GAS DISPERSION MODEL IN PEAC TOOL

Occasionally AristaTek will get an inquiry as to what gas dispersion model is used in the PEAC tool. Another question is how do the PEAC tool answers compare with answers from other models in the public domain. A third question is how does PEAC model algorithms compare with those used in the ALOHA model. The PEAC tool already displays the Initial Isolation and Protective Action Distances as listed in the 2004 (and soon, the 2008) Emergency Response Guidebook, but it also incorporates a calculator for obtaining a more accurate answer. The calculator gives the PEAC tool user more control of what he/she wants in terms of the circumstances of the released chemical, with the PEAC tool displaying the answers using the same format as in the Emergency Response Guidebook. But what algorithms do the PEAC tool use?

In answering these questions some technical concepts are discussed which are difficult to convey in a short summary, and references are made to other documents for details.

A Brief History of PEAC Tool Development

The current owners of AristaTek were employees of the University of Wyoming Research Corporation (a.k.a. Western Research Institute), a not-for-profit research institution that had contracts with the U.S. Department of Energy (DOE) from 1987 through 1999 to do public safety research relating to chemical spills. Another major not-for-profit research organization receiving this funding was the Desert Research Institute in Reno Nevada. A major part of this research was to spill chemicals or release toxic gases at the DOE HazMat Spill Center Test facility near Mercury Nevada in 1993 and 1995. Most of the releases used carbon dioxide as a toxic gas stimulant, but there were some pan evaporation tests for measuring the evaporation rate of chlorine and anhydrous ammonia performed in April 1995 at the DOE site. The summer 1995, gas dispersion release tests called "Kit Fox" simulated releases at a refinery and were funded by a consortium of 10 industrial entities making up the Petroleum Environmental Research Forum [PERF], the EPA, and the DOE. A summary of the "Kit Fox" tests is in a paper S. Bruce King, David Sheesley, Thayne Routh, and John Nordin, "The Kit Fox Field Demonstration Project and Data Set", International Conference and Workshop on Modeling the Consequences of Accidental Releases of Hazardous Materials, 1999; American Institute of Chemical Engineers, New York, N.Y. The tests were significant in that many release tests took place including the near-nighttime, very stable atmospheric stability condition. In addition, comparative tests were made for both flat surface terrain releases and releases where there were structures simulating those at a refinery, both under daytime "neutral" and near nighttime "stable" atmospheric conditions.

The U.S. Department of Energy (DOE) encouraged information transfer to emergency responders and others charged with protecting the public in the event of a toxic chemical release. The University of Wyoming Research Corporation for several years maintained a website where non-proprietary data from tests performed at the DOE HazMat Spill Test facility were freely available. Several papers have been published by different groups on model development as the result of the DOE HazMat Spill Center Tests. The Lawrence

Livermore National Laboratory SLAB Model was largely developed from earlier tests at that site. The same reference citing the "Kit Fox" tests published two other papers by different researchers on testing of the HEGADAS model and DEGADIS model with "Kit Fox" data.

The University of Wyoming Research Corporation employees (S. Bruce King, David Sheesley, Thayne Routh, John Nordin, and Vern Smith) approached the problem of information transfer differently. A 1987 University of Wyoming Research Corporation survey of over 100 industrial chemical spills where people were evacuated showed that when the accident occurred, none of the existing models were used to base evacuation distances. Under the stress of the situation, people were not familiar on how to run the models. Days after the incidents occurred, there were sometimes plenty of modelers out there to piece together what happened. But the modeling was not done under the stress of the moment of the spill. While the "Kit Fox" and other tests at DOE HazMat Spill Center Test facility illustrated some modeling deficiencies, the real problem was rapid communication of information to emergency responders who must make the decisions.

In 1996 we decided that the best way of information transfer to emergency responders would be in the form of a small hand-held computer (PEAC = Palm Emergency Action for Chemicals) which would contain information on chemicals, personnel protective clothing, and modeling information for establishing a protective action distance in case of a spill. The chemical database and personnel protective clothing information was obtained from consulting many different sources. We listened to feedback from emergency responders and other users. We incorporated additional features such as display of the Emergency Response Guidebook and other data sources intact in addition to the data sources we had developed, as often responders said that they should consult three reference sources.

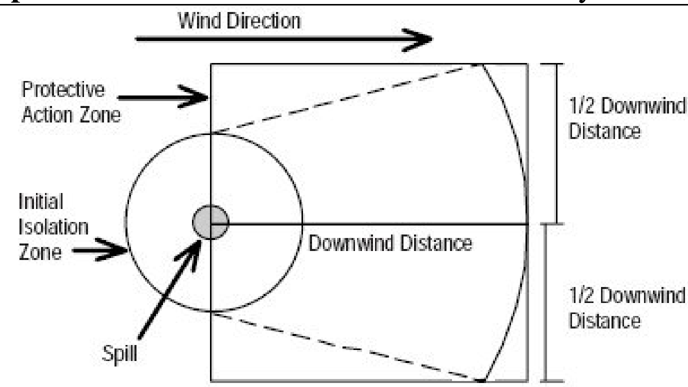
The University of Wyoming Research Corporation made a management decision in the late 1990's not to pursue public safety research contracts and concentrate its resources mostly on energy. In 1999 the employees S. Bruce King, David Sheesley, Thayne Routh, and John Nordin elected to form a for-profit company, called AristaTek, Inc., to develop and market the PEAC software. The patent rights [U.S. Patent 5724255] to the PEAC tool which incorporated gas dispersion modeling were initially licensed to Aristatek and later (December 2000) purchased from the University of Wyoming Research Corporation. [see http://www.patentstorm.us/patents/5724255.html for more details]

Overview of Input/Output in PEAC Tool for Gas Dispersion Modeling

The basic rules used by AristaTek in selecting models are (1) the calculations must be rapid and display the results in a format easily understood, (2) the responder cannot be burdened with a lot of detailed information required to run the model, (3) the responder should be able to model different situations to 'bracket" Protection Action Distances reflecting possible changing conditions, and (4) the modeling should deliver reasonably accurate results. In a real world situation of a chemical release, a first responder does not normally have information concerning meteorology or other critical details and must make rough estimates of the situation at hand. The weather conditions at an airport 15 miles away may be different from what is happening where the chemical release has occurred.

The display for "Initial Isolation Zone" and "Protective Action Distance" in the Emergency Response Guidebook is easily understood and is the basic format chosen for displaying answers in the PEAC tool.

