Technically Speaking

More examples and explanation of the patented modeling.

by Dr. John Nordin

How Does The Gas Dispersion Model in the PEAC Tool Compare with other Models?

One of the questions that PEAC tool users ask is how does the PEAC gas dispersion model compare with other gas dispersion models in the public domain. We will look at a couple of chemicals: (1) chlorine and (2) Sarin. Chlorine is widely used in industry including the manufacture of plastics and is also used in drinking water treatment. Sarin is a very poisonous chemical warfare agent which potentially be used by a terrorist. An actual chlorine spill was discussed in an earlier newsletter article [see January 2005].

The gas dispersion models that we will compare the PEAC tool to are (1) ALOHA, which is used in CAMEO; (2) the military D2PC model; (3) SLAB, developed by Lawrence Livermore National Laboratories; and (4) a passive dispersion model using Brigg's sigma expressions. We will also look at the Protective Action Distances listed in the 2004 Emergency Response Guidebook.

Some basic information on gas dispersion modeling is in the March 2005 Newsletter article [see March 2005].

2004 Emergency Response Guidebook

Before we get started, let us look up what the 2004 Emergency Response Guidebook has to say about Protection Action Distances for Chlorine and Sarin spills. The PEAC tool contains a link to the 2004 Emergency Response Guidebook, and we will reproduce the information as it appears in the Emergency Response Guidebook, Figure 1 below.

Figure 1: 2004 Emergency Response Guidebook "Green Section"

		SMALL SPILLS (From a small package or small leak from a large package)						LARGE SPILLS (From a Large package or from many small packages)					
		First ISOLATE in all Directions		Then PROTECT persons Downwind during-				First ISOLATE in all Directions		Then PROTECT persons Downwind during-			
				DAY		NIGHT				DAY		NIGHT	
ID No.	NAME OF MATERIAL	Meters	(Feet)	Kilometers	(Miles)	Kilometers	(Miles)	Meters	(Feet)	Kilometers	(Miles)	Kilometers	(Miles)
1017	Chlorine	30m	100ft	0.2km	0.2mi	1.2km	0.8mi	240m	800ft	2.4km	1.5mi	7.4km	4.6mi

		SMALL SPILLS (From a small package or small leak from a large package)						LARGE SPILLS (From a Large package or from many small packages)					
		First ISOLATE in all Directions		Then PROTECT persons Downwind during-				First ISOLATE in all Directions		Then PROTECT persons Downwind during-			
				DAY		NIGHT				DAY		NIGHT	
ID No.	NAME OF MATERIAL	Meters	(Feet)	Kilometers	(Miles)	Kilometers	(Miles)	Meters	(Feet)	Kilometers	(Miles)	Kilometers	(Miles)
2810	Sarin (when used as a weapon)	150m	500ft	1.7km	1mi	3.4km	2.1mi	1000m	3000ft	11.0+km	7.0+mi	11.0+km	7.0+mi

Example 1: 0.1 kg/sec chlorine release at ground level

This is the first example comparison we will make. We will compare the PEAC tool modeling results with several other models. We will do this for two meteorological conditions: (1) a "neutral" daytime, "D" stability condition with a wind speed of 5 meters/second and (2) a stable nighttime "F" stability condition with a wind speed of 1 meters/second. The gas dispersion models we will compare are (1) PEAC tool, (2) a passive model using Briggs' sigma values, (3) a passive model using D2PC dispersion coefficients, (4) ALOHA version 5.2.3, and (5) SLAB dispersion model. The wind speed is measured at a 2 meter height. If the model asks for a relative humidity, we used 20%. In the SLAB model, a 1-minute averaging time was used. If the models request a surface roughness, 0.1 meter or "cropland" was used. When using the PEAC tool, skies were specified as "overcast" with a wind speed of 5 meters/second to get a "D" stability condition. To get an "F" stability condition, the PEAC tool internal clock was reset to a "nighttime" condition with clear skies. When using the "F' stability condition, the PEAC tool model, SLAB, and ALOHA models default to a "dense gas" mode. The meanings of "dense gas mode", "passive mode or Gaussian mode", "D stability" and "F Stability" are discussed in an earlier newsletter article, [see March 2005, and July 2002]. The word "sigmas" refers to analytical expressions within the model that describe the degree that the toxic plume cloud mixes and spreads as it travels downwind. Briggs refers to Gary Briggs who developed some of these sigma expressions.

