Technically Speaking
A Discussion Of Gas Dispersion Models
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COMMENTARY ON USE OF GAS DISPERSION MODELS

Many of us have used a gas dispersion model to estimate downwind concentrations of a chemical contaminant in the event of an actual or potential spill. Usually a concentration representing a level of concern is established, and the gas dispersion model is run to estimate a downwind distance where the ambient concentration equals the level of concern. This downwind distance is used to establish a Protective Action Distance for the purpose of ordering a public evacuation (if there is time to evacuate) or for sheltering in place (if there is no time to evacuate). We will spend looking at these gas dispersion models, their limitations, and applying some common sense rules in getting answers for special situations.

The typical gas dispersion model allows the user to consider simple effects of (1) meteorology, (2) the chemical and amount spilled, (3) how the chemical is spilled, and (4) terrain in estimating downwind airborne concentrations as a function of distance. These effects are interrelated which makes the calculations complicated.

There are several different models in the public domain or can be purchased for a fee.

Effect of Meteorology on Gas Dispersion Modeling

Gas dispersion models consider simple effects such as wind speed and atmospheric stability. They do not consider effect of precipitation nor do the models work under an absolutely calm (zero wind speed) condition. There may also be abnormalities close to the release source. Also, to keep the calculations simple, the same terrain conditions and meteorological conditions are assumed as the chemical cloud travels downwind.

Atmospheric stability has to do with the degree of mixing of the air because of solar heating of the ground during the day or cooling at night. Hot air is less dense than cold air. During the day, under sunny skies, the ground absorbs heat from the sun and the air above the ground heats up. The air is said to be unstable; the air rises and mixes. A pilot flying his aircraft at say 1000 or 2000 feet above the ground encounters turbulence do to rising and sinking columns of air. The air is said to be unstable. If a chemical spill occurs, the resulting chemical cloud disperses rapidly due to the unstable air conditions.

At the other extreme, under clear, nighttime conditions, the ground chills. If there is little wind to mix the air, the air above the ground also chills. Cold air sinks, but the chilled air is already near the ground so air mixing does not occur. This air is said to be stable. If a chemical spill occurs, the resulting chemical cloud does not readily disperse and may stay there the whole night until winds pick up or solar heating occurs. This is the most dangerous (worst case) situation.

What happens if skies are cloudy? The sun does not heat the ground during the day nor is there much ground cooling at night. The atmosphere approaches a “neutral condition”, that is there is little tendency of the air near the surface to rise or sink because of temperature differences at different heights above the ground.

What happens under windy conditions? Wind occurs because of tight barometric pressure gradients as low or high pressure areas move across planet earth, or because of localized effects of nearby mountains or large bodies of water. Wind causes the air to mix before it has a chance to become heated due to solar heating of the ground or chilled because ground cooling at night. The atmosphere approaches a "neutral" condition.

What happens under "dead calm" conditions? The models available are not equipped to handle a "zero wind" condition; a model user might input a vary low wind speed (e.g. 1 mph; 0.5 meters per second) and keep in mind that the chemical cloud may travel in all directions. The "zero wind" condition does not exist during daytime solar heating of the ground (the air will mix due to rising and sinking columns of air), and the chemical cloud will rapidly disperse. During nighttime clear skies, there is nothing to mix the air, and the chemical cloud will just "sit there" until the air is moved. If the chemical cloud is a dense gas, it will tend to seek low terrain areas. If skies are overcast and there is "zero wind", the chemical cloud will "hop skip" around in any direction in an unpredictable way, with some areas nearby being free of the chemical and other areas further away exposed to the chemical. If the chemical is a dense gas and a massive spill occurs, the chemical cloud may follow the terrain seeking low areas.

What happens if it is raining? It depends on the chemical. Many chemicals dissolve in water. Some react with water giving off gases which in turn may dissolve in water. The rain could knock down the chemical out of the air creating a water pollution problem but also greatly shortening the length of the toxic cloud. If a thunderstorm is occurring, the atmospheric turbulence may quickly disperse the chemical cloud. Some chemicals if wetted give off enough heat that a fire may result. A lot of different things can happen.

Most gas dispersion models including the ones in CAMEO (CAMEO uses the ALOHA model) and in the PEAC tool rank atmospheric stability on a scale of 1 to 6 (sometimes letters A through F are used). A "1" or an "A" ranking represents the most unstable air condition (resulting from daytime solar heating of the ground, and little wind). Rankings 2 and 3 (B and C) represent intermediate daytime conditions, 4 or D a neutral condition, 5 or E a stable condition (near sunset or sunrise or at night), and 6 or F the most stable condition. Some models use a sliding scale called an Obukhov or Monin-Obukhov length to indicate stability (a measure of the mixing tendency of the atmosphere). Both the PEAC tool and the ALOHA model calculate the atmospheric stability internally based on Table 1.

Table 1. Pasquill-Gifford Stability Index.

Pasquill Dispersion Class	Description	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.

When a user specifies a wind speed in the PEAC tool, the wind is assumed to be at a 2 meter height (just above the height of a man). The PEAC tool internally corrects this to a 10 meter height for selection of the stability class. Ordinarily there is not much difference in wind speed measured at a two or ten meter height, but there could be a major difference if there are nearby buildings to break up the wind or under stable air conditions.