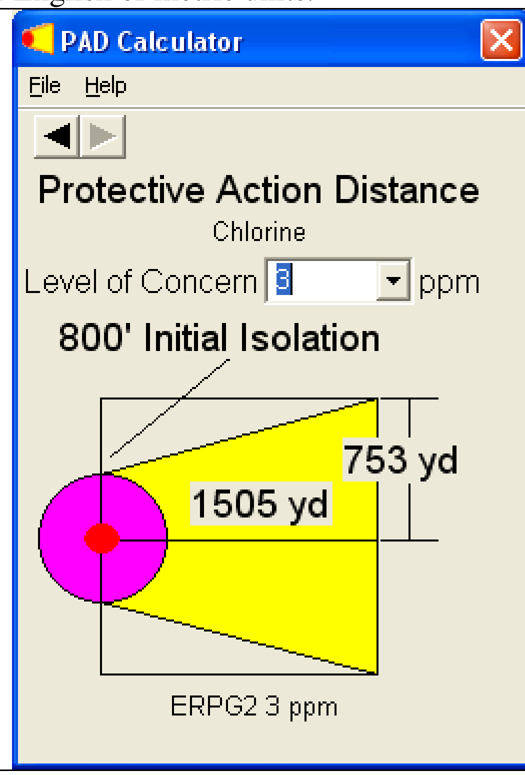
Figure 1: **The Display Chosen for the PEAC Tool is Similar to the Emergency Response Guidebook**. The PEAC tool user may use either English or metric units.



Above: Emergency Response Guidebook display

Right: PEAC tool display of results for an example situation

Notice similarities in format



The Emergency Response Guidebook (ERG) gives the user only four choices, small or large spills, daytime or nighttime releases. For most chemicals, a small spill is defined anything less than 55 or 60 gallons, and a large spill is greater than 55 or 60 gallons. For a few highly toxic chemicals such as chemical warfare agents, a lower quantity is used to distinguish between small and large spills. Daytime releases generally have lower protective action zone distances than nighttime releases because daytime solar heating of the atmosphere creates a more unstable or turbulent mixing of the air which in turn helps disperse the chemicals. There is also provision for chemicals that are water-reactive and release toxic gases. The distances for Initial Isolation and Protective Action are presented in the form of tables. At the request of PEAC tool users, we have also provided the user with the option of displaying the same numbers as the ERG.

The ERG is updated every four years. The numbers for display of the initial isolation and protective action distances also are often different for each update. The two reasons for the changes are (1) the ERG numbers are modeled to different "Levels of Concern" for different editions and (2) there are changes in the ERG modeling methodology. Details of their basis of modeling are available in a developmental document, published by Argonne National Laboratories and are available at http://hazmat.dot.gov/pubs/erg/Argonne_Report08042005.pdf.

When developing a model for the PEAC tool, the user has the option of specifying different situations:

- The total amount of chemical released, either specified as a release rate or the entire contents released in a very short time (e.g. < 15 seconds). If the release rate or total amount released is not known, the PEAC tool contains calculators for common situations.
- Basic meteorological information (wind speed, percent cloud cover, location, date, time of day). From the location, latitude and longitude is calculated. This information is used with the date, time of day, percent cloud cover, and wind speed to calculate the degree to which the chemical cloud will disperse as it travels downwind.
- Choice of three terrains: (1) flat surface, (2) brush and a few buildings here or there, and (3) urban or forests. Buildings and trees act as obstructions to the chemical cloud resulting in a more dispersed cloud, but at the same time also result in a longer time for the cloud to clear out of the area.
- The "Level of Concern" used as the basis for the Protective Action Distance". Usually the "Level 2 Emergency Response Planning Guideline" or sometimes the "Immediately Dangerous to Life and Health" level of concern is selected by the user.

There are several calculators available in the PEAC tool for estimating the mass released or a release rate if this information is not known. If rough dimensions of the container size or if standard transport tanks are used and percent full is known, the total mass can be calculated. If there is a hole in the side of a container or if there is a sheared-off pipe, the PEAC tool can estimate a maximum release rate. If the chemical is a liquid and pools on the ground, the PEAC tool can calculate an evaporation rate.

The ALOHA model used in CAMEO also contains a pool evaporation calculation methodology. The algorithms used by ALOHA for pool evaporation have been published and are in the public domain. During April 1995, the founders of AristaTek did a few pan evaporation tests using spilled liquefied anhydrous ammonia and liquefied chlorine (separate tests) in a wind tunnel at the Nevada HazMat Spill Center Test Facility. As the liquid evaporated in the one-square meter pan, the remaining liquid auto-chilled to about –70°C (lowest temperature achieved was –75.5°C for anhydrous ammonia). As the liquid temperature decreased, the evaporation rate (as measured by sensitive scales under the pan) agreed with what was predicted by the evaporation model for the different temperatures below the normal chemical boiling point. The chlorine test

was complicated by "hydrate" formation over time, which could be viewed by remote video, which tended to decrease the evaporation rate. Nevertheless, we felt that the evaporation model used in ALOHA was sufficiently accurate to be used in the PEAC tool. More details on the tests are at
http://www.aristatek.com/newsletter/0602February/TechSpeak.aspx.
Links to evaporation rate algorithms in the public domain as used in ALOHA are at the website, http://www2.arnes.si/~gljsentvid10/doc_evapo.html. The algorithms were actually not developed by the ALOHA people but are the result of earlier work developed by Kawamura, Peter, and Donald Mackay; 1985. *The Evaporation of Volatile Liquids*. University of Toronto Depts. Of Chem. Eng. and Applied Chemistry: TIPS Report EE-59, Environmental Canada (54 pages); published in: Hazardous Materials, vol. 15 (year 1987), pp. 343-364.
All these evaporation rate calculations are handled internally within the PEAC tool.

PEAC Tool Gas Dispersion Modeling

The PEAC tool follows the same practice of several models in the public domain (such as ALOHA^tm^) of internally selecting an appropriate category based on user input. The categories are:

- Continuous release, Gaussian (Passive) dispersion
- Continuous release, Dense Gas dispersion
- Instantaneous (short duration) release, Gaussian (Passive) dispersion
- Instantaneous (short duration) release, Dense Gas dispersion

Within each category, the PEAC tool assigns an atmospheric stability index (A, B, C, D, E, or F) based on wind speed and solar insolation. The reference citation is Pasquill, F. (1974), Atmospheric Diffusion, 2nd edition, John Wiley & Sons (publisher), N.Y., N.Y. The ALOHA model uses the same methodology. The SLAB model, developed by Lawrence Livermore National Laboratory, also does something similar but uses a sliding scale called a "Monin-Obukhov length" or "Obukhov length" which the user can specify.

Table 1. Pasquill-Gifford Stability Index.

Pasquill Dispersion Class	Atmospheric Stability	Surface wind speed and cloud cover Wind measured at 10 meter height
A	very unstable	daytime; strong insolation and wind < 3 m/s or moderate insolution and wind < 2 m/s
B	unstable	daytime; strong insolation with wind between about 3 and 5 m/s or moderate insolution with wind between 2 and 4 m/s or slight insolution and wind < 2 m/s
C	slightly unstable	daytime; strong insolation and wind > 5 m/s or moderate insolution with wind between 4 and about 5.5 m/s or slight insolution and wind between 2 and 5 m/s
D	neutral	All overcast sky conditions, day or night; daytime and moderate insolation and wind> 5.5 m/s; daytime and

		slight insolation and wind > 5 m/s; nighttime and wind > 5 m/s; nighttime and more than 50% cloud cover or with thin overcast and wind > 3 m/s
E	slightly stable	nighttime; thin overcast or > 50% cloud cover and wind < 3 m/s; < 50% cloud cover and wind between 3 and 5 m/s
F	stable	nighttime; < 50% cloud cover and wind < 3 m/s

Strong solar insolation is defined as a solar elevation angle > 60 degrees.
Moderate solar insolation: solar angle between (and including) 15 and 60 degrees.
Slight solar insolation: solar angle < 15 degrees.