The models were rerun at different "Levels of Concern", or different downwind concentrations. When we are done we have listings of "Centerline, Ground Level Concentrations" matched up with various "distances downwind" for various models, each under daytime neutral conditions and stable nighttime conditions. The results are graphed in Figures 2 and 3.

Figure 2: 0.1 kg/sec. Chlorine Release, D Stability, Wind 5 m/s

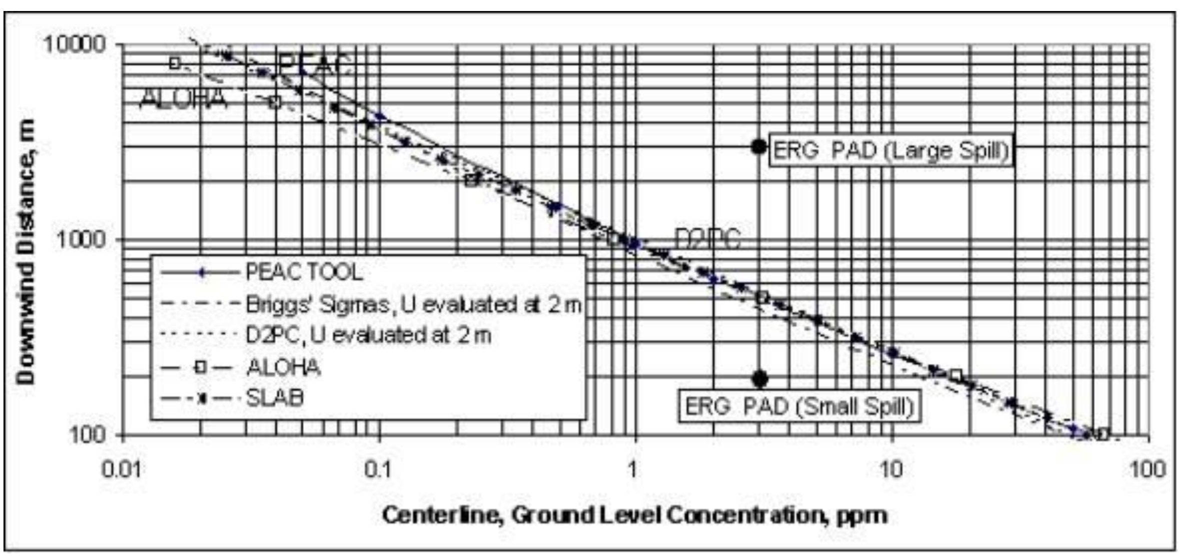
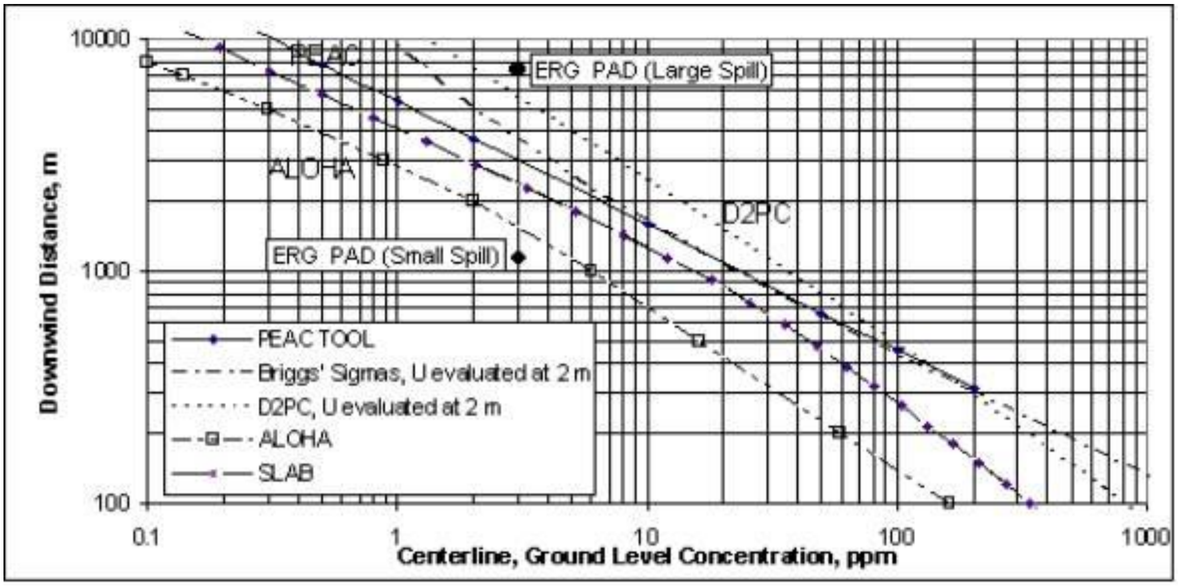


