This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-96SR18500 with the U. S. Department of Energy.

DISCLAIMER

A Comparison of EPIcode and ALOHA Calculations for Pool Evaporation and Chemical Atmospheric Transport and Dispersion

D. C. Thoman
M. W. Davis, K. R. O'Kula

Washington Safety Management Solutions LLC

Abstract

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 paper 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.

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 DNFSB Recommendation 2002-1[1] and include EPIcode (version 7.0)[2] and 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 paper is 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 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.

The first half of the paper 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 paper 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 a few common chemicals.

Atmospheric Transport and Dispersion Calculations

Gaussian Plume Model Overview

The basic form for the Gaussian plume model is given as[5]

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

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 paper, 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:

$$\chi(x,0,0)=\frac{Q}{\pi\sigma_y\sigma_z u} \qquad \text{Eq. (2)}$$

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 between 2 and 10 meters 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. 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.

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.

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[6]. Briggs developed a

different set of algebraic expressions for rural and urban environments as shown in Table 1 below.

Table 1 Briggs' Dispersion Coefficients[2].

Rural Terrain		
Atmospheric Stability Class	**σ_y [m]**	**σ_z [m]**
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		
Atmospheric Stability Class	**σ_y [m]**	**σ_z [m]**
A-B	$0.32x\ (1+0.0004)^{-1/2}$	$0.24x\ (1+0.001x)^{+1/2}$
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	$0.11x\ (1+0.0004x)^{-1/2}$	$0.08x\ (1+0.0015x)^{-1/2}$

As an illustrative example, a one g/s (1000 mg/s) release of a chemical at ground level is considered under 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 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 Equation (2):

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

EPIcode and ALOHA Gaussian Plume Models

EPIcode and ALOHA each have additional features for modeling atmospheric transport and dispersion that extend beyond the basic Gaussian plume model described above. These additional features expand input data requirements. Table 2 summarizes the input data set required for each code to replicate the results of the sample problem discussed above. A discussion follows that highlights the sensitivity of the calculated downwind concentration values to a few of the key input parameter specifications.

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 below.
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 below.
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 below.
Averaging Time	10 minutes	3 minutes* (only option)	EPIcode models plume meander due to averaging time dependency. The sensitivity of results to the averaging time specification is briefly discussed below.
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 the next subsection.

* 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 minutes for σ_y (and 10 to 60 minutes for σ_z)[7] while the EPIcode documentation assumes a time basis of 10 minutes[2] for σ_y. EPIcode makes an adjustment to σ_y for any averaging time specification other than 10 minutes.

Terrain Sensitivity

The same result of 51 mg/m^3 is obtained from EPIcode and ALOHA for the sample problem 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, however, 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 more conservative rural σ_y dispersion coefficients[7].

Table 3 Terrain Sensitivity Results.

Sample Problem Results for Base Case (Rural Terrain), (100 m)	**EPIcode 7.0 Results for "City" Terrain, (100 m)**	**ALOHA 5.2.3 Results for "Urban or Forest" Ground Roughness, (100 m)**
51 mg/m^3	4.0 mg/m^3	11 mg/m^3

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. The sample problem statement specifies a 1 m/s wind speed, but does not specify that height at which this wind speed occurs. Both 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 m and 200 m. EPIcode allows the wind speed height to be specified between 2 m 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. Both EPIcode and ALOHA use correlations of the following form to covert an input wind speed to a wind speed at the reference height[2,7].

$$u_{ref} = u_{input} \times \left(\frac{z_{ref}}{z_{input}} \right)^{p} \qquad \text{Eq. (3)}$$

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 and ALOHA use different specifications for the "p" exponent as shown in Table 4.

Table 4 Exponent "p" Specifications as a Function of Atmospheric Stability Class[2,7].

	A	B	C	D	E	F
ALOHA	0.06	0.15	0.17	0.23	0.38	0.38
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

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 Equation (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.

Table 5 Wind Speed Height Sensitivity Results.

Sample Problem Result for Base Case (1 m/s Wind Speed at Reference Height), (100 m)	**EPIcode 7.0 Result for 1 m/s Wind Speed at 10 m Height, (100 m)**	**ALOHA 5.2.3 Result for 1 m/s Wind Speed at 10 m Height, (100 m)**
51 mg/m^3	120 mg/m^3	84 mg/m^3

For the same wind speed of 1 m/s specified a 10 m, the EPIcode calculated concentration is over 40% higher than that calculated by ALOHA.

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 cm/s and 1.0 cm/s (with the remaining input specifications for the sample problem remaining the same) are shown in Table 6.

Table 6 Deposition Velocity Sensitivity Results.

