issues in the DOE Complex. Both have the capability to estimate evaporation rates from pools formed from chemical spills and to predict subsequent atmospheric transport and dispersion. This report provides an overview of the algorithms used by EPIcode and ALOHA to calculate evaporation rates and downwind plume concentrations. The technical bases for these algorithms are briefly discussed, and differences in the EPIcode and ALOHA methodologies highlighted. In addition, sample calculations are performed using EPIcode and ALOHA for selected chemicals under various environmental conditions. Side-by-side comparisons of results from sample calculations are analyzed to illustrate the impact that the different methodologies used by EPIcode and ALOHA have on predicted evaporation rates and downwind concentrations.

It is recommended that the safety analyst explicitly evaluate the strengths and limitations of any code before selecting it for a specific application. User skill and expertise can often outweigh most of the differences between ALOHA and EPIcode. Recognizing that EPIcode is inherently a scoping tool, while ALOHA is based on more detailed models, the user is recommended to perform a parameter sensitivity study to determine major dependences in the applied model and to check code output with independent techniques, such as a hand calculation, alternative computer code application, or spreadsheet techniques. A multi-tiered approach of this type will provide better confidence in overall results than to unilaterally use one code alone without questioning.

By D.C. Thoman, K.R. O'Kula, J.C. Laul, M.W. Davis, K.D. Knecht

INTRODUCTION

In June 2004, the Office of Environment, Safety and Health (EH) of the Department of Energy (DOE) issued final guidance reports for the six toolbox codes used in conducting calculations to support safety analysis and placed these guidance reports on the Central Registry web page of the EH website. The toolbox codes are the original six identified by the Implementation Plan for the Defense Nuclear Facilities Safety Board (DNFSB) Recommendation 2002-1[1] and include the Emergency Prediction Information Code (EPIcode, version 7.0)[2] and the Areal Locations of Hazardous Atmospheres (ALOHA, version 5.2.3).[3] While both have the capability to estimate evaporation rates from pools formed from chemical spills and to predict subsequent atmospheric transport and dispersion, there are differences in the models used. The objective of this report is to compare the algorithms used by these codes to perform these calculations and show how methodology differences between the two codes affect calculated evaporation rates and downwind plume concentrations.

This work is of current relevance given recent DNFSB concerns of the impact of the updated evaporation model used in EPIcode version 7.0 that has resulted in higher evaporation rates and concentrations than previously calculated with EPIcode (version 6 and earlier). Specifically, the updated evaporation model used in EPIcode 7.0, which is the Environmental Protection Agency (EPA) model that is documented in the 1999 Risk Management Program guidance (EPA-550-B-99-009),[4] uses a mass transfer coefficient of water that is a factor of 2.68 higher than that previously used. As a result, the updated evaporation model predicts evaporation rates of spilled chemical liquids and downwind plume concentrations that are higher by this same factor. These higher results have raised the issue of potential non-conservatism in safety analyses that are based on previous versions of EPIcode. While safety analyses based on ALOHA calculations are not directly affected (since ALOHA uses a different, more complex algorithm for pool evaporation), differences in results between ALOHA and EPIcode are of interest in the broader context of understanding and assessing conservatism in chemical consequence analysis.

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The first half of the report covers the atmospheric transport and dispersion algorithms of the two codes. The feature of these codes that allows the user to specify a constant release rate for the chemical of concern is used to isolate the transport and dispersion calculations. Both EPIcode and ALOHA employ the Gaussian plume model. This model is presented and used in its simplest form to perform a sample calculation for a hypothetical base-case scenario. EPIcode and ALOHA calculations for this base-case scenario and variations of it are used to compare and contrast expanded features of the Gaussian plume model that the two codes employ. In addition to the Gaussian plume model, ALOHA's dense-gas model is illustrated through sample runs and a brief discussion.

The second half of the report covers the pool evaporation algorithms of EPIcode and ALOHA. The two models are significantly different (with the ALOHA model being the more complex of the two), which makes analytical comparisons of the two models impractical. As a result, evaluation of these algorithms is limited to observations made from output generated for four common chemicals. In addition, the ALOHA evaporation rate calculations are repeated using the latest version of ALOHA, namely, version 5.3.1.[5] The effects of updates to the chemical property database in the newer version of ALOHA are shown. It is expected that ALOHA version 5.3.1 will eventually be incorporated into the toolbox (replacing version 5.2.3).

ATMOSPHERIC TRANSPORT AND DISPERSION CALCULATION

Gaussian Plume Model Overview

The basic form for the Gaussian plume model[6] is given as:

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

where

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 (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.

For the purposes of this report, a ground-level release is assumed (i.e., $H = 0$) and the receptor of interest is at ground level (i.e., $z = 0$) and on the plume centerline (i.e., $y = 0$). For these conditions, the Gaussian plume equation simplifies to the following form:

$$\chi(x,0,0) = \frac{Q}{\pi\sigma_y\sigma_z u} \quad (2)$$

Since the wind speed varies with elevation, its value in the Gaussian plume equation ideally represents 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 some fixed height typically between 2 and 10 m for a ground-level release. Information related to how EPIcode and ALOHA specifically address this issue for ground-level releases is given in the next subsection.

The horizontal and vertical dispersion coefficients (σ_y and σ_z) in the Gaussian plume 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. 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. Different atmospheric stability classes range from 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 with resultant increased dispersion are associated with unstable conditions. In addition to buoyant turbulence, mechanical turbulence contributes to dispersion. Greater mechanical turbulence is generated in urban settings from increased ground roughness due to building structures being taller and spaced closer together. Also, heat-retention capabilities of urban surfaces (e.g., concrete structures) can drive buoyant flows that increase dispersion. Different sets of dispersion coefficient curves have therefore been established for rural and urban terrain settings.

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 plume equation. Averaging time is important because greater apparent dispersion occurs with larger averaging time due to plume meander. Figure 1 shows how plume meander affects the apparent boundaries of the time-averaged plume and how these boundaries may differ from those associated from a typical snapshot of the instantaneous plume.

Both EPIcode and ALOHA use algebraic expressions for σ_y and σ_z that are a function of x and that were developed by Briggs based on established σ_y and σ_z curves.[7] Briggs developed a different set of algebraic expressions for rural and urban environments as shown in Table 1.