Figure 3: 0.1 kg/s Chlorine Release, F Stability, Wind 1 m/s



The 2004 Emergency Response Guidebook bases the Initial Isolation Zone at IDLH (Immediately Dangerous to Life and Health) conditions which for chlorine is at 10 ppm. The Protective Action Distance is the ERPG-2 (Emergency Response Planning Guideline level 2) condition of 3 ppm chlorine. It is not immediately clear whether a 0.1 kg/sec chlorine release is a large or small spill, but we will consider it a large spill. Under "small spills" the daytime 2004 ERG initial isolation distance is 30 meters and the PAD is 200 meters (0.2 km). Under "large spills" the initial isolation distance is 240 m and the PAD is 2400 m (2.4 km). This compares with 260 m at 10 ppm chlorine and 500 m at 3 ppm as shown in Figure 2. All of the models including the one in the PEAC tool gave essentially the same results in Figure 2.

Under nighttime, "F" stability conditions (Figure 3) the models gave very different results. The ALOHA model gave the least conservative results (smallest PADs) but the D2PC model gave the most conservative results (largest PADs). The PEAC tool gave an intermediate result very similar to the SLAB model. The nighttime 2004 ERG gave a PAD at 3 ppm chlorine of 7400 m (7.4 km) for their large spills and 1200 meters (1.2 km) for their small spills. This compares with 1500 km for the ALOHA model to 6000 km for the D2PC model.

Why are there these differences? One reason is that the 2004 Emergency Response Guidebook does not "fine tune" their PADs for the actual spill size or meteorological conditions and looks at everything at a 90% probability level, that is, 90% of those spills that occur during transportation accidents modeled when the tables were developed will have PADs equal to or less than the listed values.

A second reason for the differences is that the "D" stability condition is very well defined and can be created easily in a wind tunnel where chemicals or smoke can be released and their dispersal patterned studied. There are a lot of experiments available under the "D" stability or neutral stability condition to develop models. There is very little data available on dispersal patterns under the stable "F" condition or the unstable "A" condition. Therefore models are based on extrapolations.

When the owners of AristaTek released carbon dioxide at the Nevada Spill Test Facility at rates up to 4 kg/s, there was a big difference in dispersal behavior depending upon the degree to which the "F" stability developed as sunset turned to night. The model developer Gary Briggs witnessed the tests. Under the "worst case" condition, the winds died down completely and the carbon dioxide did not disperse. What is called "F Stability" by models can represent degrees of conditions from "near F" to "far F" to what some have referred to as "G" stabilities or even "H" stabilities. Because models used different data in their calibration, the results can be expected to be different.

Example 2: 2 kg/sec Chlorine Release at Ground Level

This example has the same conditions as example 1 except that the release rate is increased by a factor of 20, or 2 kg/sec. The passive models using Briggs' sigma values or D2PC sigmas do not apply because the release is considered a dense gas. The ALOHA model is set up not to display results beyond 10 km, or 1 hour cloud travel time. The modeling results are displayed in Figures 4 and 5. The PEAC tool model, SLAB, and ALOHA all operated in the dense gas mode. For the "D" stability (Figure 4), both models and the PEAC tool model essentially agreed with each other. For the "F" stability (Figure 5), the PEAC tool results essentially agreed with the SLAB model, but both SLAB and the PEAC tool predicted almost double protective action distances compared with ALOHA.

