AN AUTOMATED SHELL FOR MANAGEMENT OF PARAMETRIC DISPERSION/DEPOSITION MODELING

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ABSTRACT

In 1993, the U.S. Army tasked Argonne National Laboratory to perform a study of chemical agent dispersion and deposition for the Chemical Stockpile Emergency Preparedness Program using an existing Army computer model. The study explored a wide range of situations in terms of six parameters: agent type, quantity released, liquid droplet size, release height, wind speed, and atmospheric stability. A number of discrete values of interest were chosen for each parameter resulting in a total of 18,144 possible different combinations of parameter values. Therefore, the need arose for a systematic method to assemble the large number of input streams for the model, filter out unrealistic combinations of parameter values, run the model, and extract the results of interest from the extensive model output.

To meet these needs, Argonne National Laboratory designed an automated shell for the computer model. The shell processed the inputs, ran the model, and reported the results of interest. By doing so, the shell compressed the time needed to perform the study and freed the researchers to focus on the evaluation and interpretation of the model predictions. The results of the study are still under review by the Army and other agencies; therefore, it would be premature to discuss the results in this paper. However, the design of the shell could be applied to other hazards for which multiple-parameter modeling is performed. This paper describes the design and operation of the shell as an example for other hazards and models.

INTRODUCTION

The potential threat to the public from the storage, transportation, and demilitarization of chemical agents and weapons by the U.S. Army has given rise to the Chemical Stockpile Emergency Preparedness Program (CSEPP). As part of CSEPP, the Army has worked with appropriate regulatory agencies and state and local organizations to assure that regulatory requirements are met and that adequate emergency response plans are in place to protect the public and the environment. The immediate concern following an accidental release of chemical agent to the environment is the exposure of people downwind of the release site to the airborne agent as the cloud of agent vapor or aerosol is transported by the wind. The potential extent of the vapor hazard has been examined in earlier studies. As the emergency planning process proceeded, it became apparent that more information was needed about the potential for deposition of chemical agent aerosol on the ground and other surfaces following an accidental release.

Initially, in order to obtain preliminary estimates of the possible extent of the agent deposition hazard, the Army employed its GAPCAP (Generation of Assessment Patterns for Clouds of Airborne Particles) model (1) to estimate the downwind extent of the agent deposition pattern. Only two release scenarios and three sets of atmospheric conditions were considered and the effects of other variations in the values of the model parameters were not investigated in detail. Because of the wide range of potential release scenarios that have been developed as part of CSEPP and because of the wide range of potential release conditions and atmospheric conditions that could occur, it was decided that an extensive study of the predictions of the GAPCAP model should be made. The study would examine model predictions for wide ranges of model parameter values that represent all credible release scenarios, release conditions, and meteorological conditions. In April of 1993, the Army tasked Argonne National Laboratory to perform such a study.

DISPERSION/DEPOSITION MODEL

The GAPCAP model assumes that the concentration profiles of the material being modeled can be represented by Gaussian shapes in the vertical, crosswind, and downwind directions. The size of these Gaussian profiles are specified by standard deviation parameters (usually referred to as sigmas) that increase as simple functions of transport distance in the downwind direction. In the present application, the chemical agent is assumed to be released as small liquid droplets that are transported by the wind and eventually deposited on the ground due to gravitational settling. The assumptions that all the agent is released as liquid droplets and that the droplets do not undergo evaporation during transport are considered to be conservative in that all agent originally released remains available for deposition.

Mixing and diffusion in the vertical direction cause the vertical dimension of the cloud to increase with time and, thus, with distance downwind. However, this growth will eventually be limited by the surface of the ground below the cloud and by an atmospheric inversion cap above the cloud. The inversion cap is often characterized by a relatively rapid increase in temperature with height and represents a stable layer that creates a limit to the potential upward growth of the cloud. The layer of air between the ground and the inversion cap is referred to as the mixing layer.

The GAPCAP model formulation assumes that the wind is constant in speed and direction, that the ground surface is flat and uniform, that vertical growth of the agent cloud is limited by an impenetrable atmospheric inversion cap at a fixed height, and that meteorological conditions are uniform within the mixing layer. These assumptions are also considered to be conservative in that wind meandering, additional turbulence due to surface roughness, unlimited vertical cloud growth, and changing atmospheric conditions all should tend to increase the dispersion of the chemical agent before it is deposited resulting in lower deposition levels as the agent would be spread over larger areas.

