

## INDUSTRIAL HAZARDS TO MILITARY PERSONNEL

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### ABSTRACT

The industrial chemical health threat to the US military is growing. The increasing threat is due both to the more frequent use of industrial chemicals and infrastructure as weapons of war and opportunity, and to recent military operations in urban and industrial environments where accidents or terrorism may cause large-scale chemical releases. Using traditional single-scenario modeling techniques, it is difficult to prospectively portray the complex array of potential chemical hazards associated with specific release scenarios, but some characterization of the potential chemical concentrations and areas affected is clearly an important consideration for all phases of military operational and medical planning. This paper discusses a technique for evaluating the risks associated with chemical hazards from large-scale chemical releases, and describes a process of statistical interpretation of iterative dispersion analyses that was created to permit improved quantification of the hazards. The technique allows thousands of hypothetical releases of toxic material to be statistically combined and assessed to allow graphical representation of the statistics for the potential hazard areas where pre-determined exposure guidelines for the chemical may be exceeded.

### INTRODUCTION

While chemical and biological (CB) weapons may be the most readily identifiable airborne hazard to military personnel, they generally involve known delivery systems with understood characteristics. Non-weaponized chemical hazards may also have devastating impacts on military operations, but the spectrum of these industrial chemical hazards is far larger, and the threat is ubiquitous. In the course of military operations in urban and industrial environments, industrial chemical releases could be caused by collateral damage, acts of sabotage or terrorism, or by accidents associated with improper facility operation. In any case, an assessment of the potential consequences of such a release and the areas likely affected are important both to the civilian population and to military personnel operating in the area.

The classic example of a major industrial accident is the 1984 Bhopal gas disaster. At approximately 12:15 am local time on December 3, 1984, an intermediate storage tank containing methyl isocyanate (MIC) at the Union Carbide India Limited (UCIL) plant in Bhopal, India experienced an over-pressure event, possibly as a result of sabotage (Kalelkar, 1988). The overpressure event was caused by the introduction of a large quantity of water

into a MIC storage tank. The water, which reacts exothermically with MIC producing methylamine and carbon dioxide, caused a pressure release valve to vent, with the ultimate release of 40 tons of MIC into the early morning atmosphere. The official finding was that roughly 3,800 people died, 11,000 were disabled, and 250,000 sought medical treatment (Mehta *et al.*, 1990); unofficial estimates were as high as 8,000 killed, 30,000 disabled, and 500,000 treated. Figure 1, taken from Sharan and Gopalakrishnan (1997), shows a schematic of the Bhopal region; the four contours indicate the parts per million isopleths extracted from Singh and Ghosh (1987) and are >50 ppm, >15 ppm, >1.5 ppm, and <1.0 ppm, respectively, for regions I through IV.

The threat from industrial chemicals derives from more than classical industrial accidents though, as the use of chemicals in military conflicts is increasing. For example, use of industrial chemicals as weapons was reportedly threatened against Serbian forces in the defense of Tuzla, and Serbian forces are reported to have intentionally targeted industries in Kutina and Sisak during the conflict with Croatia. Also, crude oil production facilities were intentionally targeted for use against US forces in both wars in Iraq. In 1990, the intentional release of crude oil by the retreating Iraqi military caused the worst oil spill in world history.

## ATMOSPHERIC DISPERSION

Atmospheric dispersion is a combination of advection (the bulk motion of an atmospheric contaminant due to the wind) and diffusion (the mixing of a contaminant with the surrounding air due, primarily, to turbulence). Dispersion is driven by two primary elements – the source and the meteorology. The source determines how much material was released and over what region and time scale; hence, it determines to a great extent the severity of the problem and the size of the region affected. Meteorology impacts the size of the hazard region produced, but more importantly, it determines the location of the risk area.

It is impossible to predict when in the future such an event might occur; this makes it impossible to know the atmospheric conditions at the time. One method of assessing the potential hazard is to simulate the bounding source events discussed above using a large number of past atmospheric conditions to generate a dispersion climatology. This requires a source of historical meteorological information (to be discussed in the modeling section). The results of all the dispersion simulations can then be analyzed statistically to produce the final product.

Industrial chemical releases, whether accidental or intentional, can have widely variable released mass and spatial and temporal distributions. This makes it necessary to consider extreme limiting cases such as an instantaneous (or short-term) release of a large inventory and a continuous (or long-term) leak. These bounding cases are constructed based on assessments of the on-site inventory and probable events.

For the dispersion calculation, a number of different models are available. The 1999 Directory of Atmospheric Transport and Diffusion Consequence Assessment Models compiled by the Office of the Federal Coordinator for Meteorology (OFCM, 1999) contains more than 60 models. There are two basic types of dispersion models: Gaussian and non-Gaussian. Gaussian models are based either explicitly or implicitly on Gaussian statistics, which, in turn, are based on an assumption of constant diffusivity. This assumption can be considered reasonable in two opposite limiting cases. The first is for short-range and short-

duration events where the assumption is that the diffusivity is relatively constant over the entire four-dimensional volume of the event. The second is for chronic or continuous releases where long-term (months or years) climatic averages are being determined, and the assumption is that the *average* diffusivity is relatively invariant. These models were developed using the statistics for power plant plumes involving continuous emissions over periods ranging from weeks to months. Gaussian models are further sub-divided into plume and puff models, the former typically based on uniform, constant wind and stability conditions and the latter varying in complexity from spatially and temporally invariant atmospheric conditions to using a full four-dimensional specification of the atmosphere.

Plume models require only a personal computer and are classically based on fixed, single point wind and stability, often determined by Pasquill-Gifford turbulence (PGT) categories (Gifford, 1976) using a Morton, Taylor, Turner (MTT) entrainment ratio (Morton *et al.*, 1956). These models do not consider changing meteorological conditions (either spatially or temporally) and tend to over-predict or under-predict the peak concentration in known ways. The archetypical plume model is the ALOHA (Areal Location Of Hazardous Atmospheres) model developed in the early 1980s by the National Oceanic and Atmospheric Administration (NOAA-HMRAD, 1992).

Puff models are the next level of sophistication, with numerous variations from single point wind and stability input with constant, uniform diffusion to four-dimensional wind / temperature input to second-order closure turbulence models producing not just a mean contaminant concentration but also the concentration variance. As a result, puff models run on computer platforms varying from personal computers to large workstations. Two examples of puff dispersion models are the Vapor, Liquid, Solid TRACKing (VLSTRACK) developed by the Naval Surface Warfare Center (NSWC) (Bauer and Wolski, 1992), and the Second-order Closure Integrated PUFF (SCIPUFF) model (Sykes *et al.*, 1993) contained in the Hazard Prediction and Assessment Capability (HPAC) of the Defense Threat Reduction Agency (DTRA, 1999).