Figure 4: 2kg/s Chlorine Release, D Stability, Wind 5 m/s

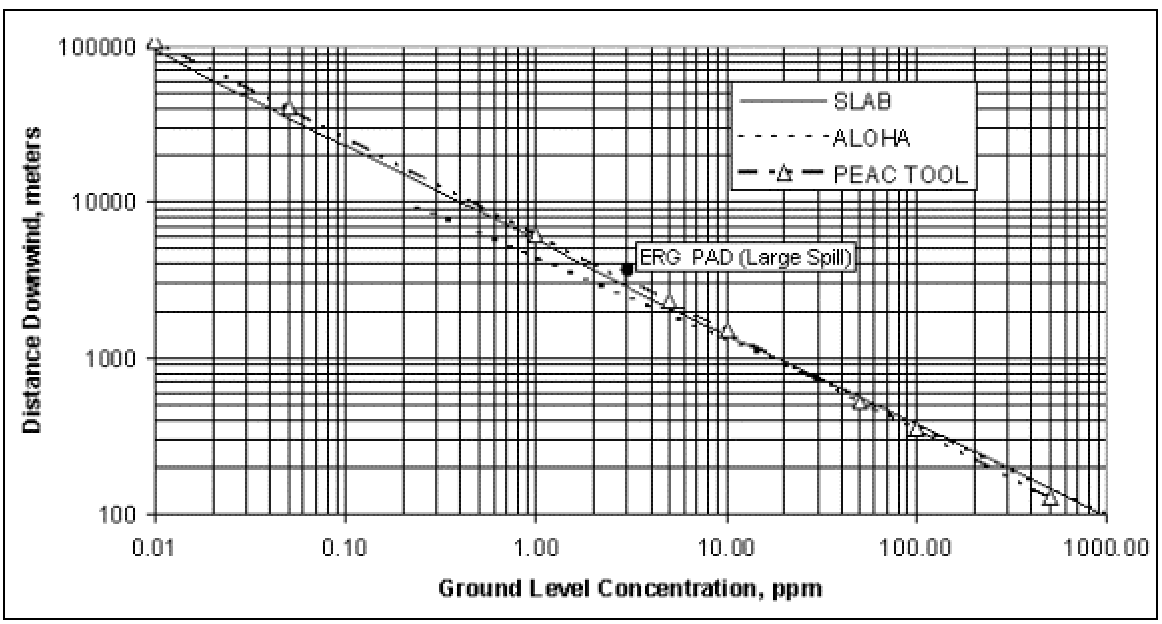
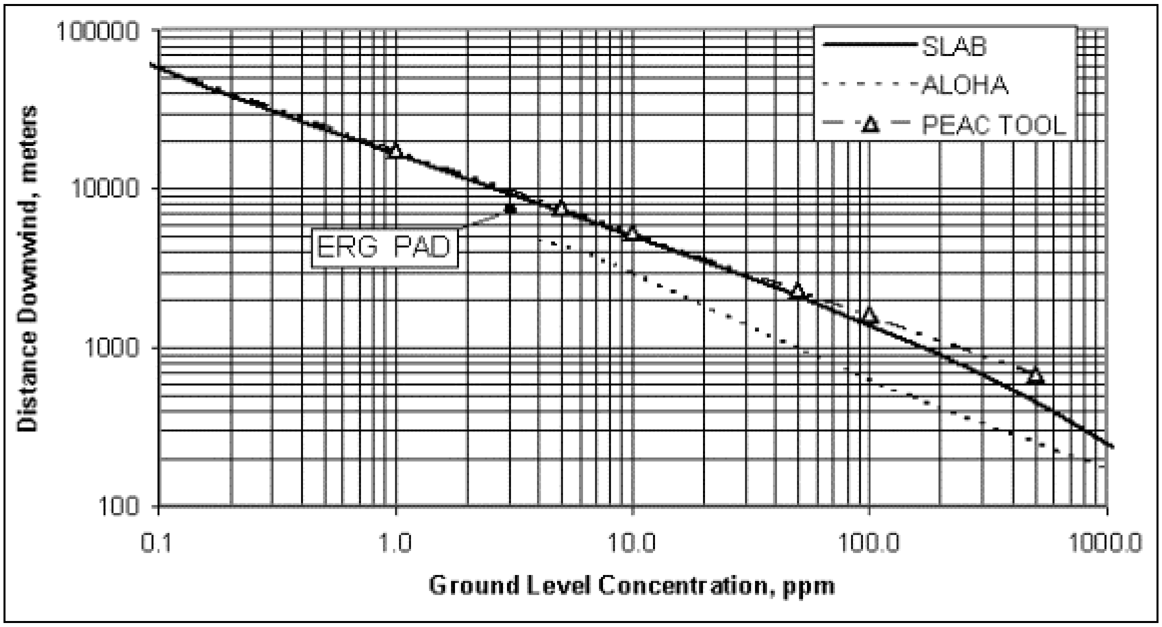


Figure 5: 2kg/s Chlorine Release, F Stability, Wind 1 m/s



There is no question that this is a large spill. The 2004 ERG lists the initial isolation zone at 240 m for large spills which compares with 1.5 km (daytime, D Stability) in Figure 3 and 5 km (nighttime, F stability) in Figure 4. The PAD for 3 ppm chlorine is set by the 2004 ERG at 1.2 km (daytime) and 7.4 km (nighttime) which is much less than what any of the models predict in Figures 3 and 4. The reason for the difference between 2004 ERG and the models lies in the definition of "large" with respect to transportation accidents. A sustained 2 kg/s release is highly unlikely in any transportation accident.