Distance Downwind	Sample Problem Result for Base Case (No Deposition), (100m)	EPIcode 7.0 Result for 0.3 cm/s Deposition Velocity, (100 m)	EPIcode 7.0 Result for 1.0 cm/s Deposition Velocity, (100 m)
100 m	51 mg/m^3	36 mg/m^3	16 mg/m^3
1000 m	0.68 mg/m^3	0.33 mg/m^3	0.06 mg/m^3

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 1000 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 minutes 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].

$$\sigma_{y,adj} = \sigma_{y,ref} \times \left(\frac{t_a}{10} \right)^{0.2} \qquad \text{Eq. (4)}$$

where:

$\sigma_{y,ref}$ = reference horizontal dispersion coefficient that is associated with 10-minute averaging time

t_a = averaging time [min] that is associated with the release scenario being analyzed

$\sigma_{y,adj}$ = 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 minutes, a downwind receptor will experience a smaller time-averaged concentration (compared to a 10-minute 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 minute and 60 minutes (with the remaining input specifications for the sample problem remaining the same) are shown in Table 7.

Table 7 Deposition Velocity Sensitivity Results.

Sample Problem Result for Base Case (10 minute Averaging Time), (100 m)	EPIcode 7.0 Result for 1 minute Averaging Time, (100 m)	EPIcode 7.0 Result for 60 minute Averaging Time, (100 m)
51 mg/m^3	82 mg/m^3	36 mg/m^3

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 (Ri_o) number above which dense gas transport effects are assumed important is assumed to be one[7].

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

For a continuous release[7]:

$$Ri_o = \frac{g \times (\rho_o - \rho_a) \times Q_c}{\rho_a \times D_o \times u_{10} \times u_*^2} \qquad \text{Eq. (5)}$$

where:

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 10m

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[7].

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.

Table 8 Sensitivity Results for Type of Dispersion Model.

Case	Chemical	Terrain	ALOHA Gaussian Plume Model Concentration, (100 m)	ALOHA Dense Gas Model Concentration, (100 m)
F Atmospheric Stability Class and 1-m/s Wind Speed				
Sample Problem 1A	Methane	Open Country	51 mg/m^3	36 mg/m^3
Sample Problem 1B	Chlorine	Open Country		28 mg/m^3
Sample Problem 1C	Benzene	Open Country		27 mg/m^3
Sample Problem 1D	Ammonia	Open Country		25 mg/m^3
Sensitivity Case 1A	Methane	Urban or Forest	11 mg/m^3	25 mg/m^3
Sensitivity Case 1B	Chlorine	Urban or Forest		18 mg/m^3
Sensitivity Case 1C	Benzene	Urban or Forest		17 mg/m^3
Sensitivity Case 1D	Ammonia	Urban or Forest		16 mg/m^3
D Atmospheric Stability Class and 2-m/s Wind Speed				
Sensitivity Case 2A	Methane	Open Country	3.6 mg/m^3	8.5 mg/m^3
Sensitivity Case 2B	Chlorine	Open Country		8.3 mg/m^3
Sensitivity Case 2C	Benzene	Open Country		8.3 mg/m^3
Sensitivity Case 2D	Ammonia	Open Country		8.3 mg/m^3
Sensitivity Case 3A	Methane	Urban or Forest	1.5 mg/m^3	5.9 mg/m^3
Sensitivity Case 3B	Chlorine	Urban or Forest		5.6 mg/m^3
Sensitivity Case 3C	Benzene	Urban or Forest		5.5 mg/m^3
Sensitivity Case 3D	Ammonia	Urban or Forest		5.8 mg/m^3

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 difference 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. The heat transfer mechanisms that are accounted for include short-wave solar influx, net longwave 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[7]. 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 temperature. 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.

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].

$$K = K_{ref} (MW_{ref}/MW)^{1/3} \qquad \text{Eq. (6)}$$

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_{ref} [cm/s] = $0.67 \times u^{0.78}$ Eq. (7)

In the previous EPIcode version, a constant of 0.25 was used in Equation (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 paper, 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 7.95m^2. The pool temperature is set to 25 °C. ALOHA requires additional input data, which for this paper 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 and ALOHA, EPIcode and ALOHA results 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 one minute 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 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).

Table 9 Sensitivity Results for Pool Evaporation Model.