The PEAC tool modeling uses the same methodology as used by ALOHA™ and other popular gas models in internally calculating a solar insolation and assigning a stability class based on user input of time of day, location, date, wind speed, terrain, and cloud cover. The wind speed in the PEAC tool is assumed to be measured at a 2 meter height, which is corrected to a 10 meter height for the purpose of table 1. Earlier versions of ALOHA (version 5.0) did not make this correction for wind speed height to conform with table 1, but later versions of ALOHA (version 5.2.3 and beyond) are reported to make this correction. The calculations are complex, but the methodology for doing this is available in the open literature.

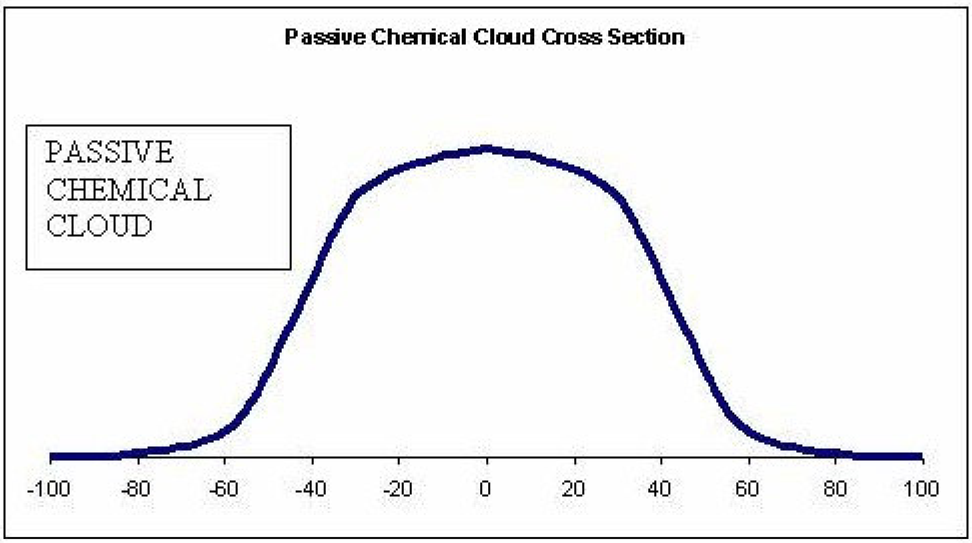
The model used in the PEAC tool makes the following assumptions, to keep things simple:

- Buoyant gases and toxic cloud liftoff are ignored. The greatest concentration is assumed at ground level
- Fires are not considered, which may result in liftoff of toxic gases
- Special terrain situations such as a valley with hills on the side, a street corridor between tall buildings, or a wake behind a large building are not considered
- The protective action distances predicted are for toxic cloud centerline, ground level locations
- The vertical momentum of the source (a jet or smokestack) is not considered.
- The modeling is for gases and vapors; the deposition aerosols and particulates is not considered
- The effect of precipitation is not considered
- Atmospheric inversion layers are not considered
- Reactions of sunlight and moisture with the airborne chemical is not considered [However, for some chemicals, a reaction product with air-water such as hydrochloric acid can be modeled instead of the original chemical]
- Distances very near the source or very far away (> 10 km) from the source must be viewed with caution. For example, ALOHA™ and the 2008 Emergency Response will not even display a Protective Action Distance far from the source. The PEAC® tool will display distances far from the source, but the emergency responder must understand that meteorology and terrain will likely not be the same, and deposition of a toxic chemical might occur. Distances very near the source will depend upon the

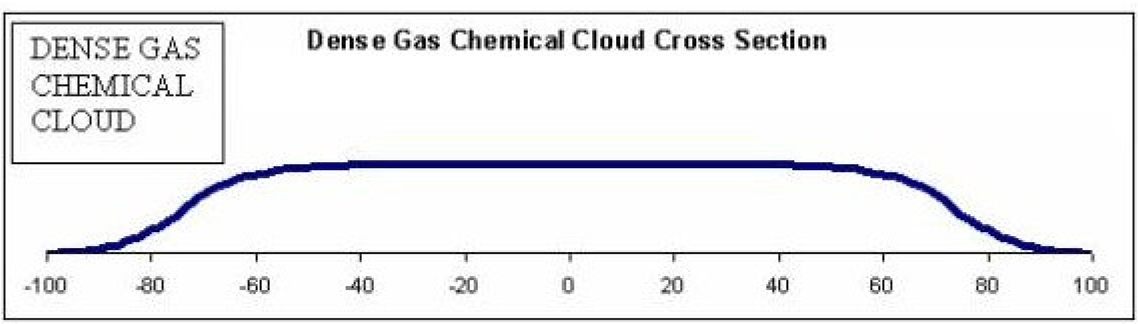
circumstances of the spill, and the PEAC tool assumes a typical release source area for user-specified release rate or quantity to calculate a distance corresponding to a downwind concentration.

Gaussian, or passive dispersion methodology is the most popular model for expressing downwind dispersion of gases. It is used in ALOHA, SLAB, the military D2PC model, and the PEAC tool. It is applicable for dispersion of gases roughly the same molecular weight and temperature of air, or for dilute gases if gas has a higher molecular weight than air. The methodology is not applicable for high concentrations of dense gases. If a cross-section of the toxic gas cloud profiles for passive and dense gases were compared at some distance downwind, it would look like the pictures below.

Figure 2: Difference between Passive and Dense Gas Cloud Profiles



The cross section of the passive gas dispersion profile is bell-shaped. The cross section of the dense gas dispersion profile is flat at the top, and the dense gas hugs the ground.



Analytical expressions for expressing concentrations at any point downwind for the passive (Gaussian-shaped) cloud are available in any textbook on Gas Dispersion modeling. The PEAC tool uses the same analytical expressions as are in the public domain. The dense gas calculations are more complex, and straight-forward analytical expressions have not been published. The simplest dense gas model assumes a boxshaped profile of “constant height” with Gaussian-shaped edges. The criteria of whether a dense gas or passive dispersion model is used is based on something called a Richardson Number. We will not get into the mathematical details of the number calculated, except to say that both the PEAC tool and the ALOHA model use the same Richardson Number concept, and the details of how the Richardson Number is calculated are available in the open literature.

As the dense gas travels downwind, it mixes in with the surrounding air. The relative density between the chemical cloud and surrounding air becomes similar, and the dense chemical cloud behaves like a passive “Gaussian” cloud as it travels further downwind.

So much for similarities. Why do models differ? The answer is that different data sets are used to calibrate the models. Also, comparisons may not be made at the same concentration averaging times for different data sets. The data sets may be outdoor releases or releases in a wind tunnel using a scale model for the terrain. Model developers also draw heavily on mixing theory to extend their projections to other circumstances because time and monetary constrains limit testing to only a few conditions. From these tests, analytical expressions called “sigma expressions” might be developed to express the degree of spreading of the chemical cloud as it travels downwind. The spreading results from atmospheric turbulence due to the wind and solar heating. During the day, the sun heats up the ground resulting in the air near the ground becoming less dense. The warm air rises resulting in mixing and dispersion of the chemical cloud. During a clear night, with little wind, the ground radiates its heat to space, and the air becomes stable, and there is little mixing of the chemical cloud with the surrounding air.