The input parameters of the GAPCAP computer model can be divided into two groups — physical parameters that describe the physical situation being modeled and control parameters that specify calculational and output options and govern the numerical computations. The physical input parameters are listed in Table 1. The source standard deviations ($\sigma_{x,o}$, $\sigma_{y,o}$, and $\sigma_{z,o}$) represent the initial size of the agent cloud at the point of release. The precise values of these parameters have little effect on the size of the cloud at downwind distances that are large with respect to the source size. The diffusion parameters (γ, α, and β) and the standard deviations at the reference distance ($\sigma_{x,R}$, $\sigma_{y,R}$, and $\sigma_{z,R}$) determine the rates of growth of the cloud as a function of downwind distance. (The reference distance is taken to be 100 meters in the GAPCAP model.) The values of these parameters are expected to be functions of the atmospheric conditions within the mixing layer. In the GAPCAP model, the wind speed within the mixing layer is assumed to be a simple function of height as described by the Frost Power Law (2) where wind speed at a specific height is determined by the wind speed at a reference height of two meters (u_R) and a power law exponent (λ).

TABLE 1 Input Parameters of the GAPCAP Model

Parameter	Description
ρ	Density of droplets
m	Mass of agent released
d	Diameter of droplets
H	Height of release
$\sigma_{x,o}$	Source standard deviation in downwind direction
$\sigma_{y,o}$	Source standard deviation in crosswind direction
$\sigma_{z,o}$	Source standard deviation in vertical direction
H_{ML}	Height of mixing layer
γ	Downwind diffusion parameter
α	Crosswind diffusion parameter
β	Vertical diffusion parameter
$\sigma_{x,R}$	Standard deviation in downwind direction at the reference distance
$\sigma_{y,R}$	Standard deviation in crosswind direction at the reference distance
$\sigma_{z,R}$	Standard deviation in vertical direction at the reference distance
K_m^*	Generalized stability parameter (used in the calculation of the droplet settling velocity)
u_R	Wind speed at reference height
λ	Frost Power Law exponent

The GAPCAP model can be used to predict agent concentration, dosage (the cumulative sum of concentration over time), and deposition at points specified by a horizontal computational grid that extends in both the downwind and crosswind directions from the point of release. In addition to reporting the input parameter values and some intermediate computational results, the output of the computer code includes the model predictions over the computational grid in tabular form.

PARAMETRIC MODEL STUDY

A parametric study of the predictions of the GAPCAP model was carried out to quantify the potential extent of chemical agent deposition downwind of an accidental release from an Army storage depot. The values of the input parameters of the GAPCAP model were systematically varied over ranges judged to span the credible release scenarios and meteorological conditions associated with the eight chemical stockpile storage depots within the continental United States. The model was used to calculate the expected downwind distances to a series of deposition levels for the various combinations of input parameter values.

The first step in carrying out the study was to relate the model input parameters to the parameters of interest to the emergency planners and to establish appropriate ranges and increments for the parameter values. Some of the model parameters are essentially the same as the parameters used by the emergency planners to specify the release scenarios while others had to be related on the basis of the reported results of other studies.

The agents considered in the study were the blister agent HD and the nerve agent VX. The agent type determines the density of the droplets (parameter ρ in Table 1) needed as input to the GAPCAP model. A series of eight masses of released agent (parameter m) was selected for the study. The masses chosen were 100, 500, 1000, 5000, 10,000, 50,000, 100,000, and 500,000 lb. These values cover the range from a relatively small release, corresponding to the agent content of a few munitions, to a value comparable to the largest credible release identified in the Emergency Response Concept Plans for the eight storage depots.

The diameter of the liquid droplets (parameter d) that would be generated during an accidental release is difficult to estimate. In actuality, a continuous range of droplet sizes would probably be produced, with the details of the distribution dependent upon the release mechanism. Droplets could range in size from a diameter of 1 µm or less, which would behave essentially like a vapor, to large drops that would rapidly settle out and not leave the immediate vicinity of the release. Even though the GAPCAP model formulation has the capability to include a distribution of particle sizes within a single cloud, for the purposes of this parametric study, releases of uniform droplet size were considered to evaluate the effect of droplet size on the predicted deposition pattern. To cover the range of droplet sizes that probably could be transported beyond the depot boundaries, a series of six diameters from 1 to 500 µm (0.5 mm) was selected (1, 5, 10, 50, 100, and 500 µm).

