A Discussion on Gas Dispersion Models

WHY DO GAS DISPERSION MODELS SOMETIMES GIVE VERY DIFFERENT ANSWERS?

The Problem:

Have you ever modeled a toxic gas release to the air using CAMEO (which incorporates the ALOHA model) and wondered why you do not always get the same answer as predicted using the PEAC tool? Or perhaps you used the ALOHA model obtained from the Environmental Protection Agency to predict a Protective Action Distance based on some toxic concentration such as ERPG-2, and then noted that result was very different from the Department of Transportation's 2000 Emergency Response Guidebook even though the same toxic concentration endpoint was used. Or perhaps you are in the Department of Defense modeling a release of a chemical warfare agent using the D2PC model, and obtained a different answer compared with models such as ALOHA or DEGADIS or any of the other models in the public domain. Why is this so?

The Answer Depends How The Model Was Formulated and What Data Sets Are Used to Calibrate

The answer why models give different results is not that one model or methodology is necessarily better than any other but that the models are formulated differently. Even when two models have the same basic mathematical formulation, different sets of data may have been used to calibrate them. Two popular mathematical formulations are (1) Gaussian-type or passive dispersion and (2) dense gas dispersion. A major difference between the two is that a cross section of the concentration profile has a "bell" shape for the Gaussian type, whereas the dense gas formulation describes a rather flat concentration profile which hugs the ground. Both the PEAC tool and the ALOHA model contains passive and dense gas formulations, but the D2PC model and DOT 2000 Emergency Response Guidebook are based on passive formulations. Passive dispersion is applicable for small releases or for large releases in situations where the molecular weight and chemical temperature is similar to the surrounding air. Dense gas dispersion is applicable for large releases of either a cold or higher molecular weight gas. Even a dense gas release becomes passive far from the source. The PEAC tool handles the decision process of whether to use a dense gas or passive formulation internally. In the case of the ALOHA model, the user can either dense gas or passive or let the model decide internally.

Regardless of whether the model uses a dense gas or Gaussian-type formulation, it must be calibrated against real data. This is because no matter how elegant the theory behind the model, the degree of how the plume cloud disperses for a given weather situation and as the cloud encounter barriers (trees, buildings, etc.) must be obtained from experiments. The people who develop the models do this ahead of time before the user runs the model. For example, the ALOHA passive dispersion model contains mathematical expressions for "Sigma Y" and "Sigma Z" which were published by Gary Briggs in 1973. Sigma Y is the standard deviation of the crosswind concentration at a distance X downwind (X = 0 at the source). Sigma Z is the standard deviation of the vertical concentration at a distance X downwind. The Sigma values describe how the cloud increases in size and becomes more dilute as it travels downwind. Gary Briggs developed empirical expressions for Sigma Y and Sigma Z for different atmospheric stability conditions

from a set of sulfur dioxide release experiments in a Kansas prairie, valid for distances between X = 100 and 10,000 meters. The original sulfur dioxide data was obtained using a 3-minute concentration averaging time and a surface roughness of 0.1 meters. ALOHA (version 5.2.3) uses another set of Sigma Z expressions if the surface roughness is greater than 0.3 meters; these Sigma Z expressions were also developed by Gary Briggs using tracer release studies in St. Louis, Missouri, and have a 60-minute concentration averaging time. Other sigma expressions developed from different data sets have been published and have been given names such as "Beals' Sigmas", "Gifford and Slade Sigmas", "Seinfeld and Turner Sigmas", etc., after the people who developed the analytical expressions from the raw data.

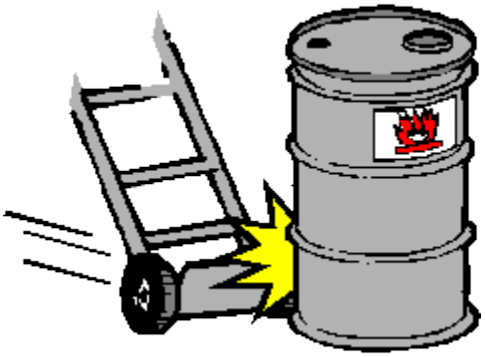
One problem is that it is not practical to run experiments under all combinations of different chemicals, different release rates, different wind speeds, different surface roughness conditions, different atmospheric stabilities, and look at different concentration averaging times. What is done is to develop empirical expressions or algorithms from a limited data set and assume that the relationships hold true for conditions not tested. Thus, in ALOHA, the same set of Briggs-developed Sigma Y and Sigma Z values (and Beals' Sigma X) are used for any passive release regardless of the chemical, wind speed, concentration averaging time, or surface roughness even though the original data set was taken under a much more limited circumstances. If a dense gas modeling is required, ALOHA uses the methodology developed by Spicer and Havens at the University of Arkansas in their DEGADIS model (description in EPA document EPA-450/4-89-019).