Let’s look at an example of a set of analytical expressions for “sigma expressions” developed from a data set, and see their use in calculating a downwind concentration.

The simplified equation for a ground level (continuous) release, Gaussian (passive) distribution is

$$C/q = (\pi\, U\, \sigma_y\, \sigma_z)^{-1}$$

where C = ground level concentration at the cloud centerline
q = release rate (continuous release, no dense gas effects)
U = wind speed
σ_y = standard deviation of the plume/cloud concentration in the cross-wind direction [“sigma expression”]
σ_z = standard deviation of the plume/cloud concentration in the vertical direction [“sigma expression”]
x = downwind direction, y = crosswind direction, z = height above ground; Release point at x = y = z = 0.

In formulating this equation, it is assumed that the plume cloud is free to expand in all directions constrained only by the ground. Therefore there are no atmospheric mixing heights, valleys, or corridors to put a cap on the expansion.

One of the most commonly used and well known expressions for "sigma expressions" are those published by Gary Briggs in 1973, using a data set for low-level sulfur dioxide releases in a southwestern Kansas field. The paper citation is Briggs, G.A., 1973, "Diffusion Estimation for Small Emissions, ATDL Contribution File No. 79, Atmospheric Turbulence and Diffusion Laboratory. The ALOHA model and the PEAC tool uses these expressions for continuous releases:

Table 2. Analytical Briggs Sigma Expressions for Passive Dispersion (x in meters)

Stability Class	σ_y meters	σ_z meters
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	$0.04x(1 + 0.0001x)^{-1/2}$	$0.016x(1 + 0.0003x)^{-1}$

These sigma expressions are valid for a concentration averaging time of 3 minutes and for a surface roughness $z_0 = 0.1$ meters. However, the same expressions have been used in models with a surface roughness of 0.3 meters and a 10 minute concentration averaging time. There are also some minor differences in how the PEAC tool handles the expressions for urban situation, which result in a slightly more conservative prediction of protective action distance for a given downwind concentration.

For the instantaneous (short duration) release, Gaussian (passive) dispersion mode, the PEAC tool and ALOHA use different sigma expressions, but both methodologies are published in the open literature. The expressions for the PEAC tool "sigma expressions" (passive dispersion mode, instantaneous release) came from the DEGADIS manual, cited below:

Spicer, T.O., and J.A. Havens, (1989). "Users Guide for the DEGADIS 2.1 Dense Gas Dispersion Model", Environmental Protection Agency, Report EPA-450/4-89-019. [comment: the manual also includes passive (Gaussian) dispersion algorithms].

The PEAC tool uses the same concentration averaging times [t_{ave}] as used in the DEGADIS manual, as follows:

Atmospheric Stability A, B, C: $t_{ave} = 18.4$ seconds
Atmospheric Stability D. $t_{ave} = 18.3$ seconds
Atmospheric Stability E. $t_{ave} = 11.4$ seconds
Atmospheric Stability F. $t_{ave} = 4.6$ seconds

The DEGADIS manual did not originally develop this work but compiled it from earlier publications, with modifications.

For the dense gas mode, the PEAC tool did not follow the DEGADIS manual. However, the ALOHA model did incorporate the DEGADIS methodology for their dense gas mode. The PEAC tool more closely mimics the SLAB Model developed by Lawrence

Livermore National Laboratory, but is not SLAB. The reference citation for SLAB model development is

Ermak, D.L. 1990. User's Manual for SLAB: An Atmospheric Dispersion Model for Denser-Than-Air Releases UCRL-MA-105607. Lawrence Livermore National Laboratory, Livermore CA.

The PEAC tool dense gas modeling uses a one-minute concentration averaging time for continuous releases, and 10 seconds averaging time for instantaneous (short duration) releases.

The developers of the DEGADIS model (Tom Spicer and Jerry Havens) examined the results of 1995 Kit Fox Dispersion tests performed at the Nevada DOE HazMat Spill Center. They concluded that the DEGADIS predictions were consistent with what was observed from the Kit Fox dispersion tests. The reference citation is Spicer, T.O., and J.A. Havens, "Description and Analysis of Atmospheric Dispersion Tests Conducted by EPA at the DOE HazMat Spill Center", International Conference and Workshop on Modeling the Consequences of Accidental Releases of Hazardous Materials; 1999. American Institute of Chemical Engineers, New York, N.Y. [comment: EPA was only one of several participants providing funding for the tests or providing direction for the tests].

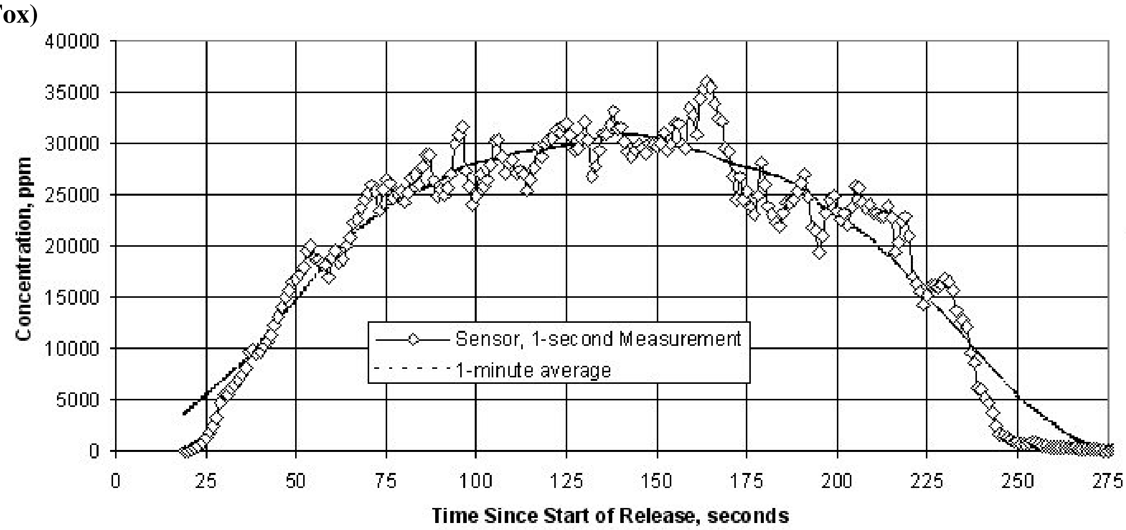
Under the "D" atmospheric stability condition, the DEGADIS model, SLAB, and model used in the PEAC tool, as well as the Kit Fox data generally gave similar results, at least within a factor of two. There were greater differences for the E stability condition and even more for the F stability condition.