The height of the release (parameter H) could range from near ground level to several hundred meters in the air, depending on the release scenario. For example, the accidental detonation of a munition during handling by a forklift would result in a release at essentially ground level; however, a release accompanied by a large fire could result in a large effective release height, because the agent might be carried upward due to the buoyancy generated by the heat of the fire. To cover a reasonably wide range of possibilities, a series of seven release heights was selected for the study. The release heights studied were 1 (corresponding to essentially a ground-level release), 50, 100, 200, 300, 500, and 700 m.

The dimensions of the effective source of the release, as specified by the source standard deviations in the model (parameters $\sigma_{x,o}$, $\sigma_{y,o}$, and $\sigma_{z,o}$), will depend on the quantity of agent involved and the manner in which the release is accomplished. However, the source dimensions have little effect on the behavior of the agent cloud as predicted by GAPCAP for downwind distances large with respect to the source size and the reference distance, x_R (100 m). In order to establish a consistent method of specifying $\sigma_{x,o}$, $\sigma_{y,o}$, and $\sigma_{z,o}$ for the parametric model study, the source dimensions contained in the database of another Army atmospheric dispersion model were examined. That model is the D2PC model (3) which has been used in previous analyses to estimate the downwind hazard from airborne chemical agents (see reference 4 for example). Based on the values of the source dimensions in the D2PC model database and on simple physical arguments, expressions for source standard deviations as a function of mass released (m), agent density (ρ), and effective release height (H) were developed for use in the parametric model study.

The remaining input parameters of the GAPCAP model except wind speed (parameters H_{ML}, γ, α, β, $\sigma_{x,R}$, $\sigma_{y,R}$, $\sigma_{z,R}$, K_m^*, and λ) are considered to be primarily functions of atmospheric conditions, particularly the atmospheric stability. Atmospheric stability is a measure of the relative amount of turbulence or mixing present in the atmosphere. Two of the primary causes of this turbulence are the uneven heating of the surface of the earth by the sun and the uneven flow of the wind over the surface of the earth due to its roughness. In a semiquantitative way, observed atmospheric stabilities are classified by meteorologists into categories. One such classification scheme, referred to as the Pasquill Stability Categories, consists of six classes designated A through F.

The rate at which air temperature changes with increasing height above the ground surface is often strongly correlated with stability. The most unstable category, with the greatest amount of turbulence, is A. Instability is often associated with a relatively large reduction in temperature and, thus, increase in density with height. Such conditions can usually exist only during the daytime, when solar radiation heats the ground surface and the air near the ground. The most stable category, with the least amount of turbulence and thus mixing, is F. This stability is often the result of an increase in air temperature with height and corresponds to a gravitationally stable condition of air density decreasing with height. These conditions usually only occur at nighttime, when solar radiation is not present to create and maintain unstable temperature and density profiles. High wind speeds tend to reduce the potential for temperature and density stratification and are usually associated with neutral stability conditions (categories C and D).

The U.S. Army D2PC model (3) also contains a database of atmospheric diffusion parameters as a function of atmospheric stability category. The values from that database were used to determine the values of the GAPCAP input parameters γ, α, β, $\sigma_{x,R}$, $\sigma_{y,R}$, $\sigma_{z,R}$, $K_m{}^*$, and λ as a function of atmospheric stability category. A series of three atmospheric stability categories was selected for the parametric study of the predictions of the GAPCAP model. Stabilities B, D, and F were chosen to cover the possible range, yet limit the number of separate model calculations required to complete the study. Stability A was omitted because such extremely unstable conditions are rarely observed; the high levels of turbulence associated with this category should lead to rapid mixing and large dilutions, resulting in smaller downwind concentration and deposition levels than other stability categories.

Although the height of the mixing layer (parameter H_{ML}) depends strongly on atmospheric stability, it is also a function of such other factors as geographic location, topography, vegetation, and season. However, very stable atmospheric conditions tend to exist only beneath low inversion caps, whereas unstable conditions tend to occur when the inversion cap is relatively high. In order to allow the parametric model study to be carried out in a generic manner, without tying it to a specific release location and specific time of year, it was decided to associate a single value for the mixing layer height with each atmospheric stability category. The database associated with the D2PC model includes tables of median mixing-layer height as a function of stability category for each of four seasons at each of the eight storage depots. Average values across the eight depots and four seasons were evaluated for each stability category. These average mixing-layer heights were used in the parametric model study to assign values to the parameter H_{ML} as a function of atmospheric stability category.