As an illustrative example, a 1 g/s (1,000 mg/s) release of a chemical at ground level is considered under

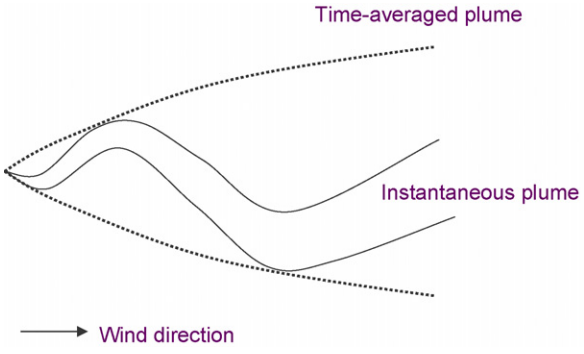

Figure 1. Effect of time averaging on apparent plume boundaries.

Table 1. Briggs' dispersion coefficients[2]

Atmospheric Stability Class	σ_y (m)	σ_z (m)
Rural terrain		
A	$0.22x(1+0.0001x)^{-1/2}$	$0.20x$
B	$0.16x(1+0.0001x)^{-1/2}$	$0.12x$
C	$0.11x(1+0.0001x)^{-1/2}$	$0.08x(1+0.0002x)^{-1/2}$
D	$0.08x(1+0.0001x)^{-1/2}$	$0.06x(1+0.0015x)^{-1/2}$
E	$0.06x(1+0.0001x)^{-1/2}$	$0.03x(1+0.0003x)^{-1}$
F	$0.04x(1+0.0001x)^{-1/2}$	$0.016x(1+0.0003x)^{-1}$
Urban terrain		
A–B	$0.32x(1+0.0004x)^{-1/2}$	$0.24x(1+0.001x)^{+1/2}$
C	$0.22x(1+0.0004x)^{-1/2}$	$0.20x$
D	$0.16x(1+0.0004x)^{-1/2}$	$0.14x(1+0.0003x)^{-1/2}$
E–F	$0.11x(1+0.0004x)^{-1/2}$	$0.08x(1+0.0015x)^{-1/2}$

meteorological conditions consisting of F atmospheric stability class and 1-m/s wind speed. Note that atmospheric transport and dispersion with the basic Gaussian plume equation is independent of any chemical property so that it is not necessary to specify a particular chemical in order to perform the calculation. The ground-level plume concentration at 100 m from this release is sought for a rural environment.

For F atmospheric stability class (rural) from Table 1 and downwind distance of 100 m:

$$\sigma_y = 0.04x(1+0.00001x)^{-1/2} = (0.04)(100)[1+(0.0001)(100)]^{-1/2} = 3.98\,\text{m}$$
$$\sigma_z = 0.016x(1+0.0003x)^{-1/2} = (0.016)(100)[1+(0.0003)(100)]^{-1/2} = 1.58\,\text{m}$$

From Eq. (2):

$$\chi(100,0,0) = \frac{1000\,\text{mg/s}}{\pi(3.98\,\text{m})(1.58\,\text{m})(1\,\text{m/s})} = 51\,\text{mg/m}^3$$

EPIcode and ALOHA Gaussian Plume Models

EPIcode and ALOHA each have additional features for modeling atmospheric transport and dispersion phenomena that extend beyond those of the basic Gaussian plume model described above. Differences exist between the codes in terms of what additional phenomena are modeled. In addition even when the same phenomena are modeled by each code, differences exist in assumptions that are employed to model the phenomena. Understanding these differences can explain how analysts can get significantly different results depending upon whether ALOHA or EPIcode is used to model a given chemical release scenario.[8] The additional features expand input data requirements beyond what was required for the sample problem discussed above. Table 2 summarizes the complete input data set required for each code to replicate the 51 mg/m^3 concentration result at 100 m of the sample problem.

The discussion that follows highlights the sensitivity of the calculated downwind concentration values to a few of the key input parameter specifications. Specifically, EPIcode and ALOHA results are shown (Tables 3–7) with input parameters changed one at a time from those specified in the base-case sample problem. The results from these sensitivity cases provide a basis for better understanding differences that can occur between ALOHA and EPIcode results.

Terrain sensitivity

The same result of 51 mg/m^3 is obtained from EPIcode and ALOHA for the base-case sample problem (Gaussian Plume Model Overview) when "standard" terrain is specified in EPIcode and when "open country" is specified for ground roughness in ALOHA and the other parameter specifications are made as indicated in Table 2. In each case, the Briggs' rural dispersion coefficients as shown in Table 1 are used.

Results from EPIcode and ALOHA do not agree, when "city" terrain is specified in EPIcode and when "urban or forest" is specified for ground roughness in ALOHA as shown in Table 3. When "city" terrain is specified in EPIcode, EPIcode uses the Briggs' urban dispersion coefficients as shown in Table 1. In contrast when "urban or forest" is specified for ground roughness in ALOHA, the Briggs' urban σ_z dispersion coefficients are used along with the generally more conservative rural σ_y dispersion coefficients.[7]

Measurement height for wind speed sensitivity

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 as shown in Figure 2. The sample problem statement specifies a 1 m/s wind speed, but does not specify the height at which this wind speed occurs. Both

Table 2. EPIcode and ALOHA input specifications for sample problem

Input Parameter	EPIcode 7.0	ALOHA 5.2.3	Comments
Terrain	Standard (rural)	Open country (rural)	The Briggs rural dispersion coefficients are used when "standard" terrain is specified in EPIcode 7.0 and when "open country" is specified for ground roughness in ALOHA 5.2.3. The sensitivity of results to city/urban terrain is briefly discussed in "Terrain sensitivity".
Atmospheric stability class	F	F	Part of sample problem statement.
Windspeed/ measurement height	1 m/s at 2 m	1 m/s at 3 m	The sample problem statement specifies a 1 m/s wind speed, but does not specify that height at which this wind speed occurs. The sensitivity of results to the measurement height specification is briefly discussed in "Measurement height for wind speed sensitivity".
Wind direction	Any direction	Any direction	Downwind concentration results are not sensitive to this input parameter specification.
Inversion height	No inversion	No inversion	Both EPIcode and ALOHA use similar modified forms of the Gaussian plume formula when the upper boundary of the plume reaches the inversion height when an inversion height is specified.
Release rate	1 g/s	1 g/s	Part of sample problem statement.
Release height	0 m	0 m	Part of sample problem statement.
Receptor height	0 m	0 m (only option)	Part of sample problem statement. Note that the default value for EPIcode 7.0 is 1.5 m.
Deposition velocity	0 cm/s	0 cm/s (only option)	EPIcode models plume depletion due to deposition. The sensitivity of results to the deposition velocity specification is briefly discussed in "Deposition velocity sensitivity".
Averaging time	10 min	3 min[a] (only option)	EPIcode models plume meander due to averaging time dependency. The sensitivity of results to the averaging time specification is briefly discussed in "Averaging time sensitivity" section.
Dispersion model	Gaussian (only option)	Gaussian	ALOHA models dense-gas dispersion either in response to user specification or based on internal algorithms that determine the dense-gas dispersion model to be more appropriate than the Gaussian model for the particular scenario. The sensitivity of results to the dense-gas dispersion specification is briefly discussed in "ALOHA Dense Gas Model" section.