Case	Chemical	EPIcode Results		ALOHA Results		
		Evaporation Rate	Concentration (100 m)	Evaporation Rate Max/Max Avg	Concentration (100 m)	
					Gaussian Model	(Dense Gas Model)
F Atmospheric Stability Class and 1-m/s Wind Speed – Rural Terrain						
Sample Problem 1A	Nitric acid	7.4 g/s	320 mg/m^3	5.3 g/s 4.7 g/s	230 mg/m^3	*88 mg/m^3
Sample Problem 1B	Chlorine	740 g/s	42,000 mg/m^3	2100 g/s 450 g/s	21,000 mg/m^3	*3000 mg/m^3
Sample Problem 1C	Benzene	11 g/s	450 mg/m^3	9.6 g/s 9.6 g/s	430 mg/m^3	*130 mg/m^3
Sample Problem 1D	Ammonia	380 g/s	22,000 mg/m^3	400 g/s 140 g/s	*6900 mg/m^3	760 mg/m^3
F Atmospheric Stability Class and 1-m/s Wind Speed – Urban Terrain						
Sensitivity Case 1A	Nitric acid	7.4 g/s	27 mg/m^3	5.3 g/s 4.7 g/s	*48 mg/m^3	61 mg/m^3
Sensitivity Case 1B	Chlorine	740 g/s	3600 mg/m^3	2100 g/s 450 g/s	4400 mg/m^3	*1500 mg/m^3
Sensitivity Case 1C	Benzene	11 g/s	39 mg/m^3	9.6 g/s 9.6 g/s	91 mg/m^3	*91 mg/m^3
Sensitivity Case 1D	Ammonia	380 g/s	1900 mg/m^3	400 g/s 140 g/s	*1400 mg/m^3	670 mg/m^3
D Atmospheric Stability Class and 2-m/s Wind Speed – Rural Terrain						
Sensitivity Case 2A	Nitric acid	13 g/s	41 mg/m^3	9.1 g/s 9.1 g/s	*32 mg/m^3	73 mg/m^3
Sensitivity Case 2B	Chlorine	1300 g/s	6000 mg/m^3	2800 g/s 670 g/s	2400 mg/m^3	*2600 mg/m^3
Sensitivity Case 2C	Benzene	18 g/s	59 mg/m^3	17 g/s 14 g/s	*49 mg/m^3	110 mg/m^3
Sensitivity Case 2D	Ammonia	650 g/s	3100 mg/m^3	540 g/s 240 g/s	*860 mg/m^3	1300 mg/m^3
D Atmospheric Stability Class and 2-m/s Wind Speed – Urban Terrain						
Sensitivity Case 3A	Nitric acid	13 g/s	8.9 mg/m^3	9.1 g/s 9.1 g/s	*13 mg/m^3	49 mg/m^3
Sensitivity Case 3B	Chlorine	1300 g/s	1300 mg/m^3	2800 g/s 670 g/s	950 mg/m^3	*1600 mg/m^3
Sensitivity Case 3C	Benzene	18 g/s	13 mg/m^3	17 g/s 14 g/s	*20 mg/m^3	74 mg/m^3
Sensitivity Case 3D	Ammonia	650 g/s	670 mg/m^3	540 g/s 240 g/s	*350 mg/m^3	869 mg/m^3
* Dispersion model that ALOHA determined to be applicable.						

Recommendations for Safety Analysis

The limited sensitivity study reported in Tables 3 – 9 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). The following are offered as recommendations to guide hazard and accident analysis of a liquid evaporation release using ALOHA, EPIcode, or another chemical dispersion model:

1. Code selection: Without comparison of code results against experimental data for a standardized test problem set, it is not possible to determine which code produces the more accurate results. Additionally, assessments of conservatism (in an absolute sense) are largely speculative without these comparisons.

2. 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.

3. Site specificity: 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. Source term consistency with dispersion assumptions: Coupling the evaporation calculations with the atmospheric transport and dispersion calculations ensures a self-consistent approach. Meteorological variables can affect both the evaporation rate and the amount of dilution of the plume during atmospheric transport. For example, wind speed can affect the evaporation rate and atmospheric dilution in opposite ways with regard to the effect produced on downwind concentrations. Parametric runs may be necessary to achieve the desired results (e.g., median, upper bound).

5. 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 two 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 paper 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 paper that are as a 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 (APAC) work[8].

References

1. DOE (2003). *Implementation Plan for Defense Nuclear Facilities Safety Board Recommendation 2002-1: Quality Assurance for Safety Software at Department of Energy Nuclear Facilities*, Report, U.S. Department of Energy, February 28, 2003.
2. EPIcode (2003). *EPIcode Version 7.0 User Documentation*, Online Help distributed with software package, Homann Associates, Inc. September 2003.
3. NOAA (1999) and EPA. *ALOHA 5.2.3 User Documentation*, Online Help distributed with software package, Office of Response and Restoration of the National Oceanic and Atmospheric Administration (NOAA) and Chemical Emergency Preparedness and Prevention Office (CEPPO) of the U.S. Environmental (EPA), Seattle, WA, 1999.
4. EPA (1999). *Risk Management Program for Offsite Consequence Analysis*, EPA 550-B-99-0009, U.S. Environmental Protection Agency, Research Triangle Park, NC, 1999.
5. S. R. Hanna (1982), G. A. Briggs, and R. P., Hosker, Jr. *Handbook on Atmospheric Dispersion*, DOE/TIC-11223, Technical Information Center, U.S. Department of Energy (DOE), Oak Ridge, TN, 1982.
6. G. A. Briggs (1973). *Diffusion Estimates for Small Emissions, Atmospheric Turbulence and Diffusion Laboratory*, ATDL Contribution File No. 79, 1973.
7. R. M. Reynolds (1992). *ALOHA Theoretical Description*, Draft Technical Memorandum NOS ORCA-65 Hazardous Materials Response and Assessment Division (HMRAD) of the National Oceanic and Atmospheric Administration (NOAA), Seattle, WA, 1992.
8. M. A. Lazaro (1997), K. Woodward, S. R. Hanna, D.J. Hesse, J. C. Huang, J. Lewis, and C. A. Mazzola. Model Review and Evaluation for Application in DOE Safety Basis Documentation of Chemical Accidents - Modeling Guidance for Atmospheric Dispersion and Consequence Assessment, ANL/EAD/TM-75, Environmental Assessment Division (EAD), Argonne National Laboratory (ANL), Argonne, IL, September 1997.