When using the PEAC tool, it is important to specify the correct geographic location, date, time of day, and cloud cover so that the solar angle and stability class can be calculated. Again, the PEAC tool takes care of this internally. The ALOHA model works similarly.

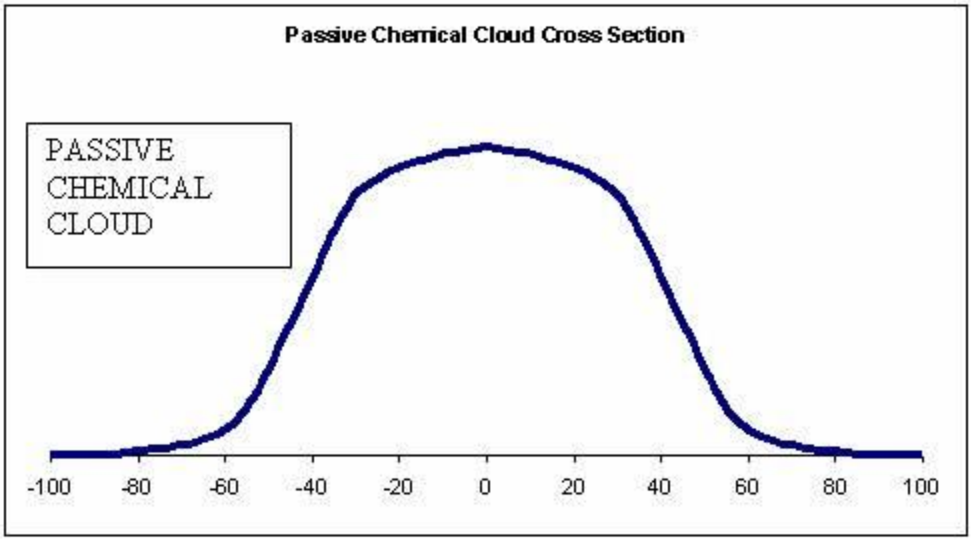
Effect of Chemical and Amount Spilled on Modeling

Obviously, the more chemical that is released the greater the concentrations in the air. Toxicity of the chemical is usually the basis for specifying a Level of Concern for the chemical. The modeling is done to estimate a downwind distance to the specified Level of Concern. For some chemicals, such as propane and ethane, an explosion hazard and resulting fireball is a greater hazard than toxicity. The modeling methodology is different for these chemicals.

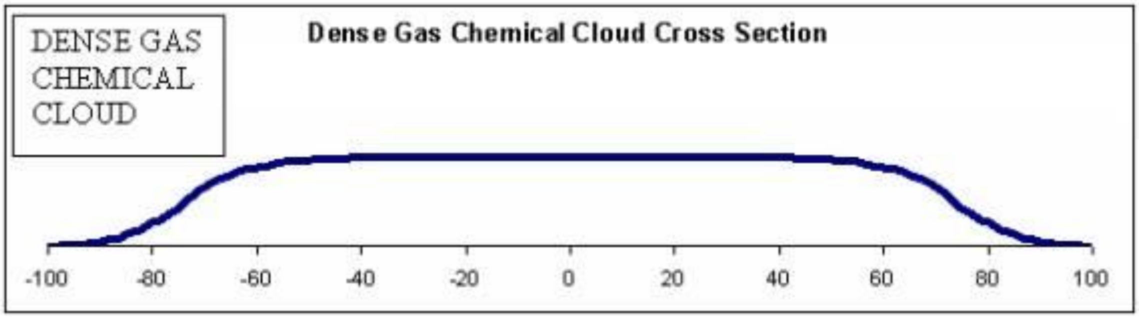
Some chemicals react with moisture in the air or if spilled in water give off toxic gases. The modeling should be done based on the toxic gases given off.

If the amount of chemical released is great enough and if the chemical is also chilled or if it has a high molecular weight, a dense gas cloud will form which hugs the ground. An example is the rupture or a valve sheared off of a chlorine tank. The dense gas dispersion uses a different modeling methodology. The terms “passive” or “Gaussian” dispersion and “dense gas” dispersion is used to distinguish between the two modeling methodologies. The PEAC tool as well as ALOHA and most other models take care of the selection internally, and the user does not have to worry about it. The military D2PC model is designed to run in the passive mode only.

Perhaps the best way of distinguishing between passive dispersion and dense gas dispersion is to look at a cross section of the chemical cloud.



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.



The worst-case situation is the combination dense gas release with a very stable ("F" Stability) atmospheric condition. The toxic chemical cloud can travel many miles from the source as there is nothing to disperse the cloud. If the spill occurs on a hillside or in a canyon, the chemical cloud will follow the terrain seeking low lying areas. This happened during the early AM hours of September 2, 1988, at the Morristown, TN water treatment plant. An estimated 2400 to 3000 lbs of chlorine was released from tanks resulting in a dense gas cloud that was described [see "Fire Engineering" magazine, Feb. 1989] as 5 miles long and up to one mile wide but only 10 feet high as it followed the terrain down the valley. Near the source of the spill, the cloud was only two feet high. When the sun rose, the winds picked up, and the cloud quickly dispersed. There were no deaths, but 4000 people were evacuated.