The non-Gaussian models use a more general formulation that drives the diffusion of the contaminant from the local turbulence statistics. The non-Gaussian models typically are based upon a particle formulation and use a three- or four-dimensional specification of atmospheric conditions, in some cases computing the evolving wind field as well. These models typically advect particles through an atmosphere that changes in space and time using the mean wind, and diffuse the particles by adding in a turbulent velocity component derived from the local turbulence statistics. Pollution concentration fields then are determined diagnostically. In some formulations, the variance also is computed diagnostically. An example of a particle dispersion system is the Operational Multiscale Environment model with Grid Adaptivity (OMEGA), developed by the SAIC Center for Atmospheric Physics (Bacon *et al.*, 2000; Boybeyi *et al.*, 2001) with support from DTRA.

The more sophisticated the physics of the model, the more capable the resulting dispersion system; however, this improvement is accompanied by an increased computational burden and a need for more detailed initial and boundary information. For example, second-order closure turbulence models require information on the Reynolds stress, a measurement that is not made operationally, though some climatological data at isolated points exist.

Some models compute not only the mean concentration, but also the concentration variance. Two examples of this are a diagnostic model due to Wilson *et al.* (1982a,b) that is included in OMEGA, and the SCIPUFF model (Sykes *et al.*, 1986), which uses a prognostic equation for the concentration variance. The variance provides a measure of the expected uncertainty of the computed mean value and thus is an important contribution to the overall solution. A key issue, however, is whether the variance has meaning in the specific context. Most variance models were developed for continuous plumes or chronic applications where the use of long-term averages is warranted. In determining the statistics for acute or isolated releases, these averages are no longer appropriate and therefore could lead to poor decision-making.

For the purposes of *potential threat* screening, the exact details of the event, the atmospheric conditions at the time of the event, and the actual response of personnel to the event all are uncertain. Accordingly, only by running a large number of hypothetical scenarios can the potential threat can be bounded. Normally, for single event simulation, non-Gaussian models should be used, with Gaussian models restricted to short-range (less than 5-10 km) and short-duration (less than 1 hour) or long-term average situations; however, since these calculations are *for screening purposes only*, with the end results used only after statistical analysis, it is appropriate to use a Gaussian model to compute the many-identical event scenario.

## **RISK ASSESSMENT AND SHORT-TERM EXPOSURE GUIDELINES**

Classical risk assessment consists of an assessment of the probability of occurrence of an event and also of the event severity *should it occur*. The probability of occurrence can vary from frequent to unlikely; the severity may vary from catastrophic to negligible. These qualitative categories must be converted to quantitative values to enable the development of objective guidance tools for effective risk management.

In the methodology presented here, the goal is not to attempt to assess the probability of an airborne release of occurring. The goal is to define the geographic region over which short-term exposure thresholds may be exceeded in the event of a chemical release. Therefore, the probability considered here is related to the weather, and most significantly to the wind direction, which varies considerably over the course of a month, season, or year.

### ***Severity***

The severity of the health impact of a chemical release is determined by the magnitude of the airborne chemical concentration, the chemical toxicity, and the duration of the exposure. The assessment of the *severity* would best be assessed using predictive (as opposed to protective) concentration thresholds for a range of specific human health endpoints. Such thresholds, which would predict specific human health outcomes associated with specific exposures, have not been established for most chemicals, largely because of the complexity of the toxicological response, the lack of experimental data, and uncertainties regarding the use of laboratory animal data to predict human health outcomes. Absent that information, severity may be estimated using established short-term exposure guidelines, which provide conservative (safer) population thresholds associated with several severity classes of health effects. In this analysis, we chose to use the Military Exposure Guidelines (MEG); other

established short-term guidelines, including the Acute Exposure Guideline Levels (AEGLE; NRC, 2002), the Emergency Response Planning Guidelines (ERPG; Kelly and Cavender, 1988), and the Temporary Emergency Exposure Limits (TEEL; Craig and Lux, 1998), could also be used.

Military Exposure Guidelines are chemical exposure guidelines established by the US Army Center for Health Promotion and Preventive Medicine (USA CHPPM, 2003). The MEG levels used in this application are the 1-hour-air-MEGs, which are derived concentrations for chemicals in air that can assist in assessing the effect of exposures to chemical hazards for a healthy military population. The definitions of the MEG levels are:

- **Minimal** is the airborne concentration above which continuous exposure for 1 hour could begin to produce mild, non-disabling, transient, reversible effects, if any.
- **Significant** is the airborne concentration above which continuous exposure for 1 hour could begin to produce irreversible, permanent, or serious health effects that may result in performance degradation and incapacitation in a small portion of individuals.
- **Severe** is the airborne concentration above which continuous exposure for 1 hour could begin to produce life-threatening or lethal effects in a small portion of individuals.

### **Probability**

The goal of the method described here is to define the extent of the potential chemical hazard area resulting from a release in advance of the actual event. The underlying assumption is that while one will never know the meteorological conditions pertaining to a potential future event, a broad enough range of past conditions provides a reasonable approximation for the range of future conditions that may pertain. Thus, a statistical analysis of a specific release scenario under meteorological conditions existing over the previous 5 years, performed four times per day each day of the assessed meteorological season over that 5 year period, reflects the distribution of hazard areas likely to result from a future event unpredictable in time of occurrence. So, in this analysis we assume that an airborne chemical release occurs, and we compute the probability that any location may exceed a given short-term exposure level.

Airborne chemical releases generally fall into one of two categories: instantaneous or short-term releases, and continuous or long-term releases. The hazards posed by these two types of events are different; hence, the processes needed to evaluate them are different. Instantaneous events typically result in exposures of short duration with little warning or chance to take protective action. Continuous events occur over longer time periods, with potentially longer exposures, and risks can be mitigated in part by personnel movement or protective postures. For this reason, we treat long duration releases as a series of 1-hour events, effectively assuming that 1 hour is the maximum exposure time before protective measures are taken, and then take the maximum exposure for each location as our metric.

An example of a short-term event is the catastrophic failure such as the rupture of a small storage tank. In this case, a metric based on cumulative exposure may be the best representation of the hazard. On the other hand, for a leaking source, where detection and

response may cause personnel to relocate once the threat is present, it may be more realistic to use a 1-hour exposure estimate rather than the cumulative exposure. These exposures can be computed mathematically from the concentration as:

$$E_{\text{instantaneous}}(x, t) = \int_0^t d\tau C(x, \tau) \quad (1)$$

$$E_{\text{continuous}}(x, t) = \max \left\{ \int_{t-1hr}^t d\tau C(x, \tau) \right\} \quad (2)$$

where  $E(x, t)$  is the exposure and  $C(x, t)$  is the concentration, both as functions of space and time. In this case, Equation (1) specifies the total integrated exposure for short-term situations while (2) defines the 1-hour trailing exposure.