Concentration Averaging Times and Toxic Cloud Duration

Some important concepts are (1) how long will the toxic cloud last and (2) what is the concentration averaging time. This might be best illustrated by looking at data obtained from the tests at the DOE HazMat Spill Center in Nevada. In these tests, various chemicals were released and resulting toxic cloud characteristics measured. During August-September 1995, for example, the series of over 70 tests identified as "Kit Fox" used carbon dioxide as a surrogate for more toxic chemicals. The carbon dioxide releases were done at ground level with carbon dioxide released at a specific rated for finite periods of time ranging from 15 seconds to 6 minutes. Chemical sensors were placed at approximately 90 different locations downwind in order to estimate the cloud centerline locations, cloud width and height, and concentrations as a function of distance downwind. The sensors recorded carbon dioxide concentrations every second. For the example illustrated below (figure 3), the carbon dioxide release rate was 1.722 kg/s for exactly 180 seconds and the sensor was located at the centerline just above ground level, 25 meters downwind. The surface roughness was 0.02 meters, the wind speed at the 2 meter height was 2.1 m/s, and the calculated Monin-Obukhov length was 5.6 meters (indicative of a F atmospheric stability). The release was done after sunset under cloudless skies. The sensor in figure 1 measured carbon dioxide concentrations as a function of time at one-second intervals. A one-minute running average concentration was calculated from the sensor measurements and also graphed on figure 3. Some general observations from the tests were

- In figure 3, based on a 2.1 m/s wind speed and sensor placed 25 m downwind, the carbon dioxide cloud should have arrived at the sensor 12 seconds after the start of the release but it actually arrived at the sensor 24 seconds after the start of the release. Even though the release was 180 seconds, the cloud lingered for almost 220 seconds before it completely passed over the sensor.
- All data taken regardless of the test or sensor showed peak one-second concentrations higher than the peak one-minute average. Obviously the peak 10-minute average would be even less. For the example in figure 3, the peak one-second sensor reading was 37,000 ppm but the peak one-minute average was 30,000 ppm.
- Even though the release start and finish had a sharp cutoff, the concentrations as seen by the sensor increased with time, leveled off, and then decreased. The parameter σ_x ["sigma x"] is used in models to measure the cloud spread in the downwind direction.

Figure 3: Example Ground-level Carbon Dioxide Sensor Measurement for a 3-Minute Release (Kit Fox)



The point to be made that a chemical release even under controlled conditions produce complex downwind behavior that is usually not accounted for with gas dispersion models in the public domain, and the emergency responder should keep this in mind when using a gas dispersion model to predict a public evacuation distance. If the release rate is small under conditions of a "D" atmospheric stability, the wind speed at the cloud level should fairly accurately predict the time that the cloud will arrive at some downwind receptor. The cloud will still spread out in the downwind and crosswind directions and increase with height. However, if the release is large such that dense gas effects occur, the cloud will tend to slow down. Also, under more stable atmospheric conditions the cloud will linger longer and take more time to clear out. One of the tests under the Kit Fox series involved a six-minute release of carbon dioxide under a far F nighttime atmospheric stability, wind speeds on order of 1 m/s; it took the cloud over 45 minutes to clear out from many downwind sensor locations. If the spill occurs in an urban setting, the downwind wake behind buildings may contain higher concentrations and take longer for the toxic cloud to clear out.

Gas dispersion models are derived from experimental data where chemicals are released under field or wind tunnel conditions. The cloud shape and spread are measured as a function of distance downwind for different meteorological conditions. The raw data for the various tests have different concentration averaging times. Most data has been taken under a "D" atmospheric stability condition, and very little (until "kit Fox") has been taken under the stable, nighttime ("F" stability) condition. Some models in the public domain allow the user to specify a concentration averaging time, and then correct σ_y by

$$\sigma_y = \sigma_{y,ref} \, (t / t_{ref})^{0.2}$$

where σ_y = lateral dispersion in the crosswind direction using the user-specified averaging time t and $\sigma_{y,ref}$ = lateral dispersion in the crosswind direction based on a reference time under which the model was originally formulated. The SLAB model contains a slightly modified expression that avoids the anomaly of σ_y approaching zero as t approaches zero.

The problem is that gas dispersion models in the public domain especially under the "F" stability condition do not agree with each other because they are formulated differently. Another issue is that minor changes in wind speed and degree of atmospheric stability in the "F" stability condition can greatly affect the behavior and dispersal of the toxic cloud. The PEAC^{tm} tool uses the models as discussed earlier but it should not be surprising that models in the public domain predict differently, especially under the "F" stability condition. While some models predict cloud arrival time and duration, data such as taken at Kit Fox can show serious disagreement under certain conditions. For this reason, the PEAC tool does not predict the cloud arrival time and duration.

More information on this subject is presented in an earlier AristaTek newsletter article, which is available at
http://www.aristatek.com/Newsletter/03%2011%20November/Technical%20Dialogue.htm.

Atmospheric Stability Index vs Monin-Obukhov Length

Both the PEAC tool and ALOHA assign stability classes A, B, C, D, E, and F based on solar insolation and wind speed. But some models such as SLAB allow the user to specify stability on a sliding scale called "Monin-Obukhov Length" (sometimes called "Obukhov length", which is an indicator of the degree of mixing of the air due to solar heating or nighttime cooling and the wind. The Monin-Obukhov length can be obtained from sonic anemometer measurements through a complex process, or approximated if accurate measurements of wind speed and temperature are available at least two different heights above the ground. A basic observation made during the "Kit Fox" tests was that meteorology did not fit exactly into C, D, or F conditions but instead there was "D borderline C", "D near E", "E changing into F", "far F", and if the winds died down at night and the air became very stable, sometimes "undefined" terms such as "G" stability or "H" stability were invented for the purpose of conversation. Gary Briggs, representing the EPA and author of the some of the "sigma formations" cited earlier, was present during the Kit Fox tests. He used these terms when the winds died down and the carbon dioxide cloud remained stationary during the night.

The SLAB model allows the user to input different Monin-Obukhov conditions. A hypothetical chlorine continuous release was modeled for several Monin-Obukhov lengths representing stable atmospheric conditions. All computer runs were done at a surface roughness = 0.1 meters and the wind speed of 1 m/s measured at the 2 meter height. The chlorine release rate was 0.126 kg/s (continuous) at 0.1 meter height.

Table 3. Calculated Downwind Distance (meters) for a Chlorine Level of Concern = 3 ppm, calculated using the SLAB Model

Obukhov length, meters	Calculated Distance, meters
28 (F near E stability)	2600
17.5 (F stability)	3200
10 (somewhat far F stability)	4865
5 (far F or "G" stability)	10200

A Monin-Obukhov length of 5 meters represents a far-F stability condition or maybe what some might call a "G" condition.

When comparing models in the public domain, the comparison for say an F stability may not be at the same Monin-Obukhov length, or the data set used for calibration of "sigma expressions may not be at the same Monin-Obukhov length, or be based on data sets taken under a different stability condition and extrapolated to a F stability condition.

For dense gas modeling, the corresponding Monin-Obukhov lengths as used in the PEAC tool are listed in table 4

Table 4. PEAC Tool Monin-Obukhov Lengths (L) for Atmospheric Stability (units: meters).