One of the largest spills of chlorine in recent U.S. history occurred on 6 January 2005 in Graniteville SC, when a 90 ton capacity chlorine tank car was breached in a train accident spilling roughly 70 or 75% of the tank contents before a seal could be placed on the tank. The release rate of chlorine could have been as much as 1 kg/s during the initial hour of the breach and then slowing down after the liquid remaining in the tank chilled and evaporated more slowly. There were several deaths from the toxic gas cloud. Critics said more people should have been evacuated.

Example 3: 2000 pounds instantaneous chlorine release at ground level

In this example, a 2000-lb chlorine tank releases all of its contents at once, for example, as the result of an explosion. The PEAC tool modeling is compared with ALOHA and SLAB for three different atmospheric stabilities: (1) "D" stability, with wind 5 m/s at 2 feet height, cloudy skies; (2) daytime "B" stability, with wind 2 m/s at 2 feet height, daytime, clear skies; and (3) nighttime "F" stability, with wind 1 m/s measured at the 2 feet height, and clear skies. A surface roughness of 0.1 m is used for all model runs. The amount released is 905.2 kg. All models including the PEAC tool operated in the dense gas mode.

The modeling results are displayed by Figures 6, 7, and 8. For the "D" and "B" stabilities, the models and the PEAC® tool essentially agree. For the "F" stability, the SLAB and ALOHA models disagree by almost an order of magnitude with the PEAC tool modeling predicting somewhat intermediate distances but closer to SLAB than ALOHA.