If we perform a series of simulations of an event using  $N$  different atmospheric conditions, then we can compute a set of metrics that span the  $N$  simulations. If each simulation produces a potential exposure  $E_i(x, t)$ , then we can compute the maximum, mean, and standard deviation of exposure for the  $N$  simulations that constitute the assessment set for the month, quarter, or year at any time after the event (since we do not know the event time):

$$E_{\text{Max}}(x) = \begin{cases} \max \{ E_i(x, \tau_{\text{Max}}) \forall i \} & (\text{instantaneous}) \\ \max \{ E_i(x, \tau) \forall i, \tau \} & (\text{continuous}) \end{cases} \quad (3)$$

$$\bar{E}(x) = \begin{cases} \frac{1}{N} \sum_i E_i(x, \tau) & (\text{instantaneous}) \\ \frac{1}{M} \cdot \frac{1}{N} \sum_i \sum_j E_i(x, j \Delta T) & (\text{continuous}) \end{cases} \quad (4)$$

$$\sigma_E(x) = \sqrt{\bar{E}^2(x) - \bar{E}^2(x)} \quad (5)$$

where  $M$  in Equation (4) represents the number of time-slices ( $\tau$ ).

These definitions show clearly that for instantaneous events it is only the final integrated exposure that matters, while for continuous events, the statistics must be computed over all simulations *and all times*.

These statistics each have advantages and disadvantages. The *maximum* represents the worst case that was seen in all of the simulations performed. This is an important consideration because outside of the region exceeding the minimum MEG level, if the input set of simulations is relatively large, risk should be minimal. On the other hand, the maximum could represent a true outlier event that may occur only once every few (or more) years. The *mean* provides a measure of the likely exposure, but since health effects typically require exceeding threshold levels of exposure, the mean may well provide little information of value by itself. The standard deviation provides a measure of variability at each point;

hence, it could be used in conjunction with the mean to generate a new measure ( $x + n \sigma_x$ ), where  $n$  typically is in the range from 1-5. However, this measure is subject to much interpretation.

A better metric is possible given the additional guidance provided by the threshold [MEG] levels – the percentage of cases that exceed these thresholds. This Probability of Exceedance (POE) metric is defined as:

$$P_{E_c}(x) = \frac{1}{N} \sum_i \begin{cases} 0 & E_i(x) < E_c \\ 1 & E_i(x) \geq E_c \end{cases} \quad (6)$$

where the summation is over all simulations *and all times*. The POE for any location is thus the percentage of cases for which the 1-hour exposure exceeds a given threshold (for example, the MEG levels). The POE is a better representation of risk than the maximum because it provides a specific measure of frequency. The maximum contour provides no information on the frequency of occurrence; on the other hand, outside the 1% POE for Minimal-MEG, there is a 99% confidence level that the Minimal-MEG will not be exceeded.

The POE metric can be displayed with variation in two parametric dimensions – the [MEG] exposure level (minimal, significant, severe) and the probability of exceedance. These two dimensions equate to severity and probability and hence provide information on the potential risk. A useful combination of graphics is shown in Figure 2 for a generic location with flat terrain involving a large (more than 10 MT) release of ammonia over a period of 12 hours. The minimal, significant, and severe 1 hour air MEG levels for ammonia are 1020, 4,620, and 45,960 mg-min/m<sup>3</sup>, respectively. The left side of the figure shows the 1% POE for the Minimal, Significant, and Severe MEG and implies that outside of these regions, there is a 99% confidence that the respective level will *not* be exceeded. The right side of the figure shows the 1% POE for the Significant MEG with overlays showing the 5% and 20% POEs. How these figures are generated is the subject of the remainder of this paper.

## THE CHEMICAL HAZARD ASSESSMENT MODELING PROGRAM

To compute the statistics discussed above, a large number of simulations must be performed automatically, in a hands-off setting. The VLSTRACK model (Bauer and Wolski, 2001), which supports command-line and batch operation, as well as operations under Windows™ and Unix, was selected as the initial dispersion model. In addition, a PC cluster computer was created to speed execution of the hundreds and thousands of simulations required to create the final POE product.

As previously mentioned, dispersion is driven primarily by the source term and by the meteorology. While VLSTRACK supports batch operation, the assembling of all of the required input files can still take a considerable amount of time. The system presented here provides the infrastructure to automate these tasks and to analyze the results of all of the simulations.

The overall control system is called the Chemical Hazard Assessment Modeling Program (CHAMP). It provides a single dialog from which the various automation functions can be called (*cf.*, Figure 3). These functions include the extraction of the meteorological

data, the generation of the source term, the creation of all of the VLSTRACK parameter input files, the statistical analysis, and the auditing functions. (In addition, CHAMP creates its output files in the format appropriate to the Windows™ or Unix operating system that is planned for use.) Each of these will be discussed in turn below.

### ***Meteorology***

For threat assessment purposes, it is impossible to know all possible combinations of the type of the event, the toxic material involved, the atmospheric conditions during and following the release, and the time of exposure. Accordingly, a predictive risk assessment requires exploring the *spectrum* of risks under different assumptions, including variable meteorological conditions, by performing a large number of analyses using historic or climatologic data. This assumes that *the past is prologue*, and uses archived meteorological data to explore what would have been the risk area if the event had occurred at some time in the past; a further assumption is that the weather patterns are such that this will be the hazard area for a future event.

The climatologic dataset selected for use in this system is the 40-year Reanalysis Project dataset (Kalnay *et al.*, 1996), which has recently been extended to a 50-year climatology (Kistler *et al.*, 2001). This joint venture between the National Centers for Environmental Prediction (NCEP) and the National Center for Atmospheric Research (NCAR) provides analyses on a roughly 1.9° grid four times a day (0000, 0600, 1200, and 1800). A 10-year extract of this data was converted to the OMEGA Packed Binary (PKB) data format that allows for direct access to the data. A routine then was developed to access and extract this data in the VLSTRACK *time-variable* and *height-time variable* meteorological data formats. This routine allows the user to put in a location (latitude / longitude), a period of time (start / stop), a duration for each output file, and the frequency of the files. The appropriate data is then accessed and the VLSTRACK formatted files are automatically written to the appropriate directory. A log file is also produced that is used by the audit sub-system in compiling all of the information about a particular analysis. This log file also contains statistical information on the surface winds, specifically, the direction probability of occurrence in 10 degree bins, formatted such that a wind direction distribution graphic (*cf.*, Figure 4) can be quickly created. In addition, a 4-bin wind speed histogram and the average surface temperature and wind speed are computed.

