Technically Speaking

Are Gas Dispersion Models Too Conservative?

by Dr, John Nordin

ARE GAS DISPERSION MODELS TOO CONSERVATIVE?

Aristatek was approached by an individual who suggested that the gas dispersion model in the PEAC tool as well as the ALOHA model in CAMEO over predict the concentrations experienced downwind from a chemical spill, and that the “actual” concentrations are much less. He cited the chlorine rail car collision in Graniteville Georgia on January 6, 2005 as an example in which 9 people were killed from chlorine gas exposure, but modeling predicted that many more people should have been killed.

An AristaTek newsletter article written in January 2005 [see “The First Responder” Jan. 2005] reviewed the nighttime Graniteville spill incident. We did not attempt to model the incident because we were uncertain of exactly how the chlorine was released and we did not know the weather conditions at the time of the release. If a modeler assumed that 60 or 90 tons of chlorine were released at once under a nighttime, low wind condition, the resulting chlorine concentrations would predict many deaths but that is not what happened. While there were initially deadly chlorine concentrations near the train wreck sufficient to kill people, the very high concentrations did not continue.

Comparison of Model Predictions With Test Spills of Chemicals

The best way of answering the question of whether gas dispersion models are too conservative is to actually release chemicals and then measure the air concentrations downwind using arrays of many sensors. Meteorology and terrain also affect how the chemical gas cloud is dispersed, so there must also be many sensors measuring wind speed, wind direction, and temperature at various locations and altitudes. These kinds of experiments are expensive to set up and carry out, but fortunately there are some useful tests performed in the United States and England. Spill tests are performed not just to develop and test models but also test mitigation procedures, do hazmat training, and test personal protective equipment under field conditions.

Many of the gas dispersion models were actually developed from field test data. The question remains, how well do the models predict other test results that were not used in the calibration of the model? The best way of answering the question is to run the model and compare with chemical concentrations as measured by downwind sensors.

Dr. Steve Hanna at Sigma Research Corporation in Concord MA is a specialist in evaluating model performance. He has published comparisons of fifteen hazardous gas dispersion models using data from eight field experiments. The results are published in

S.R. Hanna, J.C. Chang and. D.G. Strimaitis. “Hazardous Gas Model Evaluation with Field Observations” Atmospheric Environment volume 27A No 15, pages 2265-2285, 1993.

The 15 models evaluated were AFTOX, DEGADIS, HEGADAS, HGSYSTEM, INPUFF, OB/DG (a 1963 U.S. Air Force model), SLAB, AIRTOX, CHARM, FOCUS, GASTAR, PHAST, TRACE, Gaussian Plume Model, and the Bitter and McQuaid (1988) model. The eight test data sets evaluated were (1) Burro tests releasing liquefied natural gas, (2) Coyote tests releasing liquefied natural gas, (3) Desert Tortoise releasing ammonia, (4) Goldfish tests releasing hydrogen fluoride, (5) Handford tests releasing Krypton 85, (6) Maplin Sands tests releasing liquefied natural gas and liquefied propane gas, (7) Prairie Grass tests releasing sulfur dioxide, and (8) Thorny Island tests releasing freon and nitrogen dense gas. The

DEGADIS model, developed by Jerry Havens and T.O. Spicer, forms the basis of the dense gas part of the ALOHA model widely used by governmental agencies. The Gaussian Plume Model using Gary Briggs' sigmas developed from the Prairie Grass tests releasing sulfur dioxide are widely used by the U.S. Environmental Protection Agency and is also used in the ALOHA model when operated in the continuous, passive mode. Sigmas are mathematical expressions that describe the spreading and dispersal of the chemical cloud as it travels downwind and are usually developed from field test data.

The model used in the PEAC tool incorporates dense gas features which give results similar to SLAB and employs the classical Gaussian plume model equations for the passive (dilute) gas release. The military D2PC model uses Gaussian plume model equations but uses sigmas developed from different data sets than the ones developed by Gary Briggs. The details of how these models are formulated require a very lengthy dissertation.