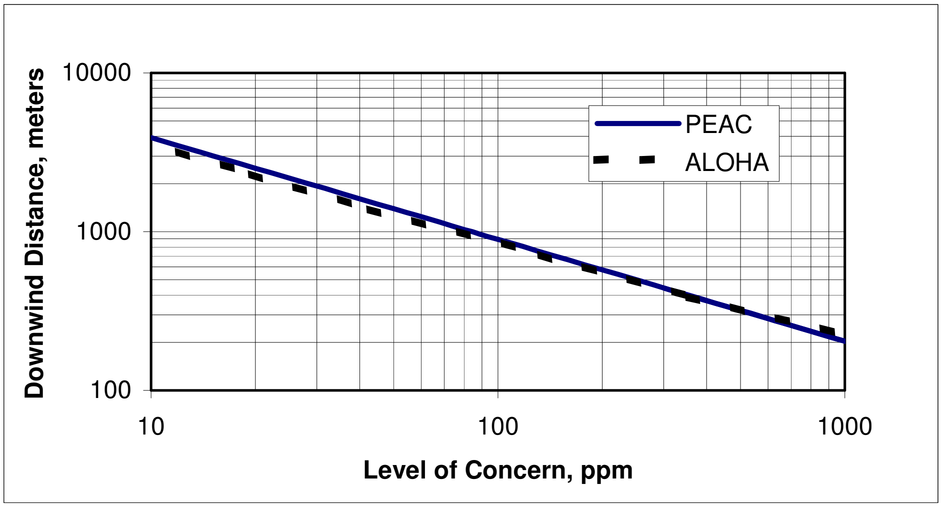
Stability	Flat Terrain	Cropland/brush	Urban/forest
A	-5.3	-9	-11
B	-7.5	-17.5	-26
C	-15.1	-61	-123
D	(1/L = 0)	(1/L = 0)	(1/L = 0)
E	15.1	61	123
F	7.5	17.5	26

<u>Example Comparisons of PEAC Tool Modeling Results With Other Models</u>

The PEAC tool model and several other models were run for several hypothetical situations. Lists of protection action distances were tabulated and then graphed for different concentrations representing Levels of Concern.

<u>**Example 1**</u>**. Anhydrous Ammonia Spill, mid afternoon, wind 5 m/s at 2 meter height**, Denver Colorado, outdoor temperature 70^{o}F. The pooled liquid evaporates from a pool at 2.5 kg/s. (we will not do the evaporation rate calculator here but simply enter a release rate for ammonia).

Figure 4: Ammonia Release at 2.5 kg/sec, wind 5 m/s at 2 meter height

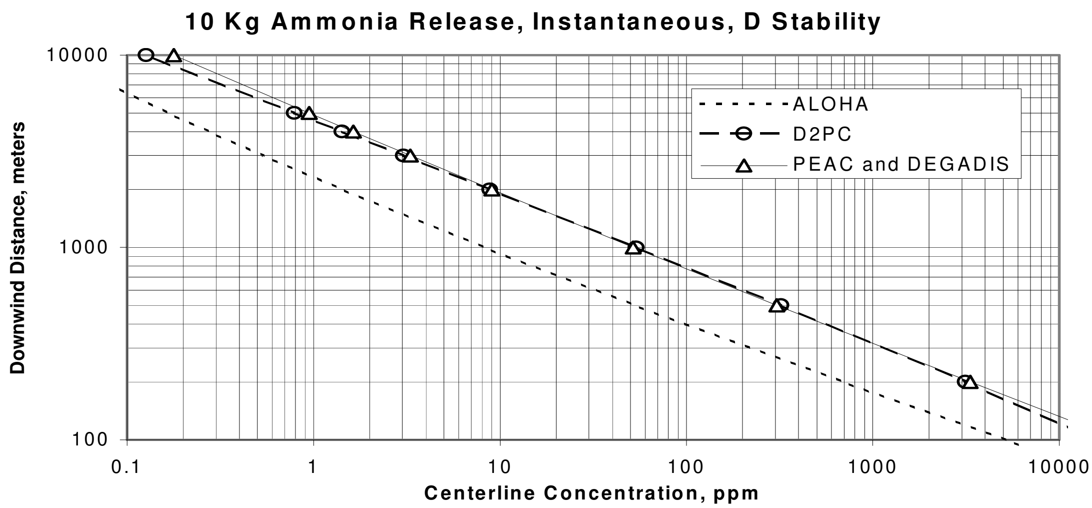


In this example, a "D" stability is computed internally by the PEAC tool and by ALOHA. At distances greater than 200 meters, the cloud behaves passively, ALOHA and PEAC use the same algorithms, and essentially the same answers are obtained.

Example 2: 10 kg Instantaneous (short duration) Ammonia Release, D Stability

In this example, 10 kilograms of anhydrous ammonia is released instantaneously (10 seconds). The meteorology is deliberately chosen to get a "D stability". The PEAC tool is set to "cropland", and the other models were set to 0.1 m surface roughness.

Figure 5: Instantaneous release of 10 kilograms of Anhydrous Ammonia, "D" stability



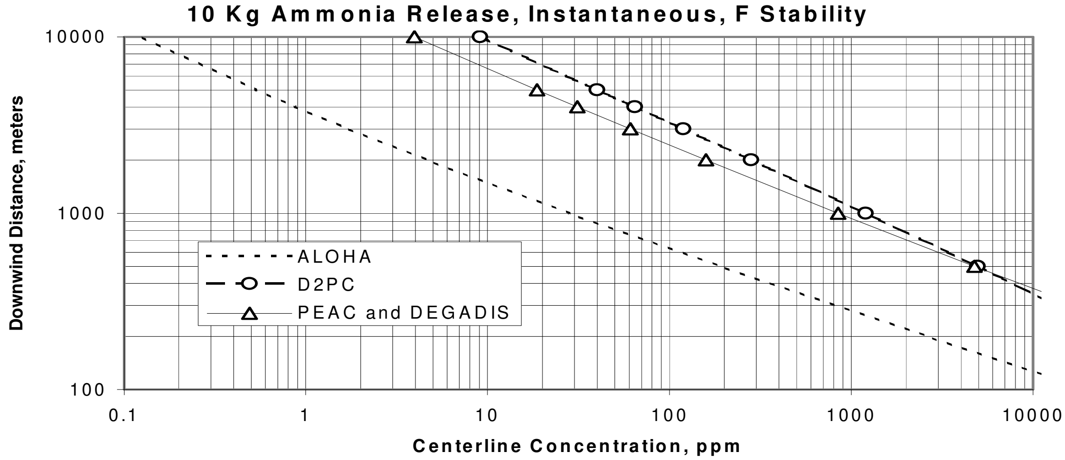
In this mode, both DEGADIS and the PEAC tool give the same answers because the same algorithms were used. The answers were also similar to those predicted by the military D2PC model, which is a Gaussian (passive) model but uses different sigma expressions. The ALOHA model sigma expressions result in a different answer.

Information including algorithms on the military D2PC model is in the following document:
Whitacre, C.G., J. H. Griner III, M.M. Myirski, and D.W. Sloop. 1987. Personal Computer Program for Chemical Hazard Prediction (D2PC) CRDEC-TR-87021. Chemical Research Development & Engineering Center, U.S. Armaments Munitions Chemical Command, Aberdeen Proving Ground, MD.