How a Chemical is Released Affects Modeling

The 2004 Emergency Response Guidebook produced jointly by Canadian, Mexican, and United States governments presents Protective Action Distances for evacuation in case a chemical is spilled. Among the choices available for certain chemicals are (1) "when used as a weapon" (as opposed to a simple spill) and (2) "when spilled in water" (as opposed to when spilled on land). When the words, "when used as a weapon" is used for chemicals such as the nerve agent Sarin, hydrogen cyanide, etc., the assumption is made that a terrorist has either attached an explosive devise to a container or otherwise rigged the container to rapidly release its contents to the air in the form of an aerosol, gas, or dust. In a simple spill, the chemical may spill onto the ground and evaporate or leak from a hole in a tank over a period of time. The modeling is different for the two cases.

Some chemicals, if spilled in water, decompose releasing toxic gases. There may be enough heat released to result in localized boiling of the water. If the chemical is simply wetted, the heat released may be sufficient to result in a fire. Some chemicals such as sodium or lithium release hydrogen gas on contact with water that may result in explosion and fire. The gas dispersion modeling is based on the toxic gases released when the chemical reacts with water, with additional attention paid to possible explosion and fire.

When someone uses a gas dispersion model, the person is confronted with two basic choices: (1) a continuous release of chemical to the atmosphere or (2) an instantaneous release of the chemical to the atmosphere. This is true of the ALOHA model, the model in the PEAC tool, and the SLAB model developed by Lawrence Livermore National Laboratories. The modeling is different with the two choices.

When the user of the model sees the words “BLEVE” or “sudden pressure release” or “instantaneous release” or “puff release” or “when used as a weapon”, the model is operating in the instantaneous mode. All of the contents of the container is released to the atmosphere at once. In the PEAC tool, if almost the entire contents of a large container or tank is released to the atmosphere within 10 seconds the model operates in the instantaneous mode. When using the model in the instantaneous mode, the user either specifies the total quantity of chemical released (e.g. kg, lbs., etc) or the container size or container dimensions.

Words such as “evaporating liquid pool”, “evaporating pool”, “horizontal jet”, “vertical jet”, “release from a pipe”, and “release from a hole in a container” signal that the model should operate in the continuous mode. In the PEAC tool, the user may either specify a mass release rate (e.g. kilograms per minute, pounds per minute) or specify a liquid pool size or a hole size in the side of a tank or a pipe release size. If a pool size is specified, the PEAC tool calculates an estimate evaporation rate (taking into account the chemical, wind speed, solar insolation, and other variables but not special circumstances such as heating from a nearby fire). If the pool size is unknown, a default area is calculated based on a 1 cm pool depth. If a hole size is specified, the PEAC tool calculates an initial release rate and base the modeling on this initial release rate (a worst case condition). As the tank is emptied, the release rate will drop off from its initial value.

The “instantaneous release” represents the worst case condition as far as predicting the greatest Protective Action Distance for a given level of concern. The toxic cloud duration over a given downwind location will probably be greater for a continuous release than for an instantaneous release, but the peak concentrations are higher for an instantaneous release assuming the same total amount of chemical is released to the atmosphere in both situations.

If a user runs a model and finds that the continuous mode gives a greater Protective Action Distance than the instantaneous mode, assuming that the same total amount of chemical is available, he has used the model incorrectly. For example, if the user specifies a 12-inch diameter hole near the bottom of a tank with no liquid pool formed, the model might calculate an initial release rate based on the hole size and shift to the continuous mode. But that release rate cannot be sustained because there is not enough material available. The user should either have specified an instantaneous release with the 12-inch hole or specify that the liquid from the tank forms a pool which evaporates into the atmosphere. If a tank capacity is say 10000 kg of chemical and there is a hole in the a tank resulting in an initial release rate to the atmosphere of 3000 kg/s, the user should specify “instantaneous release” or “BLEVE” or “sudden pressure release” as the 3000 kg/s release cannot be sustained.

Effect of Terrain on Modeling

The standard models including ALOHA model and the model in the PEAC tool considers the effect of terrain in only a crude way. A surface roughness parameter is assigned (units: meters or centimeters) for different terrain situations. The logic is that the presence of buildings, cropland, trees, or whatever will break up the air flow and aid in dispersing the chemical cloud. The surface roughness is not a measure of the height of the objects but is instead an indicator of how the average wind speed changes as a function of height near ground level due to the presence of trees or structures.

The PEAC user is offered three choices: (1) flat terrain, (2) cropland, or (3) urban/forest. The flat terrain is linked internally in the PEAC tool with a service roughness of 0.001 m, cropland 0.1 meters, and urban/forest 1 meter. Very roughly, the surface roughness is 1/15th to 1/30th of the height of the objects in the terrain.

The real world is more complicated when there are buildings or the terrain is uneven. This is the subject of another PEAC Newsletter article, available by clicking on this link.
and a Los Alamos National Laboratory paper available at this link.