A series of nine wind speeds (parameter u_R) was selected for the parametric study. The wind speeds chosen were 1, 2, 3, 5, 7, 10, 12, 15, and 20 m/s. The GAPCAP model formulation assumes the presence of a wind field that is uniform in speed and direction over both time and space. The lowest wind speed value of 1 m/s (about 2 mi/h) was selected because it is generally believed that this is approximately the lowest speed for which a relatively constant and uniform wind field can be maintained in nature (see, for example, reference 5). The upper limit on the wind speed of 20 m/s (about 45 mi/h) was selected because stronger winds are usually associated with storms or hurricanes, in which uniform wind speeds and directions are not maintained for long periods of time.

In summary, a parametric study of the GAPCAP model was devised that includes six parameters: agent type, mass of agent released, droplet diameter, effective release height, atmospheric stability, and wind speed. The parameters and parameter values used in the study are summarized in Table 2. On the basis of the number of values selected for each parameter (2 agent types, 8 release masses, 6 droplet diameters, 7 release heights, 3 atmospheric stability categories, and 9 wind speeds), there are 18,144 different combinations of parameter values possible.

TABLE 2 Parameters and Parameter Values for Model Study

Parameter	Values
Agent type	HD and VX
Mass released	100, 500, 1,000, 5,000, 10,000, 50,000, 100,000, and 500,000 lb
Droplet diameter	1, 5, 10, 50, 100, and 500 µm
Release height	1, 50, 100, 200, 300, 500, and 700 m
Atmospheric stability	Categories B, D, and F
Wind speed	1, 2, 3, 5, 7, 10, 12, 15, and 20 m/s

However, many of these combinations correspond to situations that are not physically realistic. Explicit restrictions can be applied to eliminate combinations that do not correspond to physical situations. As suggested in the D2PC model, restrictions limiting possible wind speeds for certain atmospheric stability conditions should be applied because very stable and very unstable conditions generally cannot persist unless the wind speed is sufficiently low. In addition, the release height must be within the mixing layer for the GAPCAP model to be valid. This condition adds the restriction that $H \leq H_{ML}$. These restrictions reduce the number of combinations of parameter values corresponding to physically realistic situations to 7,200.

AUTOMATED SHELL

In order to carry out the large number of computer runs required to complete the parametric study, an automated shell was designed and implemented to prepare the input for and process the output from the computer model. The actual GAPCAP computer code, which is FORTRAN, was used exactly as received from the Army with no modifications whatsoever. Using the original code eliminated the need to delve into the internal structure of the computer program and the risk of inadvertently affecting the computational results.

The automated shell was developed primarily as a "C-shell" script in a Sun/UNIX operating environment. C-shell is a command interpreter with a C-like language structure. Some specific routines used to access and manipulate the output files from GAPCAP were written in FORTRAN. Although GAPCAP can be run on a personal computer (PC), the Sun platform was selected primarily because of the excessive computation time that would be required on a PC to carry out the thousands of computer runs needed for the study.

Through a series of screen menus, the automated shell interactively allows the user to select from pre-established lists, values for the six parameters of the study (see Table 2) as well as agent deposition levels of interest. The user also has the option to enter additional values and select them for the study. Once the specific values of the parameters for the study are established, the shell systematically goes through all possible combinations of parameter values (18,144 cases in the present study). For each set of parameter values or case, the restrictions on physically realistic combinations of release height, wind speed, and atmospheric stability category are checked. If the particular case is not physically valid, an entry for that case in made directly in the appropriate output file with a flag character set to mark the case as physically invalid.

For the valid cases, the shell generates a GAPCAP input file containing values for the physical input parameters listed in Table 1 that are derived, through table look-up or simple computation, from the values of the six parameters of the study for that case. Values for most of the control parameters are constant for the entire study. However, allowance had to be made for the adjustment of a few of the control parameters during the running of each individual case. An initial value was established for each of these adjustable control parameters and a systematic scheme was developed for adjusting these control parameter values based on the output of the GAPCAP model run. The shell then repetitively runs the model until a satisfactory result is obtained or until no further adjustments in the values of the control parameters are appropriate. In either situation, an entry is made in the corresponding output file with the flag character set to mark the status of the case.