[a] Note that while both EPIcode and ALOHA use the same Briggs' dispersion coefficients for rural terrain as shown in Table 1, the EPIcode and ALOHA documentation seem to differ on the inherent time basis associated with these dispersion coefficients. The ALOHA documentation indicates the time basis to be 3 min for σ_y (and 10–60 min for σ_z)[9] while the EPIcode documentation assumes a time basis of 10 min[2] for σ_y. EPIcode makes an adjustment to σ_y for any averaging time specification other than 10 min.

EPIcode and ALOHA require a measurement height be input to correspond to the input wind speed, and results are sensitive to the measurement height input. ALOHA allows the wind speed height to be specified between 2 and 200 m. EPIcode allows the wind speed height to be specified between 2 and 100 m. For ground level releases, both EPIcode and ALOHA convert the input wind speed to a wind speed at some reference height. For EPIcode the reference height is 2 m, and for ALOHA the reference height is 3 m. The wind speed at this reference height is used in the atmospheric transport and dispersion calculations. Note that the wind speed is also used in the pool evaporation calculations (Pool Evaporation Calculations section) and that ALOHA, like EPIcode, apparently uses the wind speed at 2 m for these calculations.[9]

Table 3. Terrain sensitivity results for plume concentration (x = 100 m)

Sample Problem Results for Base Case (Rural Terrain) (mg/m^3)	EPIcode 7.0 Results for "City" Terrain (mg/m^3)	ALOHA 5.2.3 Results for "Urban or Forest" Ground Roughness (mg/m^3)
51	4.0	11

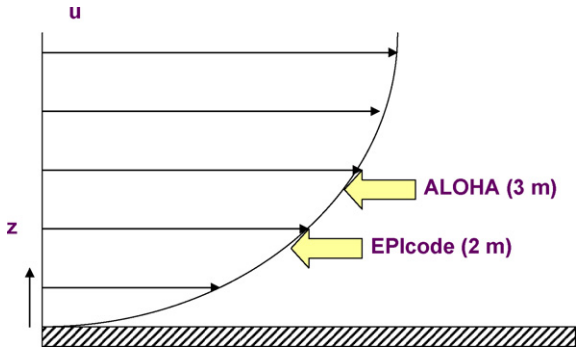

Figure 2. Atmospheric wind speed profile—ALOHA and EPIcode reference heights for atmopsheric transport and dispersion shown.

Both EPIcode and ALOHA use correlations of the following form to covert an input wind speed to a wind speed at the reference height.[2,9]

$$u_{ref} = u_{input} \times \left(\frac{z_{ref}}{z_{input}} \right)^{p} \quad (3)$$

where

z_{input}: height corresponding to wind speed input
u_{input}: wind speed input
z_{ref}: reference height for wind speed used in atmospheric transport and dispersion calculation
u_{ref}: wind speed at reference height
EPIcode specifications for the "*p*" exponent are shown in Table 4.

The National Weather Service (NWS) typically measures wind speeds at 10 m. Using the values in Table 4 for F atmospheric stability class together with Eq. (3), one can determine that a 10-m wind speed of approximately 2.4 m/s corresponds to a 1 m/s wind speed at the EPIcode reference height of 2 m and that a 10-m wind speed of approximately 1.6 m/s corresponds to a 1 m/s wind speed at the ALOHA reference height of 3 m.

To further demonstrate the sensitivity of results to the wind speed measurement height, results from EPIcode and ALOHA for 1 m/s wind speed specification corresponding to a height of 10 m (with the remaining input specifications for the sample problem remaining the same) are shown in Table 5.

For the same wind speed of 1 m/s specified at 10 m, the EPIcode calculated concentration is over 40% higher than that calculated by ALOHA and over 2.4 times that calculated for the base case.

Table 4. Exponent "p" specifications as a function of atmospheric stability class[2]

	A	B	C	D	E	F
EPIcode–standard terrain	0.07	0.07	0.10	0.15	0.35	0.55
EPIcode–city terrain	0.15	0.15	0.20	0.25	0.40	0.60

Table 5. Wind speed height sensitivity results for plume concentration (x = 100 m)

Sample Problem Result for Base Case (1 m/s Wind Speed at Reference Height) (mg/m^3)	EPIcode 7.0 Result for 1 m/s Wind Speed at 10 m Height (mg/m^3)	ALOHA 5.2.3 Result for 1 m/s Wind Speed at 10 m Height (mg/m^3)
51	120	84

Table 6. Deposition velocity sensitivity results for plume concentration

Distance Downwind (m)	Sample Problem Result for Base Case (No Deposition) (mg/m^3)	EPIcode 7.0 Result for 0.3 cm/s Deposition Velocity (mg/m^3)	EPIcode 7.0 Result for 1.0 cm/s Deposition Velocity (mg/m^3)
100	51	36	16
1,000	0.68	0.33	0.06

Deposition velocity sensitivity

Larger solid particles released in a plume will fall to the ground due to gravitational settling. Smaller particles and even gases will deposit on environmental 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) and the surface elements. Depletion of the contaminant in the plume occurs as a result. ALOHA does not model deposition. EPIcode models deposition through use of a deposition velocity that the user can specify (EPIcode default value for deposition velocity is 0 cm/s for gases and vapors and 0.3 cm/s for solids). To demonstrate the sensitivity of results to deposition, results from EPIcode for deposition velocities of 0.3 and 1.0 cm/s (with the remaining input specifications for the sample problem remaining the same) are shown in Table 6.

Plume depletion from deposition increases as the plume travels downwind. In addition to the 100-m results, results are also shown for the larger distance of 1,000 m to show this effect.