The PEAC tool when modeling passive dispersion uses the classical Gaussian equations with Sigmas from a variety of sources depending upon the circumstances, including the Briggs' Sigmas derived from the sulfur dioxide release tests and several other Sigma sources which are detailed in the DEGADIS manual (EPA-450/4-89-019). When modeling dense gas dispersion, the PEAC tool uses a matrix of power functions derived from tests performed at the DOE HazMat Spill Center in Nevada and from the dense gas model SLAB (a model in the public domain developed by Lawrence Livermore National Laboratories, who operated that Nevada DOE facility for several years).

During the summer of 1995, a massive data set labeled "Kit Fox" was taken at the DOE HazMat Spill Center. The tests, sponsored in part by ten petroleum and chemical companies, the U.S. EPA, DOE, and Western Research Institute through their DOE cooperative agreement, simulated large dense gas releases at a refinery or chemical complex under atmospheric conditions ranging from daytime neutral to near nighttime very stable which occurs when the winds are almost calm under a clear sky. The results have been recently used (S. Hanna, J. Chang, and G. Briggs, 1998) to upgrade the dense gas model HEGADAS, which was originally developed in England and is popular in the petroleum industry.

The DOT 2000 Emergency Response Guidebook

The 2000 Emergency Response Guidebook uses a somewhat different approach. The gas dispersion modeling has already been done, and the results (Protective Action Distances) have been reduced to four choices for a given chemical. The four choices are (1) daytime small spills, (2) daytime large spills, (3) nighttime small spills, and (4) nighttime large spills. Each toxic chemical has Protective Action Distances for these four choices. The information is presented in the form of look-up tables. The same information is also captured in the PEAC tool. The PEAC tool also lists the Levels of Concern upon which the Protective Action Distances are based in case the user desires to do his own modeling.



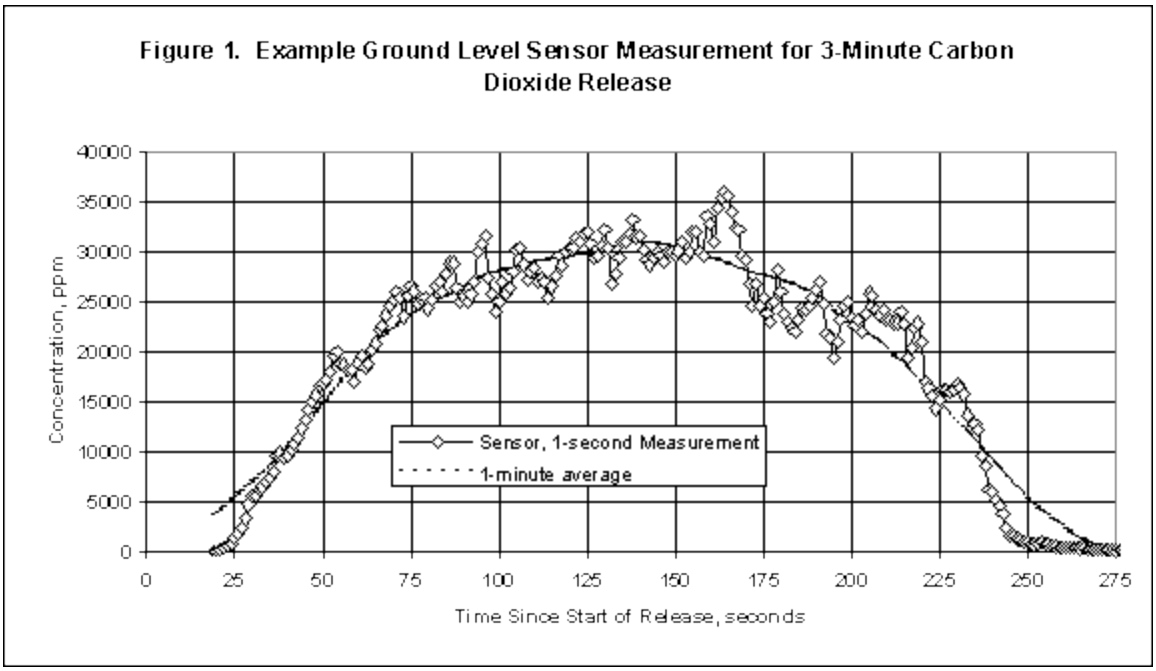
Spills 55 gallons or greater are considered large spills. Daytime spills cover unstable and neutral atmospheric conditions, and nighttime spills cover neutral and stable atmospheric conditions. Many different combinations of circumstances can occur. In developing the look-up tables, over 50,000 different combinations were modeled (different wind speeds, atmospheric stabilities, different spill situations, etc.). The results were segregated into the four categories. The number selected for the Protective Action Distance listing was based on a 90 percentile, that is 90% of the spills modeled had Protective Action Distances equal or less than the number selected for the Emergency Response Guidebook. This approach takes out some of the guesswork for the emergency responder who wants a quick answer in case of a transportation spill.