The VLSTRACK meteorology input files require additional information beyond that available in the Reanalysis Project climatology. Specifically, VLSTRACK requires information on the land surface type, the cloud cover, and the PGT index. As part of developing the overall system, the USGS 1 km land use data was coupled to the meteorological data extraction routine, with the 99 USGS land use categories mapped to the 12 VLSTRACK surface types. Additionally, a cloud algorithm, based upon the dewpoint depression throughout the vertical column of the location, was created. Finally, an algorithm to compute the PGT stability class was developed. The end result is an automated system that can extract an entire year of meteorological (.MET) files (365 days × 4 times / day for a total of 1460 files) in less than 3 minutes.

### ***Source Term***

VLSTRACK was developed for chemical and biological weapon purposes, and accordingly, its source term generator does not consider industrial sources. The VLSTRACK

model, however, will accept a *Puff Property Input* file that specifies a set of initial puffs. Each initial puff specification contains mass of the contaminant, the horizontal ( $x$ ,  $y$ ) and vertical offset from the target point, the time of the puff release relative to the start time of the simulation, the horizontal and vertical spatial standard deviations of the puff ( $\sigma_h$ ,  $\sigma_v$ ), and particle size information (for liquid and solid releases). CHAMP includes a routine to produce these Puff Property Input (.POS) files (*cf.*, Figure 5) that provides control over the amount of material released and the spatial and temporal distribution of that release. The user supplies the total amount of released material (typically based on a site assessment and some assumptions about the scenario), the release duration, and the spatial extent (horizontal and vertical) of the source. Since one of the biggest industrial hazards is the breach of a cryogenic ammonia or chlorine storage tank, CHAMP includes a cryogenic pool calculator to assist in determining the hazard from these facilities (*cf.*, Figure 6). This routine simplifies the creation of .POS files with uniform or Gaussian distributions of puffs over either elliptic or rectangular areas, and also generates a log file containing all of the user inputs.

### ***Parameter Input Files***

The primary control file for VLSTRACK is the *Parameter Input* (.DAT) file. This file links the location information with the source specification (as specified in the .POS file), the meteorology (as specified in the .MET file), and other user input, such as the output options and times. Since the source term for these analyses are always specified via the Puff Property Input file, only a limited amount of user information is required to create the Parameter Input files. The DAT routines of CHAMP provide an easy method for accepting this limited user input and creating the hundreds of Parameter Input files (as well as the single BATCH.DAT file required for automated execution of the Windows™ version of VLSTRACK). This routine also requires the user to input a standard reference number that will be used to associate the analysis with a specific industrial facility. The DAT routine also serves an important role in the analysis, audit, and housekeeping functions of the system. The standard reference number is used to build the file list that will be used for the analysis and links the facility with the end product. This file also becomes the key starting point for the audit subsystem. Finally, DAT creates a script to gather all the results of the analysis from the 13 directories over which they are scattered by VLSTRACK and consolidate them into a single directory for archival purposes. (It also creates a script to redistribute them for further analysis.)

### ***Cluster Computing***

Because a large number of runs are required to achieve reasonable statistics and confidence bounds, a PC cluster computer was built specifically to support this requirement. The cluster consists of 14 nodes each with dual AMD Athlon CPUs running Linux. Since each run is independent, conventional Gigabit interconnections were used between the boxes rather than a more expensive low-latency network. The UNIX version of VLSTRACK was compiled on this machine and a set of scripts were created to distribute the runs over a specified number of processors, execute them, and collect the results afterward. The Linux cluster is connected to a Windows™ PC that is used for the front and back end processing.

A small chemical release problem, involving the short-duration release of a modest amount of a toxic material may take only 1-2 minutes of computation for each run; nevertheless, this translates into many hours to compute 5 years of cases for a given

meteorological quarter for statistical analysis. For example, the spring meteorological quarter – March, April, May – consists of 92 days, hence 5 years of simulations using each of the 4 analysis times equates to 1,840 cases; at 2 minutes per run, these 1,840 cases would take more than 60 hours. The 28 processor cluster reduces this time to roughly 2-3 hours. Even large cryogenic releases that may require 1 hour for each simulation can be run in a few days.

To execute the large number of simulations, the meteorological (.MET), puff property (.POS), and parameter (.DAT) input files are transferred from the Windows™ front-end machine to the Linux cluster. The user then executes a C-shell script that distributes all of the simulations across the 14 nodes. A series of scripts then ensures that a run is assigned to each CPU with a new run starting as each executing run completes. Scripts also have been written to check the status of the executing runs and to collect all of the output from the individual nodes for transfer back to the front-end machine for statistical analysis.

### *Statistics Generation*

Each of the component VLSTRACK simulations is performed using a self-adjusting grid with dimensions of  $101 \times 101$  grid points (actual dimensions vary with each run). VLSTRACK adjusts the grid lower left corner ( $x_o$ ,  $y_o$ ), the grid orientation ( $\theta$ ), and the grid resolution ( $Dx$ ,  $Dy$ ) to keep the plume in the grid (Figure 7). The statistics post-processing routine first composites the domains of all input VLSTRACK simulations to define the bounding box (the dotted box in the left panel of Figure 8). A new analysis grid then is created with dimensions of  $501 \times 501$  grid points that captures the region spanned by 99 percent of the MEG exposure regions. Using this analysis grid, CHAMP computes the maximum, mean, and standard deviation for all cases as well as the percentage of cases for which the exposure exceeds the [MEG] levels input by the user.

The statistics are output by CHAMP in several formats. First, they are output in an identical format as the usual VLSTRACK grid files. This allows the use of the VLSUTIL graphics post-processor for VLSTRACK. VLSUTIL permits the generation of contour plots for user-specified contour levels and also the export of these graphics in a variety of formats including the ArcView™ shape file format for import into the ArcMap™ common mapping format. Second, the results of the statistical analysis are output directly into shape files, one each for the event location, three user-selected contours of the maximum value, and three user-selected contours of the probability of exceeding each of the three specified levels.

To illustrate this process, the 30 minute blow-down of a pressurized chlorine tank containing 2,500 kg of chlorine was assumed to occur during the spring in a generic location with flat terrain. A total of 1,840 VLSTRACK simulations were performed using 0000Z, 0600Z, 1200Z, and 1800Z meteorological data from 5 years (1996-2000, inclusive) of meteorological spring (March, April, May). Figure 9 shows the 1% POE for the Minimal (magenta), Significant (orange), and Severe (red) MEGs, respectively, on the left and the 1% (magenta shading), 5% (yellow contour), and 20% (magenta contour) POE for the Significant MEG on the right. The minimal, significant, and severe 1 hour air MEG levels for chlorine are 90, 348, and 3480 mg-min/m<sup>3</sup>, respectively.