Averaging time sensitivity

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 concentrations are averaged. This time interval is referred to as the sample or averaging time. The dispersion coefficients that are used with the Gaussian plume model reflect the averaging time over which field measurements were recorded (taken to be 10 min in EPIcode for the Briggs' rural dispersion coefficients). EPIcode adjusts the horizontal dispersion

coefficient to account for the particular averaging time that is associated with the release scenario being analyzed.[2]

$$\sigma_{y,\mathrm{adj}} = \sigma_{y,\mathrm{ref}} \times \left(\frac{t_a}{10}\right)^{0.2} \quad (4)$$

where

$\sigma_{y,\mathrm{ref}}$: reference horizontal dispersion coefficient that is associated with 10-min averaging time
t_a: averaging time (min) that is associated with the release scenario being analyzed
$\sigma_{y,\mathrm{adj}}$: horizontal dispersion coefficient that is associated with averaging time of t_a

For example, if a release scenario involves release duration of longer than 10 min, a downwind receptor will experience a smaller time-averaged concentration (compared to a 10-min release) due to increased dispersion from increased plume meander.

To demonstrate the sensitivity of results to averaging time, results from EPIcode for sample times of 1 and 60 min (with the remaining input specifications for the sample problem remaining the same) are shown in Table 7.

ALOHA Dense Gas Model

If the density of the initial chemical cloud is greater than that of the ambient air, then the possibility exists for dense-gas type of atmospheric transport and dispersion (ALOHA uses the term heavy gas in place of dense gas). In dense-gas atmospheric transport and dispersion, the dense-gas cloud resists the influences of the hydraulic pressure field associated with 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 spreading that occurs with a neutrally buoyant release.

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 ($\mathrm{Ri_o}$) number above which dense gas transport effects are assumed important is assumed to be one.[9]

- $\mathrm{Ri_o} \leq 1$ For neutrally buoyant atmospheric transport and dispersion
- $\mathrm{Ri_o} > 1$ 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 $\mathrm{Ri_o}$ values as low as one and become more pronounced as $\mathrm{Ri_o}$ is increased.

For a continuous release[9]:

$$\mathrm{Ri_o} = \frac{g(\rho_o - \rho_a)Q_c}{\rho_a D_o u_{10} u_*^2} \quad (5)$$

where

g: acceleration of gravity
ρ_a: ambient air density
ρ_o: released chemical density at source
Q_c: continuous volumetric release rate
D_o: scale dimension of the source
u_{10}: mean wind speed at a height of 10 m
u_*: friction velocity

Unlike the Gaussian model used by ALOHA for neutrally buoyant transport and dispersion, the dense-gas set of equations used by ALOHA is too complicated to be presented and discussed in a condensed manner. ALOHA documentation identifies the 14 equations that the ALOHA code solves simultaneously to arrive at a solution for downwind concentration.[9]

Table 7. Averaging time sensitivity results for plume concentration (x = 100 m)

Sample Problem Result for Base Case (10 min Averaging Time) (mg/m^3)	EPIcode 7.0 Result for 1 min Averaging Time (mg/m^3)	EPIcode 7.0 Result for 60 min Averaging Time (mg/m^3)
51	82	36

To demonstrate the sensitivity of results to the type of dispersion model used, results from using the dense gas model of ALOHA are shown in Table 8 for the sample problem as well as for several other cases. Unlike Gaussian plume transport and dispersion, dense gas transport and dispersion is sensitive to properties of the chemical released. The four chemicals considered are methane, chlorine, benzene, and ammonia. Dense-gas releases can potentially occur with gases that have a density greater than air due to either a high molecular weight (e.g., chlorine, benzene) or being sufficiently cooled (e.g., refrigerated ammonia, refrigerated methane). A chemical cloud with sufficient aerosol content (e.g., release of liquefied chlorine or ammonia) can also result in the bulk cloud density being greater than that of the ambient air.

The results show that sometimes the Gaussian plume model predicts higher concentrations and sometimes the dense-gas model predicts higher concentrations. Up to nearly a factor of four differences is observed between the Gaussian plume concentration and the dense-gas plume concentration.

POOL EVAPORATION CALCULATIONS

ALOHA Evaporation Model

As part of the pool evaporation solution, ALOHA solves the mass and energy conservation equations to calculate the change in pool temperature with time as shown in Figure 3. The heat transfer mechanisms that are accounted for include short-wave solar influx, net long wave radiation flux between the pool and the atmosphere, ground-to-pool heat conduction, atmosphere-to-pool sensible heat flux, and latent heat flux from evaporation.[9] The evaporation rate varies with time in response to the changing pool temperature.

The liquid is non-boiling if the boiling point of the liquid is greater than the ground temperature. The vapor pressure of the chemical at each time step determines the time-dependent evaporation rate (i.e., evaporative mass transfer) for non-boiling liquids and is a strong function of the pool tempera-

Table 8. Type of dispersion model sensitivity results for plume concentration (x = 100 m)

Case	Chemical	Terrain	ALOHA 5.2.3 Gaussian Plume Model Concentration (mg/m^3)	ALOHA 5.2.3 Dense Gas Model Concentration (mg/m^3)
F atmospheric stability class and 1-m/s wind speed				
Sample problem 1A	Methane	Open country	51	36
Sample problem 1B	Chlorine	Open country		28
Sample problem 1C	Benzene	Open country		27
Sample problem 1D	Ammonia	Open country		25
Sensitivity case 1A	Methane	Urban or forest	11	25
Sensitivity case 1B	Chlorine	Urban or forest		18
Sensitivity case 1C	Benzene	Urban or forest		17
Sensitivity case 1D	Ammonia	Urban or forest		16
D atmospheric stability class and 2-m/s wind speed				
Sensitivity case 2A	Methane	Open country	3.6	8.5
Sensitivity case 2B	Chlorine	Open country		8.3
Sensitivity case 2C	Benzene	Open country		8.3
Sensitivity case 2D	Ammonia	Open country		8.3
Sensitivity case 3A	Methane	Urban or forest	1.5	5.9
Sensitivity case 3B	Chlorine	Urban or forest		5.6
Sensitivity case 3C	Benzene	Urban or forest		5.5
Sensitivity case 3D	Ammonia	Urban or forest		5.8

ture. The sum of all the heat fluxes at each time step will either increase or decrease the internal energy of the puddle, and will change proportionately to the change in internal energy.

If the boiling temperature of the liquid is less than the ground temperature, then the chemical vapor pressure is equal to the atmospheric pressure, and the liquid boils. The pool temperature remains constant in time at the chemical boiling point. There is no change in the internal energy of the puddle as the evaporative heat flux balances the heat flux from the other heat flux sources. Thus, the net heat flux from these other sources at each time step determines the time-dependent vaporization rate. The term cryogenic refers to chemicals that have a very low boiling point, such that the ground-to-pool heat conduction is the dominant heat flux. ALOHA accounts for cooling of the ground beneath a cryogenic pool.