Dr. Steve Hanna's paper concluded that the models generally predicted plume centerline concentrations within a factor of two when compared with actual tests. The models Bitter and McQuaid, CHARM, GASTAR, SLAB, HEGADAS, HYSYSTEM, PHAST, and TRACE most consistently gave good performance. The better models for dense gas release were AIRTOX, HGSYSTEM, PHAST, and SLAB. The models somewhat under-predicted the hydrogen fluoride concentrations in the Goldfish series of tests. But none of the models accurately predicted the observed variation in concentrations with averaging time [real world concentration fluctuations as measured by the tests were greater than what would be predicted]. Also there were some discrepancies in the chemical cloud width and height when modeling was compared with actual tests. Models that might under-predict plume cloud centerline concentrations for one set of tests might over-predict concentrations in another lest.

AristaTek has also done model comparisons independent of Steve Hanna's paper. We have posted a summary of the results in an earlier Newsletter article [see "The First Responder", June 2002]. The conclusion was that models generally agreed with each other under "neutral" atmospheric conditions (little temperature difference with height from ground) but there can be major differences, sometimes as much as an order of magnitude under nighttime clear sky conditions ("the "F" stability"). The reason is that most calibration tests were done under "neutral" atmospheric conditions, sometimes called the "D" stability, but there was essentially nothing under the stable nighttime, low wind conditions where cold air settles near the ground ("F" stability). The models extrapolate what might occur under "F" stability conditions without verifying tests.

In 1995, funded in part by the U.S. Department of Energy, the EPA, and 10 petroleum and industrial companies completed a series of tests at the Nevada Test Site near Mercury Nevada identified as the Kit Fox series of tests. The personnel who now are owners of AristaTek set up and ran the tests. The tests used carbon dioxide as a dense gas simulate. Over 90 releases were done under a variety of conditions ranging from daytime neutral "D" stability conditions to nighttime "far F" stabilities. Approximately 100 real-time carbon dioxide sensors were placed in arrays at various locations and heights downwind from the releases. Comparisons were done with and without structures in place to break up the air flow, simulating structures at a refinery. Independent air flow tests were also done using small scale models of a refinery in a wind tunnel (by EPA and by a private contractor). Both Drs. Steve Hanna and Gary Briggs witnessed the tests and had access to the test results. Steve Hanna used the test results to calibrate/adjust the HEGADAS model [see S.R. Hanna and J.C. Chang, "Testing of the HEGADAS Model Using the Kit Fox Field Data", International Conference and Workshop on Modeling the Consequences of Accidental Releases of Hazardous Materials, 1999, ISBN 0-8169-0781-1, AIChE, N.Y., N.Y.] . The HEGADAS model agreed with test data, but minor adjustments were made (HEGADAS version 3+). Gary Briggs commented, if the models agree by a factor of two with test data there is good agreement.