These products provide a considerable amount of information in a readily acceptable format. The region outside of the 1% Probability of Exceedance (POE) contour for a specified exposure level has a 99% confidence factor that the exposure level will not be exceeded. Thus the 1% POE graphic depicts the 99% confidence level for non-exposure at

the Minimal, Significant, and Severe MEG levels. The 1%, 5%, and 20% POE for the Significant-MEG provide information on the gradient in probability space so that the unit commander can understand if increasing the probability level decreases the area significantly. **It is important to remember that this represents the probability that a certain location would be affected if an event were to happen. Accordingly, the true probability also must consider the potential for the event to occur in the first place.**

### *Audit Functionality*

The fact that hundreds or thousands of individual simulations are necessary to generate the final product makes it critical that the chain of steps be documented. The audit function collects all of the information on the meteorology used, including the location of the actual meteorological analysis point, the material and its properties, the source term including the amount, duration, and geometry, the analysis methodology, and additional comments and audit information (*cf.*, Figure 10). All of this information then is written into a text file.

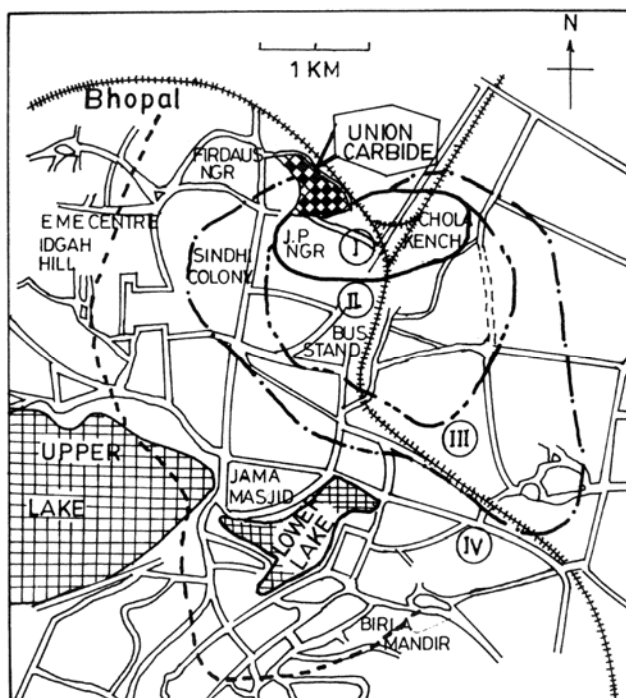
## CONCLUSIONS

We have developed an analytical method to prospectively define the probabilistic distribution of the geographic extent of the potential hazard area associated with a large-scale release of an industrial chemical. This method *assumes* that an event does occur, and computes the exposure using historic weather data to determine the statistical likelihood that any given location exceeds a specified set of threshold exposure values. A system to execute this method was constructed based on the VLSTRACK dispersion model consisting of both additional software – CHAMP – that simplifies the configuration, execution, and analysis of hundreds or thousands of VLSTRACK simulations, and hardware – a 14-node, 28-CPU PC cluster running Linux – that greatly reduces the clock time for completion of the simulations.

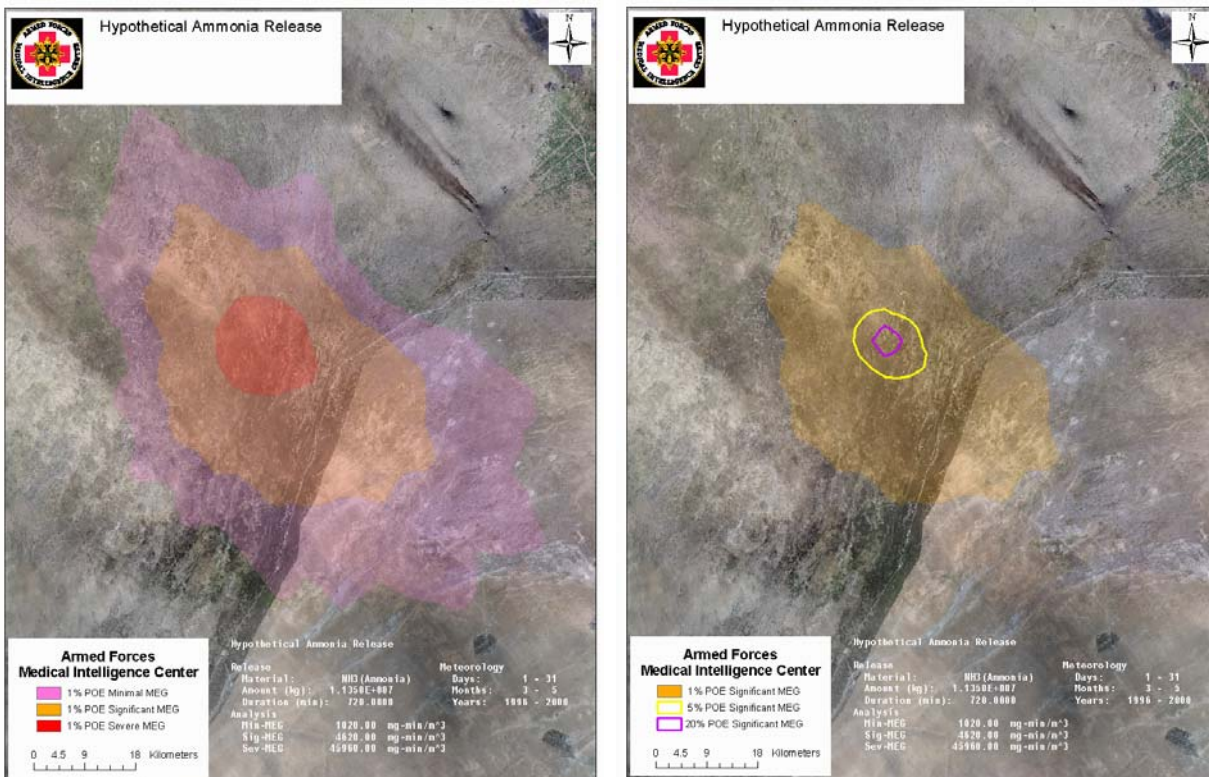
The methods described here allow us to estimate the area where short term exposure guidelines might be exceeded in the event of a large-scale chemical release. This information is useful for predeployment operational planning to allow avoidance of chemical hazards. In addition, this method of statistical representation of iterative dispersion analysis may prove useful for civilian risk management efforts, allowing probabilistic risk area assessment for either short or longer term releases to complement existing worst case scenario analyses.