Figure 6: 2000 lb. Instantaneous Chlorine Release, D Stability, Wind 5 m/s

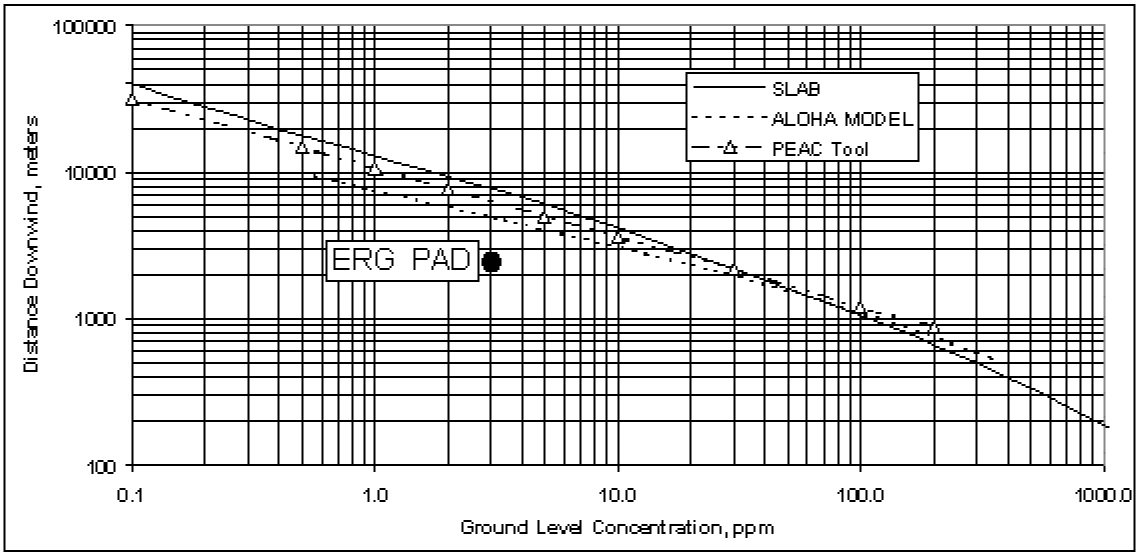


Figure 7: 2000 lb. Instantaneous Chlorine Release, B Stability, Wind 2 m/s

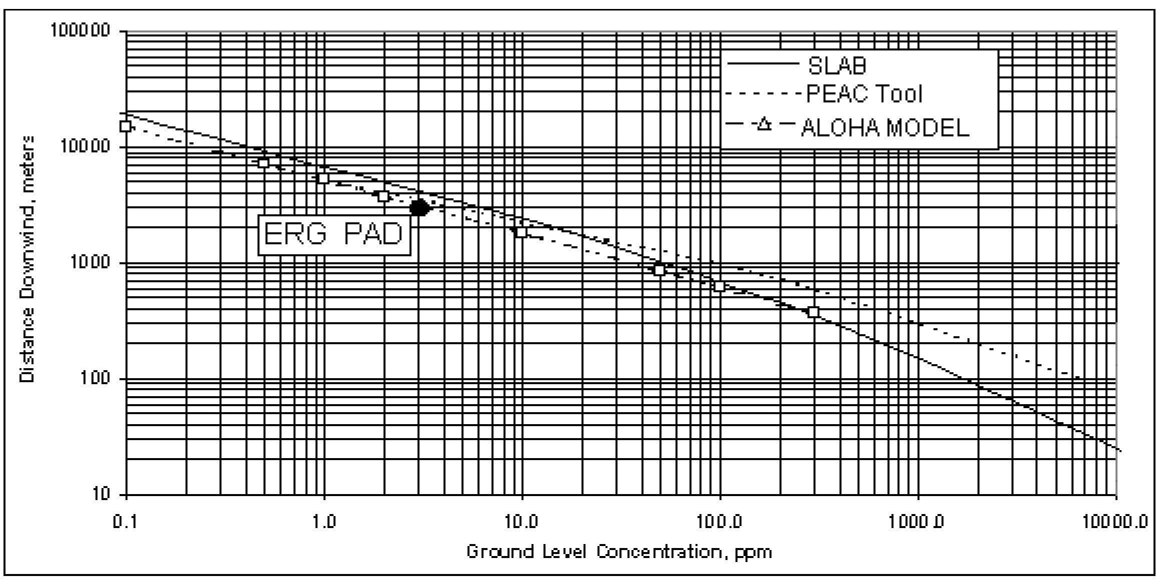
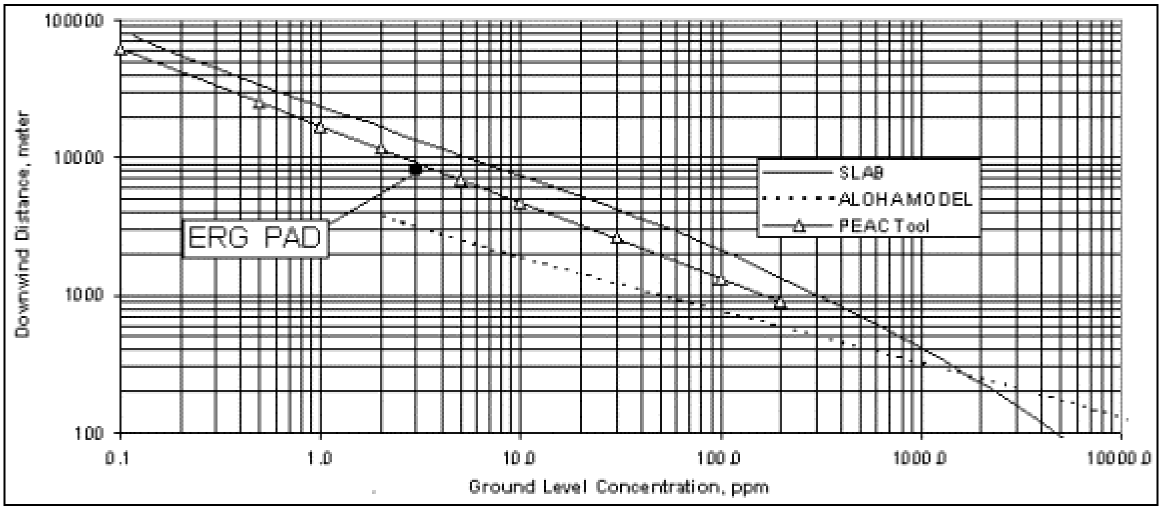