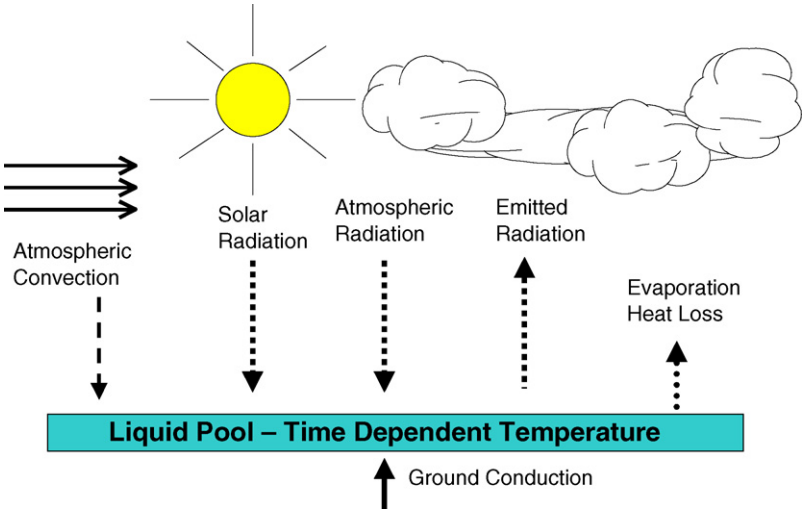

Figure 3. ALOHA energy balance for evaporation calculations.

EPIcode Evaporation Model

EPIcode uses the simpler EPA evaporation model that is documented in the 1999 Risk Management Program guidance (EPA-550-B-99-009).[4] The model is an easy-to-use screening tool that approximates the evaporation rate based on the pool area and temperature and the chemical-specific properties of molecular weight, vapor pressure, and gas-phase mass-transfer coefficient. The gas-phase mass-transfer coefficient (K) is estimated from the mass-transfer coefficient of a reference compound using the following empirical correlation.[4]

$$K = K_{ref}\left(\frac{MW_{ref}}{MW}\right)^{1/3} \quad (6)$$

where

K_{ref}: gas-phase mass-transfer coefficient of reference compound
MW_{ref}: molecular weight of reference compound
K: gas-phase mass-transfer coefficient of spilled chemical
MW: molecular weight of spilled chemical

The EPA model uses water as the reference compound and the following correlation.[4]

$$K_{\text{ref}}\left(\frac{\text{cm}}{\text{s}}\right) = 0.67u^{0.78} \quad (7)$$

In the previous EPIcode version, a constant of 0.25 was used in Eq. (7) instead of 0.67 following the EPA model that was in use at the time. Thus, EPIcode 7.0 uses a mass transfer coefficient of water that is factor of 2.68 higher than previously used. As a result, the updated evaporation model predicts evaporation rates of spilled chemical liquids and downwind plume concentrations that are higher by this same factor.

Pool Evaporation Results

The sample problem for the pool evaporation calculations has the same set of input specifications as shown in Table 2 except that the constant release rate input of 1 g/s is replaced by input data for pool dimensions and temperature. For this report, a pool volume of 21 gallons is assumed to spread such that the pool has a uniform depth of 1 cm, which gives a pool surface area of 7.95 m^2. The pool temperature is set to 25 °C. ALOHA requires additional input data, which for this report consisted of the following specifications: date/time of 06/29/04 and 23:59, cloud cover of 50%, 50% relative humidity, air and ground temperature of 25 °C, and "default" ground type. Since pool evaporation is dependent on chemical properties (most importantly vapor pressure), four chemicals are considered: nitric acid, chlorine, benzene, and ammonia.

To demonstrate the sensitivity of results to the pool evaporation models of EPIcode (version 7.0) and ALOHA (version 5.2.3), EPIcode and ALOHA results at 100 m are shown in Table 9 for the sample problem as well as for three sensitivity cases. The ALOHA output shows two evaporation rates corresponding to the maximum computed over a time step and the maximum average sustained that is averaged over a time period of 1 min or more. The average release rates for up to five time periods are used by ALOHA to calculate downwind concentrations.

Note that in all 16 cases analyzed, the EPIcode calculated evaporation rate is higher than the maximum average evaporation rate calculated by ALOHA. Differences of up to a factor of 2.7 times higher are observed. Thus, differences between ALOHA and EPIcode in calculated evaporation rates can equal the difference of 2.68 between version 7.0 and previous versions of EPIcode.

Generally the higher evaporation rates calculated by EPIcode translate to higher calculated downwind concentrations than ALOHA. For the 8 rural terrain cases, the EPIcode 100-m concentrations are typically observed to be a factor of two to four

Table 9. Sensitivity results (x = 100 m) for pool evaporation (EPIcode 7.0 & ALOHA 5.2.3)

		EPIcode 7.0 Results		ALOHA 5.2.3 Results		
					Plume Concentration ($x = 100$ m)	
Case	Chemical	Evaporation Rate (g/s)	Plume Concentration ($x = 100$ m) (mg/m^3)	Evaporation Rate (Max (g/s)/ Max Avg (g/s))	Gaussian Model (mg/m^3)	Dense Gas Model (mg/m^3)
F atmospheric stability class and 1-m/s wind speed–rural terrain						
Sample problem 1A	Nitric acid	7.4	320	5.3/4.7	230	[a]88
Sample problem 1B	Chlorine	740	42,000	2,100/450	21,000	[a]3,000
Sample problem 1C	Benzene	13	560	9.6/9.6	430	[a]130
Sample problem 1D	Ammonia	380	22,000	400/140	[a]6,900	760
F atmospheric stability class and 1-m/s wind speed–urban terrain						
Sensitivity case 1A	Nitric acid	7.4	27	5.3/4.7	[a]48	61
Sensitivity case 1B	Chlorine	740	3,600	2,100/450	4,400	[a]1,500
Sensitivity case 1C	Benzene	13	48	9.6/9.6	90	[a]91
Sensitivity case 1D	Ammonia	380	1,900	400/140	[a]1,400	670
D atmospheric stability class and 2-m/s wind speed–rural terrain						
Sensitivity case 2A	Nitric acid	13	41	9.1/9.1	[a]32	73
Sensitivity case 2B	Chlorine	1,300	6,000	2,800/670	2,400	[a]2,600
Sensitivity case 2C	Benzene	22	73	17/14	[a]49	110
Sensitivity case 2D	Ammonia	650	3,100	540/240	[a]860	1,300
D atmospheric stability class and 2-m/s wind speed–urban terrain						
Sensitivity case 3A	Nitric acid	13	8.9	9.1/9.1	[a]13	49
Sensitivity case 3B	Chlorine	1,300	1,300	2,800/670	950	[a]1,600
Sensitivity case 3C	Benzene	22	16	17/14	[a]20	74
Sensitivity case 3D	Ammonia	650	670	540/240	[a]350	870

[a] Dispersion model that ALOHA determined to be applicable.

higher (a factor of 14 is observed for one case) than ALOHA. The urban results show that sometimes EPIcode predicts higher concentrations and sometimes ALOHA predicts higher concentrations (up to a factor of two difference).