In the future, the system could be enhanced by introducing high spatial and temporal resolution climatologic data for specific sites and also automatic generation of seasonal and annual statistics.

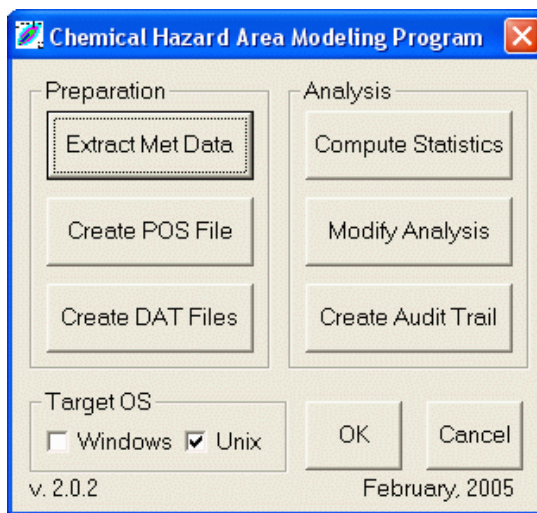
## FIGURES



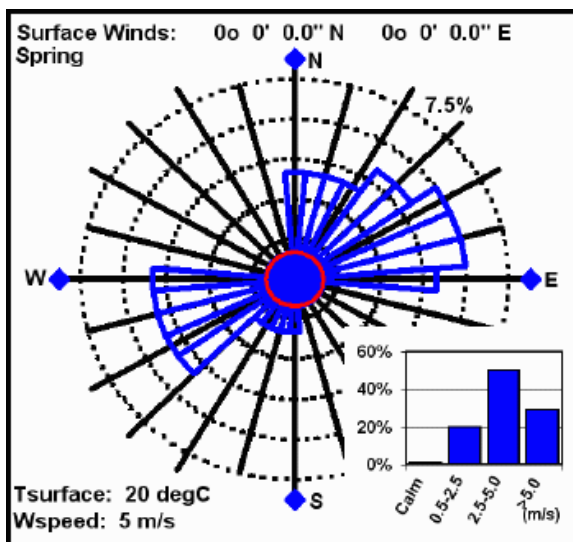
**Figure 1.** The Bhopal gas disaster killed thousands and caused hundreds of thousands of people to seek medical treatment. (Figure taken from Sharan and Goplakrishnan (1997)).



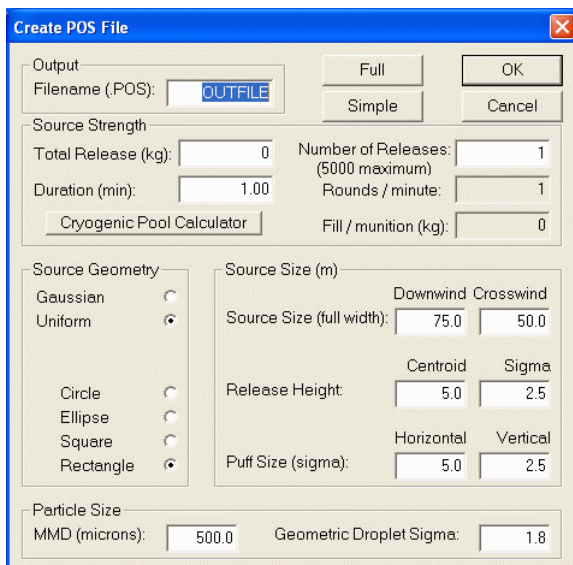
**Figure 2.** The 1% Probability of Exceedance (left) for the Minimal (magenta), Significant (orange), and Severe (red) MEG levels and the (right) 1%, 5%, and 20% POE for the Significant MEG (orange shading, yellow contour, and red contour, respectively) for a hypothetical large ammonia release (more than  $10^7$  kg released over 12 hours).



**Figure 3.** Primary CHAMP Dialog



**Figure 4.** The CHAMP meteorological data extraction routine also computes the wind direction statistics (blue arcs) in 10 degree bands (the red circle is the probability of calm winds), and a histogram of the wind speed. In addition the average surface temperature and wind speed are computed.



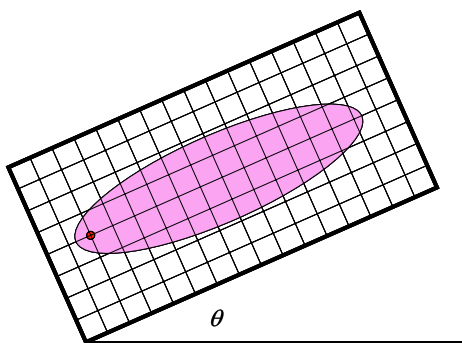
**Figure 5.** Create POS File Menu

The image shows a software window titled "Cryogenic Pool Evaporation" with a standard Windows-style title bar (minimize, maximize, close buttons). The window contains several input fields and buttons for calculating evaporation parameters. The "Material" dropdown is set to "NH3(Ammonia)" and the "Surface" is set to "Concrete / Sand".

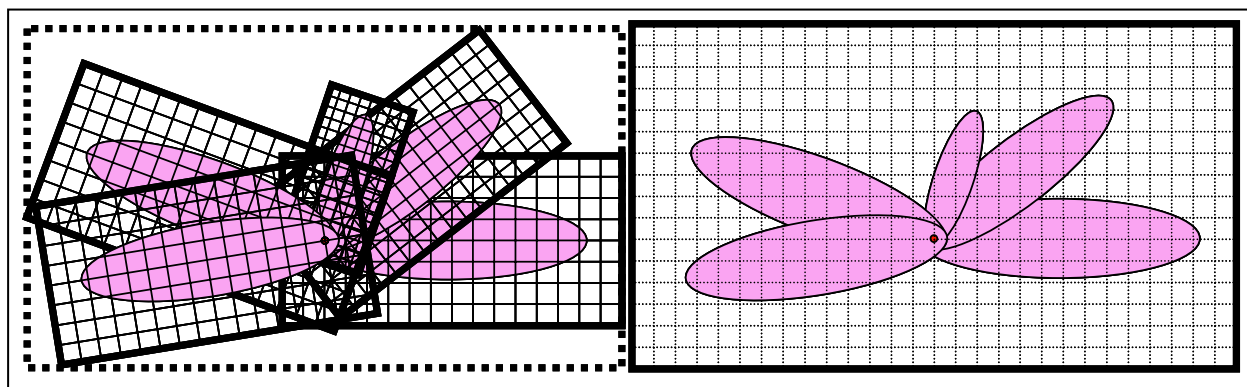
Section	Parameter	Value
Physical Properties	Liquid Density (g / cc):	0.602
	Heat of Vaporization (MJ / kg):	1.370
	Boiling Point (C):	-33.33
	Density (kg / m <sup>3</sup> ):	1600.0
Physical Properties	Heat Capacity (J / kg-K):	800.0
	Thermal Conductivity (W / m-K):	0.300
	Ground Temperature(C):	0.00
Mensuration	Release Volume (ML):	0.000
	Dike Length (m):	10.0
	Width (m):	10.0
Ambient Conditions	Air Temperature (C):	0.00
	Wind Speed (m / s):	5.00
	BL Depth (m):	10.00
Total Release (kg):		0
Evaporation Times (hr) - Ground Heat:		0
Air Heat (hr):		0

Buttons for "OK" and "Cancel" are located to the right of the "Ambient Conditions" section.