Figure 8: 2000 lb Instantaneous Chlorine Release, F Stability, Wind 1 m/s



Example 4: 2 kg SARIN evaporating in a pan in a 50°C environment

In this hypothetical example, 2 kg of liquid toxic nerve agent Sarin (also called GB) is placed in a shallow pan 0.49 m in diameter and is located at a spot where the air temperature is 50°C (e.g. an exhaust from a building). Sarin is unstable if heated at too high a temperature, but at 50°C no changes in chemical composition is assumed. During the daytime, with a wind speed of 5 m/s at a 2-m height, the PEAC tool model predicts an evaporation rate of 0.0003 kg/s. At night, with a wind speed of 1 m/s at the 2 m height, the PEAC tool model predicts an evaporation rate of 0.0001 kg/s. An "F" stability condition exists at night, and a "D" stability condition exists during the day. At an evaporation rate of 0.0001 kg/s, it will take 5.5 hours before the before the toxic chemical completely evaporates. The PEACtool model and the ALOHA model defaults to the passive mode. The dense gas model SLAB does not display results. There was some difficulty in running the ALOHA model, with warning messages saying that ALOHA does not predict accurately at very low concentrations. The results, graphed in Figures 9 and 10, show that the PEAC tool gives similar results to the passive models using either the Briggs' sigmas or the D2PC sigmas (with 10-minute averaging time for D2PC) and with ALOHA.

Figure 9: 0.0003 kg/s SARIN Release, D Stability, Wind 4 m/s

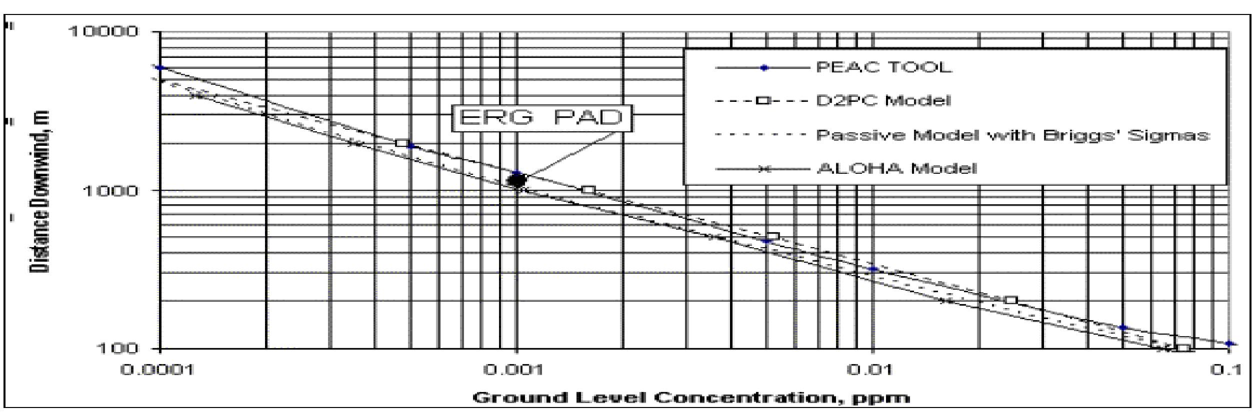
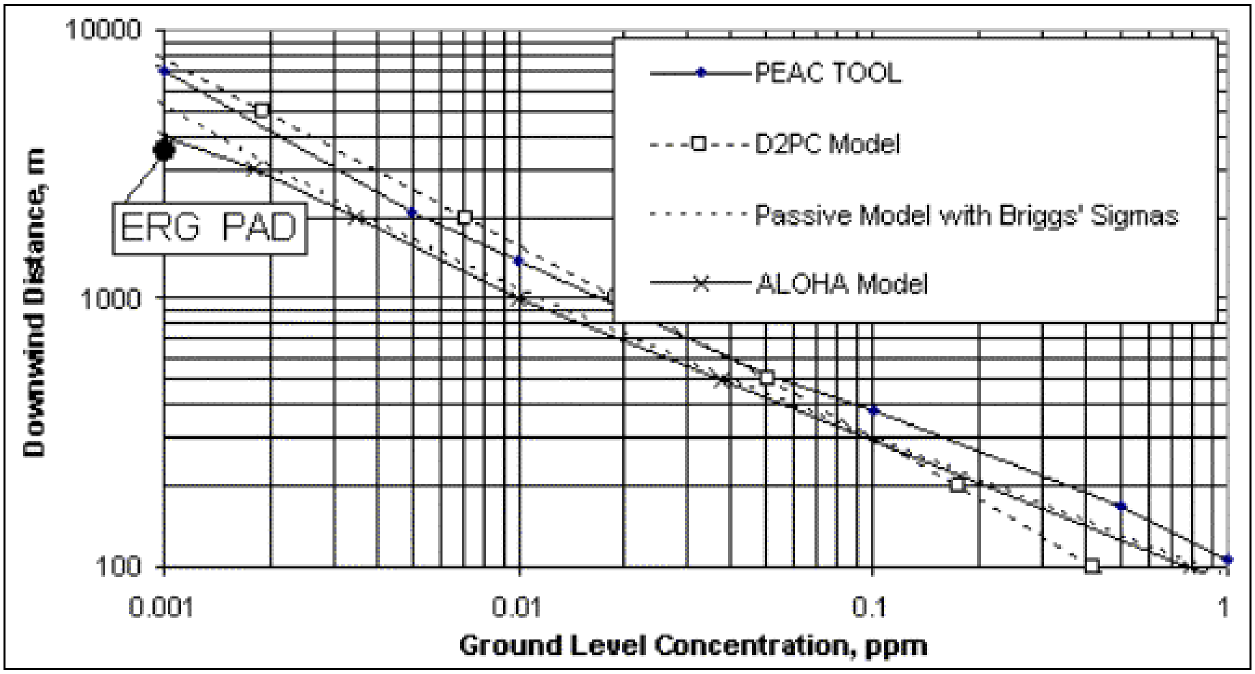