The coupled evaporation rate and atmospheric dispersion calculations are repeated using the latest version of ALOHA, namely, version 5.3.1.[5] The chemical property database was updated in this newer version of ALOHA. It is expected that ALOHA version 5.3.1 will eventually be incorporated into the toolbox (replacing version 5.2.3). Evaporation rates and 100-m concentrations from ALOHA 5.3.1 are shown in Table 10 alongside the ALOHA version 5.2.3 results. Only minor differences (typically 10% or less) are seen in the nitric acid and benzene results between the two ALOHA versions. An interesting result with the second nitric acid result (F atmospheric stability class and 1 m/s wind speed–urban terrain) is that ALOHA 5.3.1 selected the dense gas model to be applicable in contrast to the Gaussian model that was selected by ALOHA 5.2.3. Differences up to 25% are observed with the ammonia cases. The largest change occurs with the chlorine and the releases under meteorological conditions of F stability class and 1 m/s wind speed. The predicted evaporation rate with ALOHA 5.3.1 is twice that predicted with the previous ALOHA version.

Finally, concentration results at 2 km are investigated. Comparison of EPIcode (version 7.0) and ALOHA (version 5.3.1) results at 2 km are shown in Table 11. These results show similar trends to those reported in Table 9 for 100-m concentrations. In all cases for rural terrain, EPIcode results are consistently higher at both 100 m and 2 km (when compared against ALOHA results using the dispersion model that ALOHA determined to be applicable). The higher EPIcode concentration rates are consistent with the higher evaporation rates determined by EPIcode that were noted above. In general the EPIcode concentration results are a factor of 2–4 higher, although differences as high as a factor of ten were observed. For the urban terrain cases there was no clear trend. Recall from the urban terrain sensitivity case shown earlier for dispersion (Table 3), that the ALOHA results were almost a factor of 3 higher. This dispersion effect tended to offset the higher evaporation rates of EPIcode, leading to the results shown in Tables 9 and 11 of ALOHA sometimes predicting higher concentration and EPIcode sometimes predicting higher concentrations in the urban terrain cases (within a factor of 3 in all cases).

It cannot be stressed enough that the above findings were made with a very limited data set and care must be made not to over-generalize these results. Further investigation is recommended

Table 10. Sensitivity results (x = 100 m) for pool evaporation (ALOHA 5.2.3 & ALOHA 5.3.1)

	ALOHA 5.2.3 Results			ALOHA 5.3.1 Results		
		Plume Concentration ($x = 100$ m)			Plume Concentration ($x = 100$ m)	
Chemical	Evaporation Rate (Max Avg) (g/s)	Gaussian Model (mg/m^3)	Dense Gas Model (mg/m^3)	Evaporation Rate (Max Avg) (g/s)	Gaussian Model (mg/m^3)	Dense Gas Model (mg/m^3)
F atmospheric stability class and 1-m/s wind speed–rural terrain						
Nitric acid	4.7	230	[a]88	4.8	240	[a]90
Chlorine	450	21,000	[a]3,000	900	38,000	[a]5,900
Benzene	9.6	430	[a]130	8.7	430	[a]130
Ammonia	140	[a]6,900	760	180	[a]8,200	810
F atmospheric stability class and 1-m/s wind speed–urban terrain						
Nitric acid	4.7	[a]48	61	4.8	49	[a]62
Chlorine	450	4,400	[a]1,500	900	7,900	[a]2,600
Benzene	9.6	91	[a]91	8.7	89	[a]91
Ammonia	140	[a]1,400	670	180	[a]1,700	720
D atmospheric stability class and 2-m/s wind speed–rural terrain						
Nitric acid	9.1	[a]32	73	7.9	[a]28	62
Chlorine	670	2,400	[a]2,600	910	3,200	[a]3,400
Benzene	14	[a]49	110	14	[a]50	110
Ammonia	240	[a]860	1,300	190	[a]680	1,100
D atmospheric stability class and 2-m/s wind speed–urban terrain						
Nitric acid	9.1	[a]13	49	7.9	[a]11	44
Chlorine	670	950	[a]1,600	910	1,300	[a]2,000
Benzene	14	[a]20	74	14	[a]20	76
Ammonia	240	[a]350	870	190	[a]270	720

[a] Dispersion model that ALOHA determined to be applicable.

Table 11. Sensitivity results (x = 2 km) for pool evaporation model (EPIcode 7.0 & ALOHA 5.3.1)

		EPIcode 7.0 Results		ALOHA 5.3.1 Results		
					Plume Concentration ($x = 2$ km)	
Case	Chemical	Evaporation Rate (g/s)	Plume Concentration ($x = 2$ km) (mg/m^3)	Evaporation Rate (Max Avg) (g/s)	Gaussian Model (mg/m^3)	Dense Gas Model (mg/m^3)
F atmospheric stability class and 1-m/s wind speed–rural terrain						
Sample problem 1A	Nitric acid	7.4	1.6	4.8	0.99	[a]0.58
Sample problem 1B	Chlorine	740	210	900	38	[a]7.5
Sample problem 1C	Benzene	13	2.8	8.7	1.8	[a]1.0
Sample problem 1D	Ammonia	380	110	180	[a]12	5.3
F atmospheric stability class and 1-m/s wind speed–urban terrain						
Sensitivity case 1A	Nitric acid	7.4	0.18	4.8	0.25	[a]0.41
Sensitivity case 1B	Chlorine	740	16	900	9.6	[a]5.9
Sensitivity case 1C	Benzene	13	0.32	8.7	0.45	[a]0.73
Sensitivity case 1D	Ammonia	380	7.4	180	[a]3.0	4.3
D atmospheric stability class and 2-m/s wind speed–rural terrain						
Sensitivity case 2A	Nitric acid	13	0.23	7.9	[a]0.14	0.21
Sensitivity case 2B	Chlorine	1,300	33	910	6.6	[a]10
Sensitivity case 2C	Benzene	22	0.41	14	[a]0.26	0.39
Sensitivity case 2D	Ammonia	650	16	190	[a]1.6	2.5
D atmospheric stability class and 2-m/s wind speed–urban terrain						
Sensitivity case 3A	Nitric acid	13	0.038	7.9	[a]0.039	0.15
Sensitivity case 3B	Chlorine	1,300	3.1	910	1.8	[a]7.5
Sensitivity case 3C	Benzene	22	0.068	14	[a]0.070	0.27
Sensitivity case 3D	Ammonia	650	1.3	190	[a]0.42	1.8