The DOT lookup tables have limitations. The lookup table would over predict the Protective Action Distance for a spill of a pint-sized container of liquid onto the ground, but probably under predict a catastrophic release of chlorine from a tanker-trailer. A slow leak of sulfuric acid from a tank onto the ground probably would not require a major public evacuation because of the very low vapor pressure of sulfuric acid, but if the same tank were in a fire, an extensive evacuation may be necessary. The DOT modeling effort also does not consider terrorist activity, where a large amount of chemical might be released at once because of explosives.

Obviously, the DOT lookup tables can sometimes predict very different Protective Action Distances compared with modeling the situation directly.

Concentration Averaging

The raw data used to calibrate models may have very different concentration averaging times. Even if the chemical released to the atmosphere is carefully controlled, as the dispersion cloud travels downwind the concentration as seen by a sensor in the cloud path will fluctuate because of local atmospheric turbulence. In addition, the cloud itself may meander in and out of the sensor location. Thus a one-second peak concentration at a given location downwind will be greater than a one-minute averaged peak concentration, which in turn will be greater than a one-hour average concentration, even though the amount released at the source is the same. If there is a "puff" or instantaneous release, the differences become even greater.

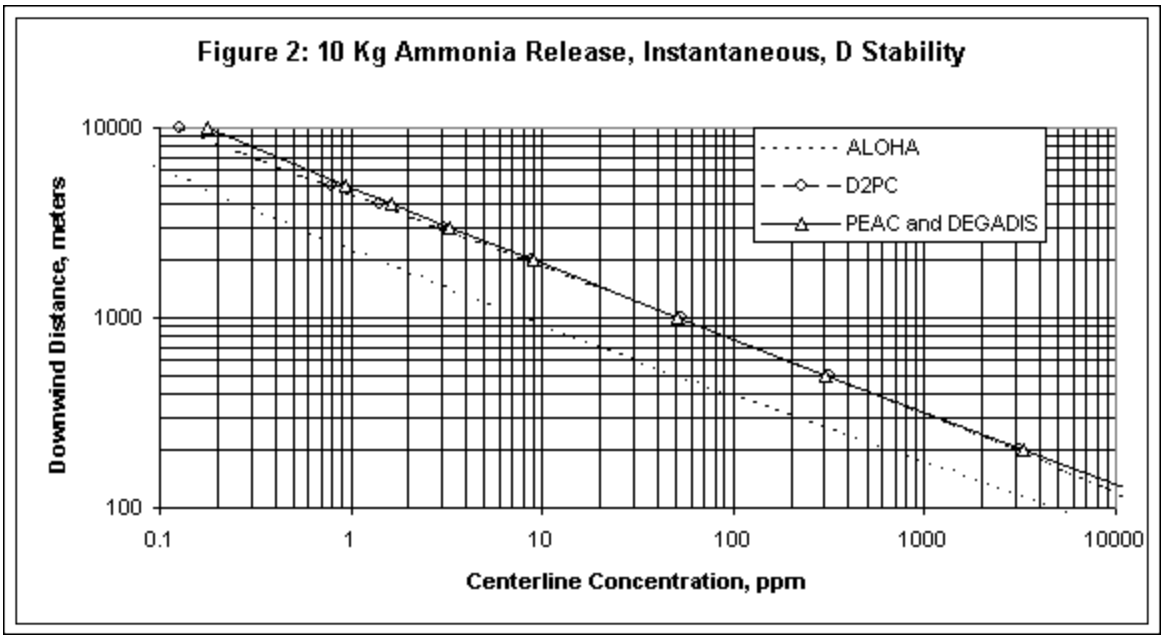


An example of a sensor plot with time is illustrated by Figure 1. In this test at the DOE HazMat Spill Center, 1.722 kg/s of carbon dioxide was released for exactly 180 seconds, and the resulting plume cloud concentration measured by a sensor placed 25 meters downwind. The peak 1-second concentration was 37000 ppm but the peak 1-minute concentration was 30000 ppm. An average 1-hour concentration would be much less, in fact, the cloud only lasted about 225 seconds as it passed over the sensor.

Sometimes data is taken using a sampling pump or other device to capture a volume of gas over a time period (e.g. one hour). This method is commonly used in tracer gas studies, where sulfur hexafluoride or some other chemical is released in a test. The gas captured is collected and then analyzed using a gas chromatograph. The concentration obtained was the average concentration over the sampling period. The Figure 1 data was collected using a real time, quick response sensor, which measured the concentration every second.

Whether the user should model a 1-minute peak concentration or say a 1-hour average concentration depends how the data is to be used. In the workplace, maximum concentrations that a worker can be exposed to a chemical are sometimes expressed as 8-hour time-weighted averages. With some chemicals, a 15-minute ceiling limit is imposed, meaning, that this is the maximum concentration the worker can be exposed during a 15-minute period. On the other hand, inhalation of a chemical warfare agent can be fatal in a single breath; therefore a two or three second peak concentration is of interest.

Thus, models can give different results depending upon the concentration averaging time and Sigmas developed from the calibration data, as illustrated by Figure 2 for a 10 kg instantaneous ammonia release under passive conditions and neutral ("D" atmospheric stability) conditions.