Figure 10: 0.0001 kg/s SARIN Release, F Stability, Wind 1 m/s



The various modeling results shown in Figures 9 and 10 gave very roughly the same results. The military D2PC model gave the most conservative results (e.g. greater PADs), and the ALOHA model gave the least conservative results. The PEAC tool gave an intermediate result, not too different from the classical passive model using Briggs sigma analytical expressions.

NIOSH (National Institute for Occupational Safety and Health) and OSHA have recently published (April 2005) interim values for IDLH and 8-hour worker exposure limits (Time Weighted Average, or TWA) for Sarin. The values are 0.01 mg/m^3 (0.00175 ppm) for IDLH and 0.00003 mg/m^3 (0.00000525 ppm) for the TWA worker exposure limit. Details are at the website (click here to see).

The 2004 Emergency Response Guidebook (Figure 1) recommends a 1.7 km PAD for daytime spills and 3.4 km for nighttime spills. The initial isolation zone is set at 150 meters. It is not clear what Levels of Concern were used by the 2004 ERG as NIOSH and OSHA published their values after the 2004 ERG was published but it is probably 0.001 ppm . The lethal concentration of Sarin in air for 1-hour exposure of laboratory test animals (rat) is 0.1 ppm, called the LC50 value. The PAD in the ERG is usually set at 1% of LC50 if a ERPG-2 value has not been published. The 1.7 km PAD for daytime in the 2004 ERG compares with about 1.2 km at 0.001 ppm in Figure 9. The 3.4 km PAD in the ERG for nighttime compares with 3 to 7 km at 0.001 ppm predicted by various models in Figure 10.

Fortunately, Sarin hydrolyzes (reacts with) moisture in the air over time producing less toxic byproducts. As the toxic cloud travels downwind , the Sarin will slowly disappear as the Sarin reacts with air moisture. Sunlight will hasten the destruction. The time frame for its disappearance is several days. The models do not account for the destruction of the Sarin chemical in the toxic cloud. The Sarin will still be potent during the initial release and for perhaps a few kilometers downwind, but after several kilometers, its concentration will be less than predicted by modeling. A good rainstorm will wash the chemical out of the sky.

The 2004 ERG lists Sarin (when used as a weapon). The container size used by the US Department of Transportation ERG modeling was 2 kg for a small spill, the same of what was used in our example. Usually when ERG uses the description “when used as a weapon” it means that the entire contents are released quickly as by an explosive device, but in our example the “terrorist” chose a different way of getting the Sarin liquid into the air, by evaporating it in a hot stream of air.

Conclusions

- The PEAC tool gas dispersion model gives comparable answers to other gas dispersion models in the public domain.
- No one model or methodology is necessarily better than any of the others examined. The military D2PC model appears to be more conservative. The ERG tables are quick and easily to use but do not allow the user to differentiate between container sizes or meteorology except by “day” or “night” or “large spill” or “small spill”.
- Models are different because they are formulated differently. They are different because the use different data sets to calibrate the models in their development. Data sets are easy to come by for the daytime, “D” stability condition which can be done in a wind tunnel simulation but are very difficult to obtain for the nighttime “F” stability condition. Air flow around objects and terrain complicate plume cloud dispersal.
- In an emergency response condition, the model must be kept simple. The user cannot be prompted for detailed information input which he/she does not have an answer. The model in the PEAC tool requests some basic information with default conditions (which can be overridden by the user).