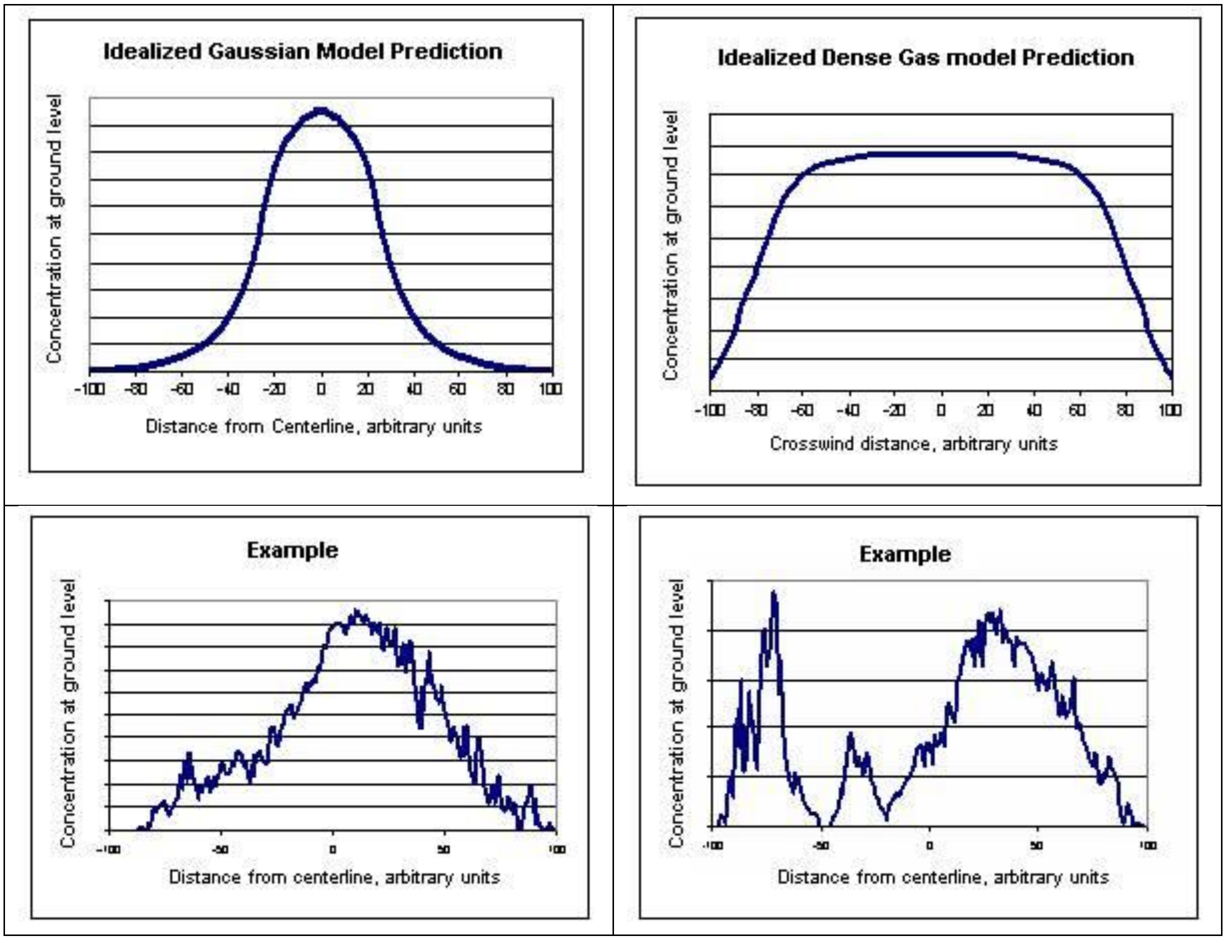
The Kit Fox series of tests has not been fully analyzed because of lack of government funding. AristaTek personnel completed comparisons with the SLAB model on their own and concluded that the SLAB model generally predicted chemical cloud centerline concentrations within a factor of two, but there was a lot of natural or stochastic variability in the tests. There was also a big difference in "near F" and "far F" stability conditions at sunset and night depending upon the wind speed and the temperatures measured as a function of height. Many modelers prefer to use a sliding scale called "Obukhov Length" or Monin-

Obukhov length to measure atmospheric stability rather than letter designations ranging from A to F. When structures were put in place (simulating a refinery), the chemical cloud height was considerably greater than predicted by the SLAB model. Dr. Steve Hanna concluded the same thing.

Both AristaTek and Dr. Steve Hanna were frustrated by the variability of the data which made analysis difficult. Models are based on averages and are formulated to smooth out the variability. But the real world is not that way. AristaTek personnel have examined real world chemical spills resulting in a toxic chemical cloud and have noted, especially under low wind conditions, the cloud can sometimes move in unpredictable ways. Based on witness accounts of odor and sometimes visual observations, some areas may get the blunt of the chemical cloud and other areas may escape. This was also noted in many of the Kit Fox test results. Some cross sectional snapshots of the chemical cloud width at a particular time are illustrated below. Sometimes the chemical cloud wandered off outside the range covered by the sensor array previously set up.