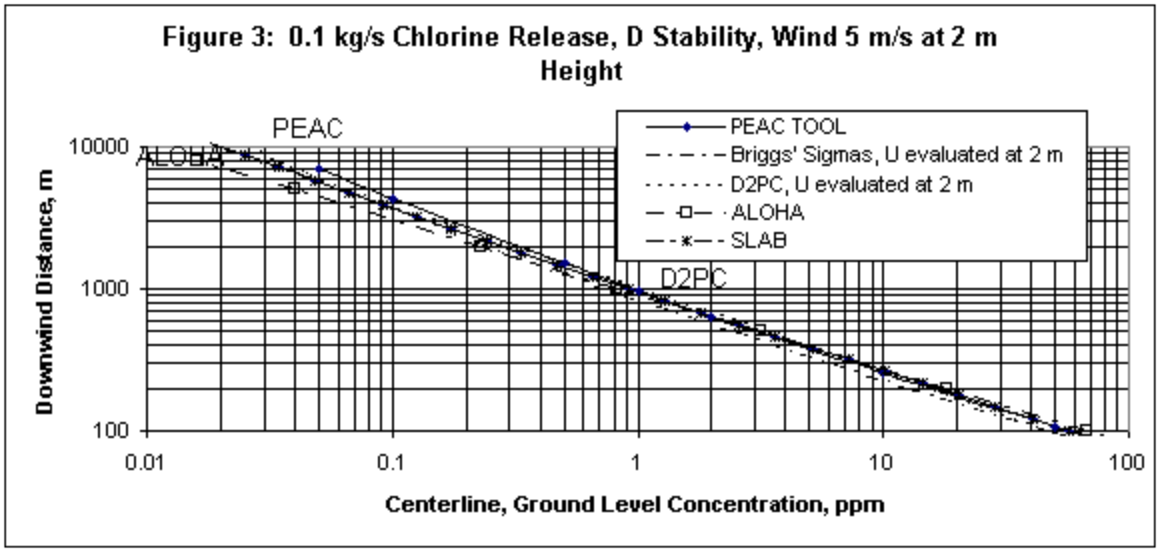


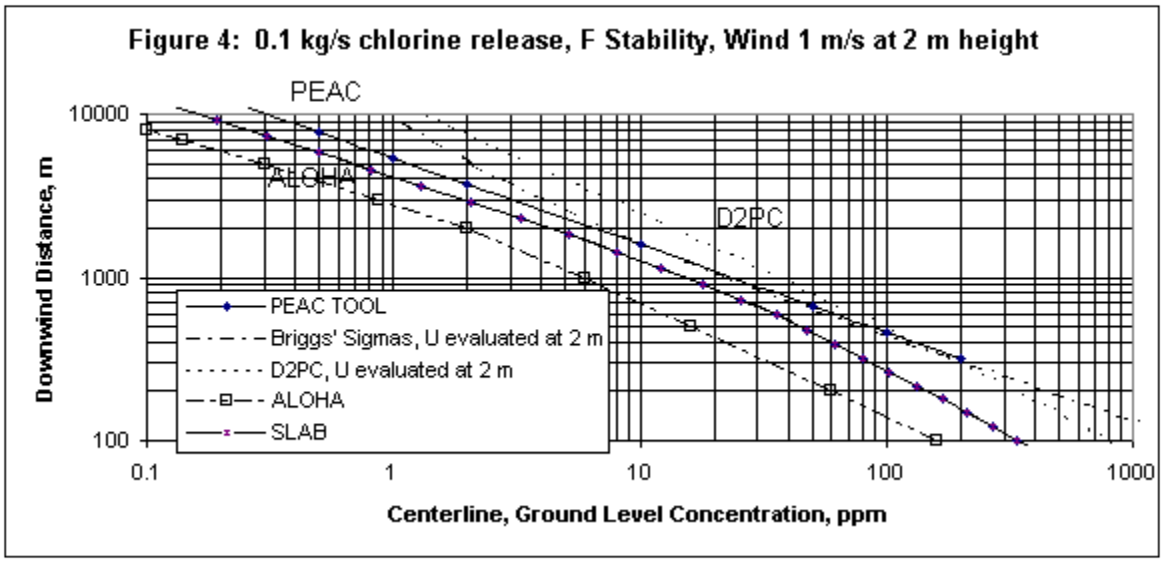
The ALOHA model (version 5.2.3) was based on Brigg's Sigma Y and Sigma X, and Beals Sigma X values. The PEAC tool and the DEGADIS model gave the same answers for this application, as both used the Seinfeld and Turner Sigma Z and the Gifford and Slade Sigma Y, and the model set Sigma X = Sigma Y. The D2PC model was developed from another set of Sigma values and happened to give approximately the same result as DEGADIS and the PEAC tool.

Lack of Calibration Data For Stable Atmospheric Conditions

Another reason why models differ is there is a lack of good calibration data under stable atmospheric conditions. Stable atmospheric conditions occur under clear or mostly clear skies, low wind conditions, and near sunset or at night. Under these conditions, the ground loses heat by radiant cooling. A dense layer of cold air settles near the ground. This condition is the most dangerous in case of a spill because the toxic cloud does not readily disperse and can meander far from the source almost intact. This is in contrast to a neutral atmospheric condition, which typically occurs during windy conditions or cloud cover. The turbulence generated by the wind causes the cloud to disperse. Unstable atmospheric conditions occur during sunny days and low wind speeds when sun radiation heats the ground causing the air near the ground to rise creating updrafts and downdrafts. The cloud disperses even more readily under unstable conditions than under neutral conditions. Modelers sometimes classify atmospheric stability by the letters A, B, C, D, E, and F with A being the most unstable, D being neutral, and F being the most stable.

Most calibration data have been taken under neutral atmospheric conditions because it is the easiest to do and the easiest to define. Very little data have been collected under the stable night time condition or under the very unstable day time condition. The stable F condition is of particular interest as this is the "worst case". Figure 3 illustrates that the models agree fairly well under the neutral or "D" stability condition. Figure 4 shows the models depart significantly under the very stable "F" condition.





What Does This Mean to the User?

Models are used by the user as rough guidelines for estimating Protective Action Distances and public evacuations and do not give absolute results. Completing well-designed tests at locations such as the HazMat Spill Center and elsewhere can decrease uncertainties. The user should look at information from a variety of sources and model the situation under different scenarios.

*Mr. John Nordin received his BS in Chemical Engineering in 1961 from the University of Minnesota. In 1965 he received his Ph.D. from the University of Minnesota in Biochemical Engineering.