[a] Dispersion model that ALOHA determined to be applicable.

for verification. The main value of the above results is to demonstrate the variability of results that one can expect between ALOHA and EPIcode when modeling evaporation rates and resulting downwind concentrations.

GUIDANCE FOR SAFETY ANALYSIS

The limited sensitivity study reported in Tables 3–11 above indicates that the results are sensitive to meteorology (stability category and wind speed), surface roughness (urban, rural), specific chemical being released and its properties, dispersion model (dense gas, neutrally buoyant), and complexity of the code (EPIcode, ALOHA). This section offers guidance for performing a hazard or accident analysis of a liquid evaporation release using ALOHA, EPIcode, or another chemical dispersion model. This guidance summarizes information and recommendations that have been previously documented in other references[10–15] and builds upon them in light of the findings of the current effort that is documented in this report.

1. **Code selection**: The ultimate goal for the analyst is to use the code that will generally produce the most accurate results with a conservative bias for the scenarios being analyzed. Without comparison of code results against experimental data for a standardized test problem set, however, it is not possible to make this determination. Additionally, assessments of conservatism (in an absolute sense) are largely speculative without these comparisons. That being said, the following factors should be considered in selection of a code for analyzing downwind concentrations from liquid chemical spills.
   a. ***Meteorological data for atmospheric transport and dispersion calculations***–Both ALOHA and EPIcode use specifications of a single wind speed and single atmospheric stability class. Neither ALOHA or EPIcode allow for statistical treatment of site meteorological data as discussed below. The analysis for many sites use default specifications of F atmospheric stability class and 1–2 m/s wind speed.[10] These specifications are chosen to represent "unfavorable" meteorological conditions for accident analysis of the offsite receptor and ideally are based on analysis of site meteorological data. In defining unfavorable meteorological conditions for chemical releases, it seems reasonable to follow the practices that are used for radiological consequence analysis of the offsite receptor as prescribed by Appendix A of DOE-STD-3009.[16] Specifically, radiological consequences are based on the

95th percentile of the distribution of doses as determined from the statistical treatment of results that are calculated using hourly site meteorological data over a period of one year or more. In context of chemical releases, unfavorable meteorology would thus refer to the meteorology that coupled with the source term would lead to concentration exposures for chemicals that are exceeded less than five percent of the time based on site meteorological conditions.

Some sites use the capability of MACCS2 (MELCOR Accident Consequence Code System 2)[17,18] to generate a 95th percentile χ/Q value based on statistical analysis of results generated using one year of hourly site meteorological data.[10] MACCS2 was designed for calculation of radiological consequences from user-specified source term releases and therefore does not have an evaporation rate algorithm. So, the evaporation rate must be determined from a hand calculation or from a code such as ALOHA or EPIcode to use with the MACCS2 generated χ/Q value. The decoupling of the source term (i.e., evaporation rate) calculation from the atmospheric transport and dispersion (i.e., χ/Q) calculation is somewhat undesirable (see item 2 below) but an analyst may feel that this is an acceptable tradeoff in order to use a 95th percentile χ/Q value based on site meteorology and other MACCS2 capabilities (e.g., building wake modeling).

b. ***Increased initial dispersion from building wakes***–Neither ALOHA or EPIcode models the dispersion effects behind building wakes. Since wake effects near the source tend to enhance dispersion that provides additional dilution, it is generally believed that neglecting these effects in estimating chemical concentrations at downwind locations for ground-level releases is conservative. MACCS2 allows the user to model enhanced dispersion due to dispersion through specification of an initial plume cross-section. The initial plume dimensions scale to the building cross-section, and dispersion is modeled mathematically through creation of a virtual source that is upwind of the building/source location. The specification of reasonably conservative building dimensions may require some effort since the analyst may need to consider (e.g., usually through parametric study) various combinations of release locations and line-of-sight obstruction dimensions that are dependent upon the wind direction.

c. ***Terrain specification***–Most DOE sites have terrain characteristics between the rural and urban extremes that are available with ALOHA and EPIcode. As a result, the use of the rural-terrain dispersion coefficients are generally recommended for these sites since more conservative results are obtained with these for non-buoyant, ground releases. As a result, the different specification schemes of the σ_y dispersion coefficients between ALOHA and EPIcode for city or urban generally is not an issue. In contrast, MACCS2 allows for intermediary specifications for the σ_z dispersion coefficient through the use of a surface roughness length correction factor to the rural σ_z dispersion coefficient. The surface roughness length is a 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. Generally, a surface roughness length of 3 cm is associated with the rural dispersion coefficients, and a surface roughness length of 100 cm is associated with the urban dispersion coefficients. As a general rule, the surface roughness length is considered to be approximately 0.1 times the average height of roughness elements located in the transport region of interest.

d. ***Deposition***–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 a plume occurs as a result. The most conservative results are generally obtained with the deposition velocity set to zero. Both EPIcode and MACCS2 allow for deposition to be modeled through the specification of a deposition velocity, but ALOHA does not (EPIcode uses default values of 0.3 cm/s for particles and 0 cm/s for gases).

e. ***Averaging time***–The dispersion coefficients that are used with the Gaussian plume model reflect the averaging time over which field measurements were recorded (taken to be 3–10 min for the Briggs' rural dispersion coefficients as indicated in the Table 2 note). The time-averaged concentration decreases as the averaging time increases due to plume meander as was shown in Figure 1. In the Gaussian dispersion model, the effect of averaging time, when different from the experimental basis, is typically addressed through a correction factor to the horizontal dispersion coefficient as done in EPIcode and MACCS2 (ALOHA does not incorporate averaging-time correction).