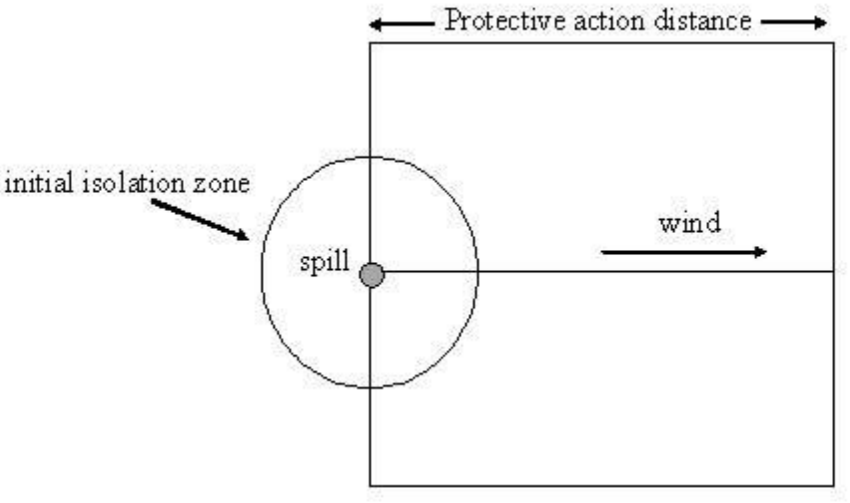
Figure 1 presents theoretical ground level concentrations as a function of distance from an arbitrary centerline compared with what might be measured by sensors at a point in time. The numbers plotted are not important. Sometimes the chemical cloud will split up as shown in the lower right because of micrometeorology and interaction with structures or objects in the cloud path. A time plot of any sensor at a particular location will also display considerable scatter even if the chemical is released at a constant rate because of micrometeorology.

Figure 1. Comparison with Model Predictions with Field Test Data



What can we conclude from this discussion? The models that are available depict actual concentrations in the air within the limits of data and field tests used to calibrate the models, in other words, there are no deliberate attempts to incorporate safety factors to make them more conservative. But there is a lot that is unknown and there are too few good field tests available to calibrate and develop models. Because of unknown real-world situations, there is a tendency to think "worst case" when ordering public evacuations or shelter in place. It is better to order more people to evacuate to be on the safe side rather than have people die or suffer permanent disabilities because the situation turned out worse.

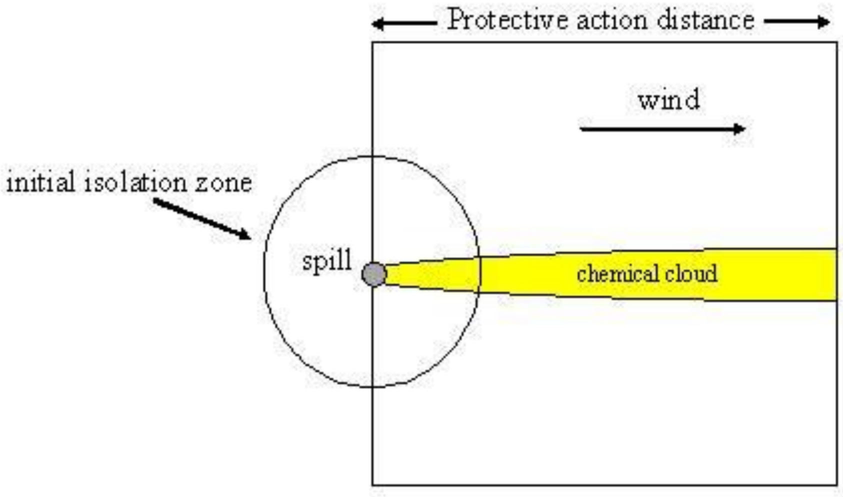
Protective Action Distances for Public Evacuation



The 2004 Emergency Response Guidebook (as well as earlier editions) displays a diagram called a protection action zone for public evacuation like the one shown above. The width of the protection action zone is the same as the length. The length is based on gas dispersion modeling using a level of concern either equal to the ERPG-2 level for the chemical or 1/100 of the 1-hr LC50 value for rats. [ERPG-2: Emergency Response Planning Guideline level 2 concentration]. The PEAC tool display also has adopted the Emergency Response Guidebook format for display of the Protective Action Distance [PAD]. A person might think that all space within the Protection Action Zone might see concentrations representing the level of concern, but this is far from true

The truth is that the width of the toxic plume cloud is relatively narrow compared to the length. The models predict the centerline concentration within the cloud, the worst case condition usually at ground level. The actual width of the cloud is a function of several variables, including wind speed, atmospheric stability, nature of the chemical release, terrain, and whether there are structures in the way to break up the air flow. The cloud may be several miles long but only a few hundred feet wide. When the Kit Fox dense gas releases were performed under a "D" atmospheric stability, the cloud width was roughly 10 meters wide at 225 meters downwind.