Example 3: 10 kg Instantaneous (short duration) Ammonia Release, F Stability

In this example, 10 kilograms of anhydrous ammonia is released instantaneously (10 seconds). The meteorology is deliberately chosen to get a "F stability". The PEAC tool is set to "cropland", and the other models were set to 0.1 m surface roughness.

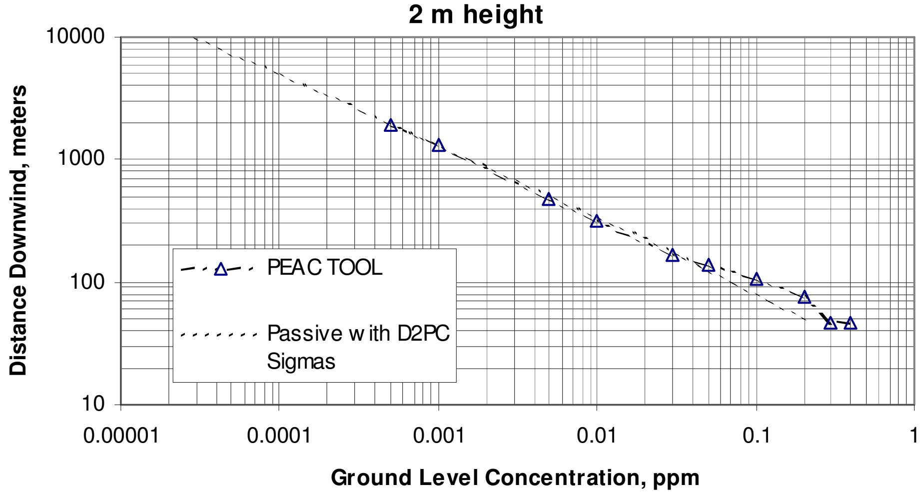
Figure 6: Instantaneous release of 10 kilograms of Anhydrous Ammonia, "F" stability



In this mode, both DEGADIS and the PEAC tool give the same answers because the same algorithms were used. Both answers were a little less conservative than those predicted by the military D2PC model, which is a Gaussian model but uses different sigma expressions. The ALOHA model sigma expressions result in less conservative answer.

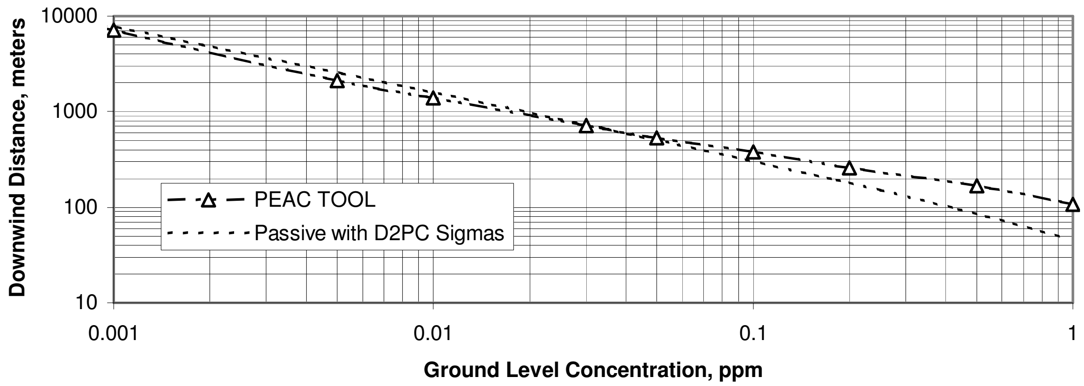
Example 4: Sarin Release. In this example we will compare the PEAC tool results with the military D2PC model. This is a passive (Gaussian) model designed for modeling chemical warfare agent releases. For the PEAC tool, we will deliberately choose parameters to get a D Stability condition, and model for a 0.0003 kg/sec release of Sarin as from an evaporating pool. We do not have the D2PC model itself to run, but we do have the algorithms for this model, which were programmed in an Excel spreadsheet. The comparison is in Figure 7.

Figure 7. 0.0003 kg/s SARIN release, D Stability, Wind 5 m/s at 2 m height



The comparisons were repeated for conditions deliberately chosen to get an F stability condition (figure 8, note change in release rate and wind speed):

Figure 8. 0.0001 kg/s SARIN release, F Stability, Wind 1 m/s at 2 m height



In this example, the D2PC model and the PEAC model give similar answers.

Example 5: 2 kg/sec Chlorine Release at Ground Level. In this example, chlorine is released at ground level at continuous release rate of 2 kg/sec. At this release rate, the chlorine cloud is a dense gas, at least near the source. The passive model D2PC does not apply. In figure 9, meteorological conditions were deliberately chosen to get a D stability (overcast, wind 5 m/s at 2 meter height). In figure 10, meteorological conditions were deliberately chosen to get a F stability (clear nighttime, wind 1 m/s at 2 meter height). For the SLAB modeling comparisons, we set the SLAB Monin-Obukov length to the same value as used in the PEAC tool.