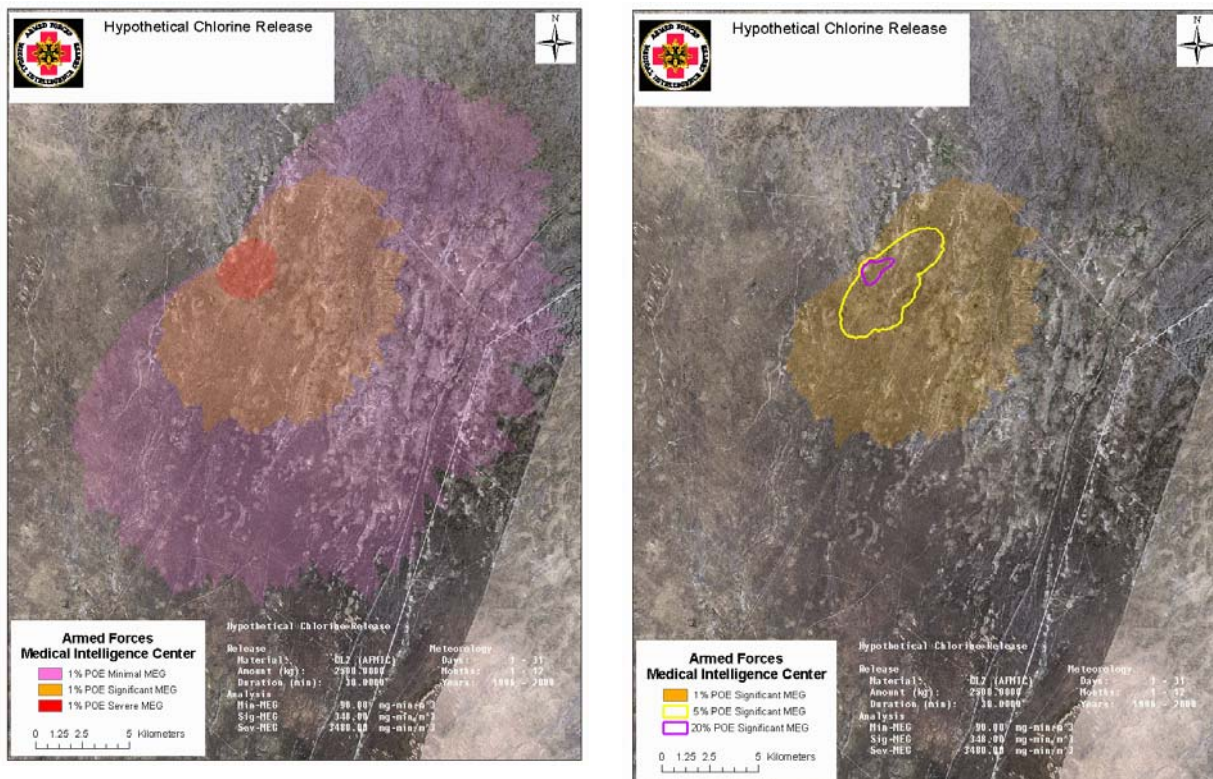
**Figure 6.** Cryogenic Pool Calculator



**Figure 7.** The self-adjusting VLSTRACK grid maintains the plume in its domain.



**Figure 8.** To analyze a large number of VLSTRACK simulations, it is first necessary to make an overlay of the input VLSTRACK grids (left) and find the *bounding box* (dotted line). A new *analysis grid* (right) is then created and used to compute the statistics by computing the interpolated value of each component run at each analysis grid point, then computing the maximum, mean, standard deviation, and the percentage of cases that exceeded specified threshold exposure levels (typically the MEG levels).



**Figure 9.** The 1% Probability of Exceedance (left) for the Minimal (magenta), Significant (orange), and Severe (red) MEG levels and the (right) 1%, 5%, and 20% POE for the Significant MEG (orange shading, yellow contour, and magenta contour, respectively) for a hypothetical chlorine release (2,500 kg released over 30 minutes).

**Audit**

Analysis Name  
LOG File: 1234567-0001-0001-STAT.LOG

Case Name  
DAT File: test0001.DAT # GRD Files: 1000

Meteorological Data  
Met Location: 19° 59' 58.2" N 70° 18' 45.0" E  
Start - Stop Year/Month/Day: 1996 - 2000 / 01 - 12 / 01 - 31  
Analysis Times: 0000 0600 1200 1800  
Months: FULL YEAR  
Met File Type: 2 / Altitude Mode: 0  
Sfc / PGT / Cloud Flags: -1 / -1 / -1  
Offset (km): 71.89

Quantity / Temporal - Spatial Distribution  
Output Mode: FULL  
Total Release (kg): 2500.0000  
Number of Releases: 100  
Duration (min): 5.000  
Distribution: UNIFORM  
Geometry: RECTANGLE  
Downwind Munition Spread (m): 50.00  
Crosswind Munition Spread (m): 25.00  
Release Height / SigmaZ (m): 2.50 / 2.50  
Puff SigmaXY / SigmaZ (m): 10.00 / 2.50  
MMD / SigmaMMD: 500.00 / 1.80

Material  
Cl2 (AFMIC)  
'Cl2 (AFMIC)' 'Cl2' 3 2.54 100. 350.0 2.00 -34.6 'Cl2'  
0.0019 4.30e9

Facility Information  
BESuffix: 1111-02222  
Surrogate Key: 10001000 1234567  
Tank ID / Scenario: 0001 / 0001  
Latitude: 20° 0' 0.0" N  
Longitude: 71° 0' 0.0" E

Analysis Configuration  
NX, NY: 501 501  
MODE: CUMULATIVE  
Min-MEG 90.0000 mg-min/m<sup>3</sup>  
Sig-MEG 348.0000 mg-min/m<sup>3</sup>  
Sev-MEG 3480.0000 mg-min/m<sup>3</sup>  
EXCEEDANCE PROBABILITIES  
1.000 5.000 7.500 20.000 33.000

Comments  
Summary Title

Audit  
Analyst: DPB  
Date: January 25, 2005  
PR Log #: 0000

**Figure 10.** The CHAMP Audit system collects all information relating to the meteorology, material, source, analysis, and additional commentary.