The illustration below shows a possible chemical plume cloud superimposed on the 2004 Emergency Response Guidebook display for a PAD. Even then, the concentrations upon which the PAD is based occur at the cloud centerline. There will be broad areas within the Protective Action Zone that may see no chemical or very low air concentrations.



Someone may ask, “Why not have a computer model display the chemical cloud width overlaid on a map and evacuate that area only?” The problem is accurate meteorological information is usually not available at the time of the spill. Even if conditions are known, they may be different 15 minutes later. Terrain and local meteorology can cause the cloud to shift and change direction. Sometimes the winds can die down completely, and the chemical cloud may move in any direction from the spill.

The June 18, 1988 Springfield MA chlorine fire chemical cloud was described as several city blocks wide and four or five miles long. Winds were blowing from the SW at 7 to 10 miles per hour. Particles from the fire made the cloud visible. However, chlorine was released at the source during the previous night under conditions of dense fog and no wind. There was no apparent predictable pattern of the chemical cloud movement. Chlorine odor was the only means of detection.

Because of uncertainties surrounding a release, authorities may order an evacuation in all directions, or use a PAD pattern similar to the display in the Emergency Response Guidebook , or evacuate selected neighborhoods. To be on the safe side, more people may be evacuated or told to shelter in place because knowledge on the extent of the release or potential release and weather conditions is incomplete. Does this mean that the models are too conservative? No. Our knowledge at the time of the spill is usually incomplete, and it is better to err on the side of safety.

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The cloud half width is defined as:

Half Width = $[\,3 \int dy\, y^2\, C\,]^{1/2}$ where C = concentration at location y, y = crosswind direction from centerline at y = 0, and y is integrated over all y ($-\infty$ to ∞). If the cloud shape is symmetrical and the cloud is not buoyant, we can use ground level concentrations for C; otherwise use center-of-gravity concentrations with respect to height.

Knowledge of Meteorology is Incomplete

Our knowledge of the exact weather conditions including atmospheric stability required to run gas dispersion models is incomplete. The ALOHA model as well as the one in the PEAC tool tries to make best educated guess on atmospheric stability by asking the user to estimate a wind speed and cloud cover; Using this information plus the date, location, and time of day an estimate of the stability (A through F, with A being the most unstable, D neutral, and F most stable) for use in the model. The "worst case" or most conservative case is the F stability at a low wind speed. This condition occurs at night or just before sunrise or after sunset under clear skies and low wind conditions. When doing modeling for a potential release, "worst case" conditions are often selected. For example, the EPA off site consequence analysis in case of a possible spill of hazardous chemicals requires that the user run atmospheric dispersion models under an "F" stability at a 1.5 m/s wind speed. Does this mean that the model is too conservative? No, the model user is running the model under "worst case" conditions.

Comment: If winds die down completely under clear skies, an even more "worse case" situation than using a 1.5 m/s wind speed will occur. However, gas dispersion models are not designed to run under a zero wind condition.

Knowledge of Release Situation is Incomplete

The first responder coming on a scene of an accident does not know the release rate of the chemical to the air. The responder may not even know whether the chemical container has been breached. There may be a chemical odor, but in case of a train derailment or transportation accident, there could be more than one chemical involved. The site of the accident may be obscured by smoke or fire or debris. Close inspection may be impossible or very hazardous.

The worst case condition for modeling is if all of the chemical is released to the atmosphere at once. The amount released is based on size of the storage tank. The PEAC tool permits the user to estimate a PAD for a "worst case" situation by choosing "BLEVE or sudden pressure release" and container size.