Figure 9. 2 kg/s Chlorine Release, D Stability, Wind 5 m/s at 2 m height

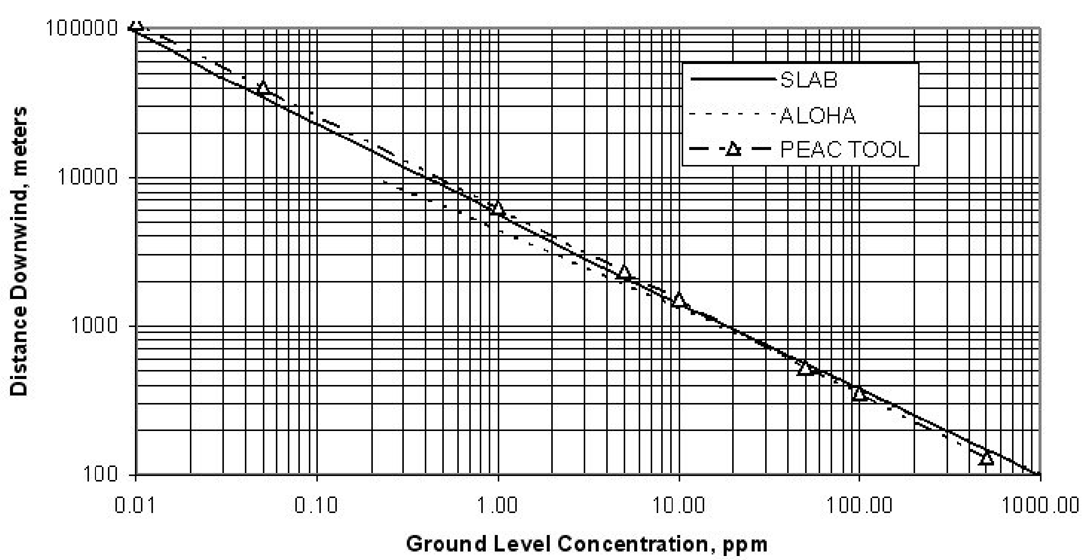
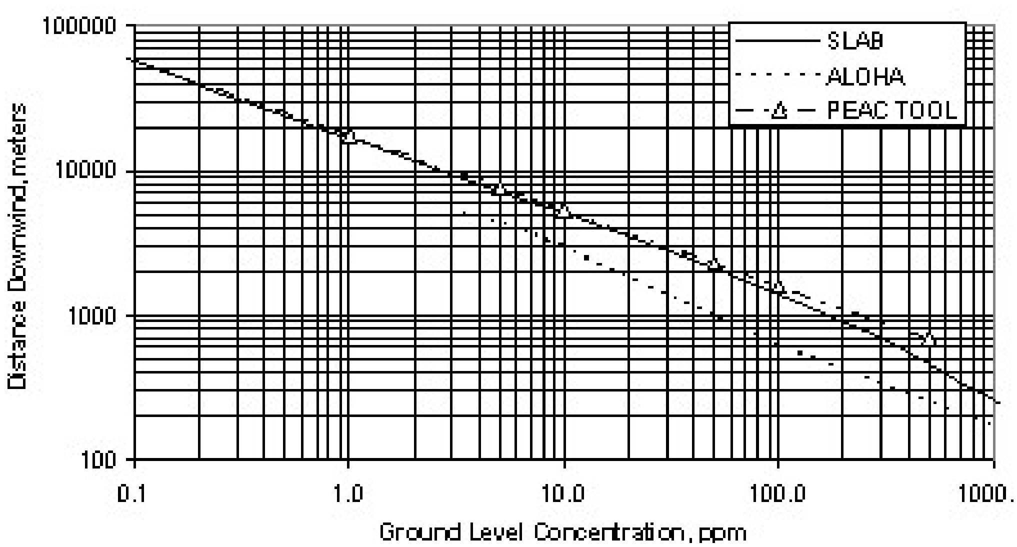


Figure 10. 2 kg/s Chlorine Release, F Stability, Wind 1 m/s at 2 meter height



Example 6: A Terrorist blows up a 90-ton Rail Car Containing Chlorine, and all of the Chlorine is Released to the Atmosphere at Once.

For this situation, the models were set to a D stability condition using a wind speed of 5 m/s at a 2 meter height, urban setting for the PEAC tool (or 1 meter surface roughness for SLAB), and 50^{o}F ambient temperature (Figure 11). For the F Stability, a clear nighttime sky was specified using a 1.5 m/s wind speed at a 2 meter height.

Figure 11: 90-Ton Chlorine Instantaneous Release, Daytime D Stability

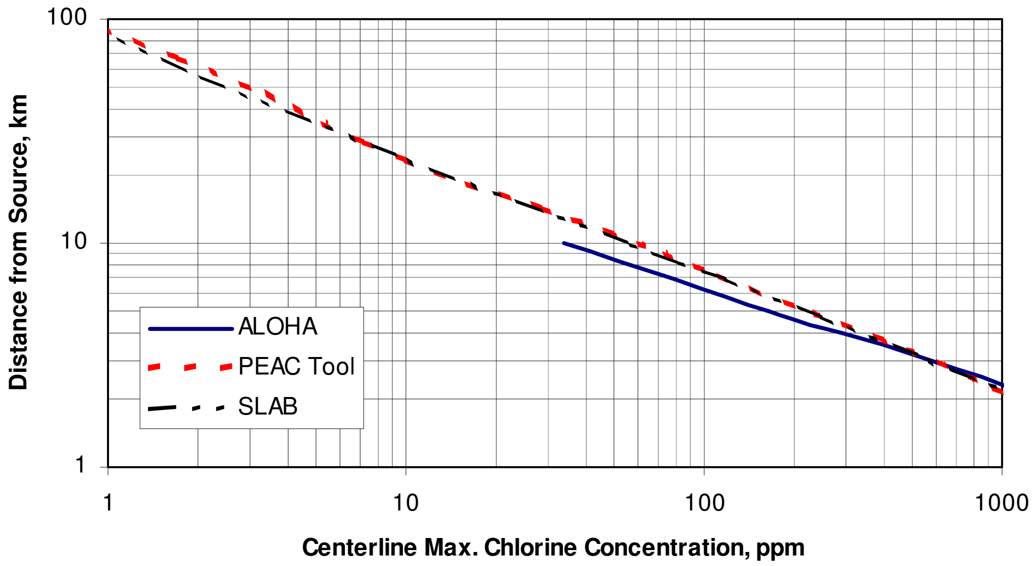
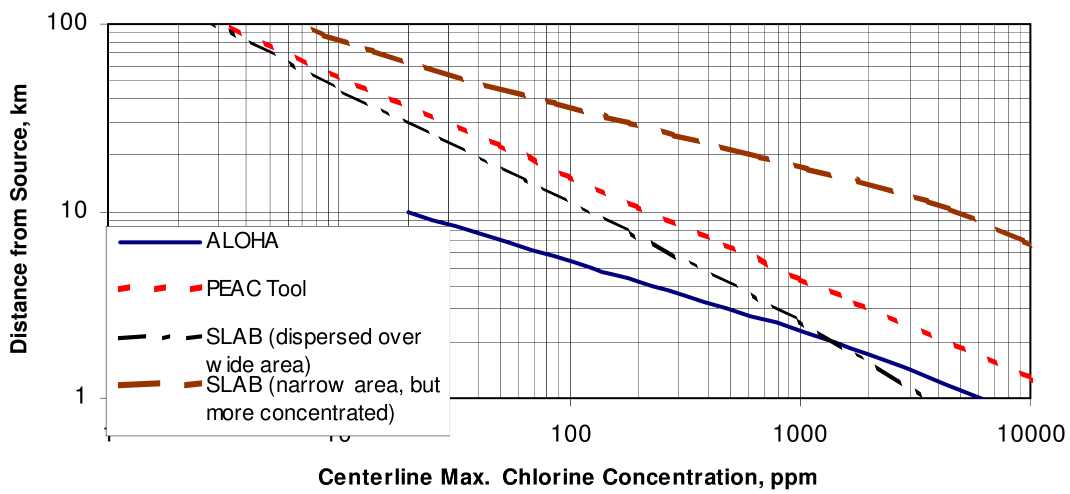


Figure 12: 90-Ton Chlorine Instantaneous Release, Clear Nighttime Conditions, "F Stability"



For the SLAB model, the user must specify an effective cross sectional area after the explosion. No guidelines are provided with the SLAB model on how to do this, so two extreme situations were modeled (dispersed over a wide area or a more narrow area). The maximum cloud centerline concentrations are plotted near ground level.

Conclusions

The PEAC model methodology compares favorably with established models in the public domain. Generally, the available models give similar result for the “D” stability condition, but have some differences when the F stability is modeled. The PEAC modeling methodology uses fairly short concentration averaging times and therefore presents a more conservative distance corresponding to a given Level of Concern than if a longer averaging time were used. The “Kit Fox” tests showed a wide variance in results for the “F stability” depending upon the degree of air stability, and this is a major reason why models can differ considerably when a F stability is specified.