The 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.[4] Published exposure guidelines include the Emergency Response Planning Guidelines (ERPGs), Temporary Emergency Exposure

Limits (TEELs), and Acute Exposure Guideline Limits (AEGLs). AEGLs have been developed in terms of five emergency exposure periods (10 and 30 min, 1, 4, and 8 h). Since the DOE has not provided definitive exposure guidelines for chemical exposures for use in accident analysis, the specific use of ERPGs, TEELs, and AEGLs in accident analysis and specification of averaging time remain largely open issues.

A 15-min averaging time has been used historically in accident analysis in terms of determining the peak 15-min time weighted (TWA) chemical concentration for comparison with the exposure guideline.[10,11] Since the time basis for the rural dispersion coefficients used in ALOHA, EPIcode, and MACCS2 are less than 15 min, use of results from these codes without averaging time correction to represent a 15-min TWA adds conservatism for scenarios with releases lasting longer than 15 min. Note that MACCS2 also allows for the use of Tadmor-Gur dispersion coefficients (3-min time basis for σ_y).[19]

f. ***Measurement height for wind speed***–The MACCS2 code uses hourly meteorological data that includes wind speed reported at 10 m (NWS typically measures wind speeds at 10 m). These wind-speed values are used in the atmospheric transport and dispersion calculations consistent with Nuclear Regulatory Commission guidance.[20] Both ALOHA and EPIcode use a single wind-speed value that the analyst specifies along with the measurement height associated with this wind speed. For ground level releases, both EPIcode and ALOHA convert the input wind speed to a wind speed at a reference height, which is 2 m for EPIcode and 3 m for ALOHA. The wind speed at this reference height is used in the atmospheric transport and dispersion calculations. As evidenced by the Table 5 results presented earlier, the wind-speed adjustment by ALOHA and EPIcode can add significant conservatism to the calculated concentration with respect to the approach used by MACCS2.

g. ***Dense gas release***–Only ALOHA models dense-gas atmospheric transport and dispersion.

h. ***Other factors***–ALOHA has a one-hour limit for plume travel time. Calculations are terminated before the plume reaches far-field receptors under light winds. For example, the leading edge of a puff or plume will travel a distance of about 5.4 km for a wind speed of 1.5 m/s, which is commonly used along with F atmospheric stability class for consequence calculations under unfavorable conditions. Therefore, ALOHA is incapable of making concentration predictions for receptors beyond approximately 5.4 km for a wind speed of 1.5 m/s.

Both EPIcode and MACCS2 have the capability to print out results (concentration predictions and χ/Q estimates, respectively) as a function of downwind distance from the release. This feature is very useful for elevated (i.e., stack) releases. For elevated releases of neutrally buoyant gases, 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 to reach ground level.

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 when using ALOHA or EPIcode. EPIcode has a useful feature that can aid in this process. When viewing the plume centerline concentrations as a function of distance graphically, the user has the option of requesting that EPIcode display results for each of the six stability classes simultaneously. The parametric approach is not needed with the MACCS2 code due to the statistical algorithms built around the sampling of site meteorological data. At each downwind location, the 95th percentile χ/Q value (as well as the other metrics that are included in the output) is determined from the distribution of results at that location that are calculated using hourly site meteorological data over a period of one year.

2. **Source term consistency with dispersion assumptions**: Coupling the evaporation calculations with the atmospheric transport and dispersion calculations ensures a self-consistent approach. Meteorological variables affect both the evaporation rate and the amount of dilution of the plume during atmospheric transport. For example, wind speed affects the evaporation rate and atmospheric dilution in opposite ways with regard to the effect produced on downwind concentrations. For example, a high wind speed promotes higher evaporation rates, but also supports greater dilution during atmospheric transport. Parametric runs may be necessary to achieve the desired results (e.g., median, unfavorable,

upper bound). There is some evidence that the dominant influence of the meteorological variables generally occurs with atmospheric dispersion and dilution such that meteorological conditions that produce conservative χ/Q values also produce conservative downwind chemical concentrations when the evaporation rate calculation is coupled with the atmospheric transport and dispersion calculation.[13] This finding can be used to develop a reasonably conservative approach for the situation described in 1a (Code Selection) above in which an analyst chooses to decouple the source term and dispersion calculations by using MACCS2 to calculate a 95th percentile χ/Q value based on site meteorology. A reasonable approach would be to use the wind speed associated with the 95th percentile χ/Q value for the evaporation rate calculations or a slightly higher wind speed for added conservatism.

3. **Input data and modeling assumptions**: The documentation accompanying the analysis should include the bases for key input data and modeling assumptions. The reasoning behind including or omitting phenomenological effects should be given. Selection of an appropriate meteorology should be consistent with the purpose intended. Other characteristics of the analysis should use input values applicable to the region of transport.
4. **Use of results**: Decisions (e.g., need for safety controls) based on the results of a code should consider the inherent uncertainty in the results as evidenced by the variability that can exist between the results of different codes modeling the same scenario.

CONCLUDING REMARKS

The universally higher evaporation rates and downwind concentrations calculated with EPIcode version 7.0 by a factor of 2.68 in comparison with those calculated with previous EPIcode versions have raised the issue of potential non-conservatism in safety analyses that are based on previous versions of EPIcode. The factor of 2.68 difference must be considered in the broader context of the variability of results that one can expect between the results of two different computer codes that model evaporation rates and resulting downwind concentrations. The comparisons in this report highlight the variability of results obtained from the simple screening tool model of EPIcode and the more complex model of ALOHA. The variability is magnified when the pool evaporation model is coupled to atmospheric transport and dispersion models to predict downwind chemical concentrations. The observed differences seen in this report that are as high as an order of a magnitude are consistent with other published results such as those documented in the DOE-sponsored Accident Phenomenology and Consequence Assessment work.[12] A lower or higher result with one code versus the other only provides an indication of relative conservatism. Comparison of code results against an extensive experimental data set is needed to evaluate the accuracy of these codes and assess conservatism in the absolute sense.

It is recommended that the safety analyst explicitly evaluate the strengths and limitations of any code before selecting it for a specific application. User skill and expertise can often outweigh most of the differences between ALOHA and EPIcode. Recognizing that EPIcode is inherently a scoping tool, while ALOHA is based on more detailed models, the user is recommended to perform a parameter sensitivity study to determine major dependences in the applied model and to check code output with independent techniques, such as a hand calculation, alternative computer code application, or spreadsheet techniques. A multi-tiered approach of this type will provide better confidence in overall results than to unilaterally use one code alone, without questioning the technical model basis.

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