The PEAC user also has the option of estimating a release rate either directly or from calculation of an evaporation rate from a liquid pool or from a hole size in a tank that has been breached. There are many variables that affect the evaporation rate from a spilled pool, including the pool area, wind speed, solar radiation, and temperature. The PEAC tool uses the same method of calculation as in the ALOHA model for liquid pool evaporation. If the release is from a hole in a tank, the release rate will depend on the size and location of the hole. If the tank is under pressure, there will be an initial higher release rate but which should decrease as the pressure decreases. A tank containing a liquid such as chlorine or anhydrous ammonia if breached may spill liquid or gaseous chemical depending upon the location of the hole. If the hole is at the top of the tank, the gas under pressure will be released. The liquid within the tank will start to boil releasing more gas out the hole. As the liquid boils, the temperature inside the tank will decrease. The boiling rate will then decrease, and the gas escaping out of the hole will decrease. If the hole is near the bottom of the tank, the liquid will escape forming a pool. If the pool is a cryogenic liquid (such as chlorine or anhydrous ammonia), there will be considerable chilling of the pool as the chemical evaporates. Chemical spill tests at the Nevada Spill Test Facility showed that a spilled pool of chlorine or ammonia chilled to roughly -68^{o}F compared with a normal boiling point of about -35^{o}F. The evaporation rate of chlorine or ammonia is much less at -68^{o} F; therefore the release rate to the atmosphere would be less, and the PAD based on gas dispersion modeling would be less than if the modeling assumed a warmer temperature.

The PEAC tool modeling, using a release rate based on a tank hole breach, assumes a worst case, which is the initial release rate. The calculations do not consider that the release rate will decrease with time as the tank is emptied and the liquid remaining in the tank evaporates at a slower rate because of chilling. Calculations can be refined to give a better estimate, but more detailed information will be required of the user. The first responder is not likely to know the required information. Therefore it is better to err on the side of safety and assume worst case.

On 6 January 2005 at about 2:30 AM, a 42-car freight train struck a parked train in Graniteville South Carolina causing a breach in a 90 ton capacity chlorine tank car carried by the freight train. Eight people in the area were killed by chlorine inhalation; the engineer of the freight train also died from a combination of injuries sustained by the accident and chlorine inhalation. Over 250 people were hospitalized because of chlorine inhalation. Some apparently suffered lingering disability. About 5400 people were evacuated.

The ALOHA model was reported not to work very well for this particular spill [see http://www.chemicalspill.org/railcar.html]. The modeling was done to predict an evacuation distance based on IDLH of 10 ppm. [IDLH = Immediately Dangerous to Life and Health]. The ALOHA modeling further predicted that the chlorine rail car tank would empty within hours. This is not what happened as there was still considerable chlorine left within the tank after a couple of days.

After several days it was determined that there were about 30 tons of chlorine still left in the tank, and the chlorine escaped through a fist-sized hole above the liquid level. A patch was eventually placed on the hole. The chlorine was drained from the tank.

AristaTek was unable to determine the weather conditions at the time of the accident. Apparently there were low wind nighttime conditions with possible mist or fog. By next morning, there were strong and gusty winds. Fish kills were reported where storm drains from the area fed into waterways, suggesting either some liquid chlorine entering the drains or precipitation possibly scrubbing out some of the chlorine. Models do not work well under low wind or if there is any precipitation.

The fist-sized hole was probably near the top of the tank. There was considerable chlorine left in the tank after several days. There would have been an initial breach after the accident resulting in emission of gaseous and possibly some liquid chlorine. The chlorine left in the tank would have chilled thereby decreasing the evaporation rate. The fact that the chlorine pool was contained within the tank would have allowed the tank to chill even more reducing the evaporation rate even further. The problem with the ALOHA modeling is that a too large emission rate was used, not that the ALOHA model itself was too conservative. These types of situations are very difficult to model.

If the chlorine emission rate was less, the emission duration would be longer. Therefore modeling should have been done to a 1 ppm endpoint, not the 10 ppm IDLH endpoint. Chlorine continued to be emitted over a several day period. There was a high initial rate at the time of the breach, followed by a much lower continuous rate which lasted several days. The problem is not that the ALOHA model is too conservative. The problem is what emission rate to properly use in the models and what meteorology conditions to use.

Conclusion

The models themselves display chemical cloud dispersion in so far as they can be calibrated with test spills. The problem is during a HazMat incident or potential incident, all of the required information to run the models is not known. Because of the unknowns, sometimes a “worst case” situation is selected, and this may give the appearance that the model is too conservative.