## REFERENCES

- Bacon, D. P., N. Ahmad, Z. Boybeyi, T. Dunn, M. S. Hall, P. C. S. Lee, A. Sarma, M. D. Turner, K. T. Waight, S. H. Young, and J. W. Zack, 2000. A Dynamically Adapting Weather and Dispersion Model: The Operational Multiscale Environment model with Grid Adaptivity (OMEGA), *Mon. Wea. Rev.* **128**, 2044-2076.
- Boybeyi, Z. and D. Bacon, 1996. The accurate representation of meteorology in mesoscale dispersion models, in *Environmental Modeling – Vol. 3 (Computer Methods and Software for Simulating Environmental Pollution and its Adverse Effects)*, P. Zannetti, Ed., Computational Mechanics Publications, Southampton.
- Bauer, T., and M. Wolski, 2001. Software User's Manual for the Chemical / Biological Agent Vapor, Liquid, and Solid Tracking (VLSTRACK) Computer Model, Version 3.1. US Naval Surface Warfare Center, Systems Research and Technology Department, NSWCDD/TR-01/83.

- Boybeyi, Z., N. N. Ahmad, D. P. Bacon, T. J. Dunn, M. S. Hall, P. C. S. Lee, R. A. Sarma, and T. R. Wait, 2001. Evaluation of the Operational Multiscale Environment Model with Grid Adaptivity against the European Tracer Experiment. *J. Appl. Met.* **40**, 1541–1558.
- Craig, D. K., and C. R. Lux, 1998. Methodology for Deriving Temporary Emergency Exposure Limits (TEELs). Westinghouse Savannah River Company, WSRC-TR-98-00080, Aiken, SC 29808.
- DTRA, 1999. Hazard Prediction and Assessment Capability (HPAC) User's Guide Version 3.2. Defense Threat Reduction Agency, HPAC-UGUIDE-01-U-RAC0.
- Gifford, F. A., 1976. Turbulent Diffusion – Typing Schemes: A Review. *Nuclear Safety*, **17**, 71.
- Kalelkar, A. S., 1988. Investigation of Large-Magnitude Incidents: Bhopal as a Case Study. Arthur D. Little, Inc., Cambridge, MA, May, 1988.
- Kalnay, E., M. Kanamitsu, R. Kistler, W. Collins, D. Deaven, L. Gandin, M. Iredell, S. Saha, G. White, J. Woollen, Y. Zhu, A. Leetmaa, B. Reynolds, M. Chelliah, W. Ebisuzaki, W. Higgins, J. Janowiak, K.C. Mo, C. Ropelewski, J. Wang, Roy Jenne, Dennis Joseph, 1996. The NCEP/NCAR 40-Year Reanalysis Project. *Bull. Am. Met. Soc.*, **77**, 437–472.
- Kelly, D. P. and F. L. Cavender, 1988. Emergency Reponse in Encyclopedia of Toxicology, Vol. 1. P. Wexler, Ed. Academic Press, San Diego, 527-531.
- Kistler, R., E. Kalnay, W. Collins, S. Saha, G. White, J. Woollen, M. Chelliah, W. Ebisuzaki, M. Kanamitsu, V. Kousky, H. van den Dool, R. Jenne, M. Fiorino, 2001. The NCEP-NCAR 50-Year Reanalysis: Monthly Means CD-ROM and Documentation. *Bull. Am. Met. Soc.*, **82**, 247–268.
- Mehta, P. S., A. S. Mehta, S. J. Mehta, and A. B. Makhijani, 1990. Bhopal tragedy's health effects. A review of methyl isocyanate toxicity. *JAMA*, **264**, 2781-2787.
- Morton, B. R., Taylor, G. I., and Turner, J. S., 1956. Turbulent Gravitational Convection from Maintained and Instantaneous Sources. *Proc. Roy. Soc. (London) Ser. A.*, **234**, 1-23.
- National Research Council, Committee on Toxicology, 2002. Acute Exposure Guideline Levels (AEGs) for Hazardous Substances, Volume 2. National Academy Press, Washington, DC.
- NOAA-HMRAD, 1992. ALOHA (Areal Locations of Hazardous Atmospheres), 5.0 Theoretical Description. National Oceanic and Atmospheric Administration, Hazardous Materials Response and Assessment Division, Contribution No. HMRAD 92-5 (draft).
- OFCEM, 1999. Directory of Atmospheric Transport and Diffusion Consequence Assessment Models. Office of the Federal Coordinator for Meteorological Services and Supporting Research, FCM-3-1999.

- Sharan, M. and S. G. Gopalakrishnan, 1997. Bhopal gas accident: A numerical simulation of the gas dispersion event. *Env. Modeling & Software*, **12**, Nos. 2-3, 135-141. Elsevier Science Ltd.
- Singh, M. P. and Ghosh, S. 1987. Bhopal gas tragedy: Model simulations of dispersion scenario. *J. Hazardous Materials*, **17**, 1-22.
- Sykes, R. I., S. F. Parker, D. S. Henn, and W. S. Lewellen, 1993. Numerical Simulation of ANATEX Tracer Data Using a Turbulence Closure Model for Long-Range Dispersion. *J. Appl. Met.*, **32**, 929-947.
- Sykes, R. I., W. S. Lewellen, and S. F. Parker, 1986. A Gaussian Plume Model of Atmospheric Dispersion Based on Second-Order Closure. *Journal of Climate and Applied Meteorology*, **25**, 322-331.
- USA CHPPM, 2003. Chemical Exposure Guidelines for Deployed Military Personnel, US Army Center for Health Promotion and Preventative Medicine, USA CHPPM TG 230.
- USA Field Manual 100-14, 1998. Risk Management. Headquarters, Dept. of the Army, Washington, DC.
- Wilson, D. J., A. G. Robins, and J. E. Fackrell, 1982a. Predicting the spatial distribution of concentration fluctuations from a ground level source. *Atmospheric Environment*, **16**, 497-504.
- Wilson, D. J., J. E. Fackrell, and A. G. Robins, 1982b. Concentration fluctuations in an elevated plume: a diffusion-dissipation approximation. *Atmospheric Environment*, **16**, 2581-2589.