As mentioned earlier, the GAPCAP model generates a rather extensive output file. However, for the purposes of the present study, the only model results of immediate interest are the downwind distances to the points where the predicted deposition level drops below the deposition levels of interest to the emergency planners. Because of the symmetric nature of the GAPCAP dispersion model, this distance will always lie along the centerline of the predicted deposition pattern in the direction of travel of the wind. Once the shell has determined that a satisfactory model run has been completed, the GAPCAP output file is searched to identify, for each of the deposition levels of interest, the two grid points along the centerline of calculational grid where the predicted deposition levels bracket the deposition level of interest. Linear interpolation is then used to estimate the downwind extent associated with the deposition level. If the end of the computational grid occurs before the smallest deposition level of interest is reached, values of the appropriate control parameters of the GAPCAP model are adjusted and the model is run again.

After all the downwind distances corresponding to all the deposition levels of interest are found or when the limits of the model are reached, the results are written to an output file. In order to simplify further processing of the study results and to avoid any potential for misinterpretation of the individual results, each record in the output file is complete and self-contained. That is, each record contains the values of the six parameters used in the calculation, the specific deposition level of interest, the predicted distance to that deposition level, and a flag character that indicates the status of the GAPCAP computer run. Because 72,576 output records were generated for this study (18,144 combinations of parameter values times four deposition levels), a series of output files were created rather than producing one large file that would be difficult to manipulate.

When the model runs were complete, the information from the output files was loaded into a commercial database application on a personal computer. The database application provided a convenient way to sort and group the results; to examine means, extremes, trends, and other statistics representative of the results; and to produce formatted tables of results for inclusion in project reports.

APPLICATION TO OTHER HAZARDS

While this study focused on one man-made hazard, the concept of an automated shell could be applied to other hazards for which multiple-parameter modeling is performed. For example, consider the modeling of coastal flooding caused by hurricanes (6). Such modeling is a complex problem involving interactions among water, wind, atmospheric pressure, land, and earth rotation. Like the modeling of chemical agent dispersion, modeling of hurricane-induced flooding involves many parameters such as pressure at a given radial distance, peripheral pressure, pressure at maximum wind, a density coefficient, a Coriolis parameter, forward speed of the hurricane, and wind stress over the water surface. For purposes of emergency planning, the prediction of hurricane effects must account for many additional uncertainties such as the time, location, and direction of landfall. Also, like the present study, the results of hurricane and flood models are typically calculated for a large-scale spatial grid. Such a situation could readily lend itself to the use of an automated shell to manage a very large number of computer runs. The hurricane and flood hazard is but one example of a multiple-parameter modeling situation. Others can be readily conceived.

CONCLUSIONS

The results of the parametric study of the predictions of the GAPCAP model are still under review by the Army and other agencies; therefore, it would be premature to discuss the specifics of the results in this paper. However, based on the success of using an automated shell for the present study, the concept of using such a shell to conduct similar extensive parametric studies deserves consideration. Often emergency planners need to know the possible range of consequences of a class of accidents or natural disasters in a general geographic region rather than the detailed consequences of a specific event at a specific location. Computer models may exist that can be used to make predictions for specific conditions. However, it may be very difficult and time consuming to prepare input for numerous cases, run the model repetitively, and examine the results of each case. The use of an automated shell such as has been described in this paper can significantly simplify and speed-up this process.

ACKNOWLEDGMENT

This work was supported under a military interdepartmental purchase request from the U.S. Department of Defense, Office of the Assistant Secretary of the Army for Installations, Logistics, and Environment through U.S. Department of Energy contract W-31-109-Eng-38.

REFERENCE LIST

1. Daniel L. Wu and Dale W. Sloop, *A Package of Transport and Diffusion Models for Biological Toxin Agents*, U.S. Army Chemical Research, Development, and Engineering Center, Aberdeen Proving Ground, Maryland, CRDEC-TR-86034, June 1986.

2. O.G. Sutton, *Micrometeorology*, McGraw-Hill Book Company, New York, 1953, p. 238.

3. C. Glenvil Whitacre, Joseph H. Griner III, Michael M. Myirski, and Dale W. Sloop, *Personal Computer Program for Chemical Hazard Prediction (D2PC)*, U.S. Army AMCC Report CRDEC-TR-87021, January 1987.

4. MITRE Corporation, *Risk Analysis Supporting the Chemical Stockpile Disposal Program (CSDP)*, December 17, 1987.

5. Innovative Emergency Management, Inc., and M. Myirski, U.S. Army Edgewood Research, Development and Engineering Center, *Reference Manual: D2 and Hazard Analysis*, Baton Rouge, Louisiana, August 24, 1993.

6. Y. J. Tsai, *Simulation of Coastal Flooding Caused by Hurricanes and Winter Storms*, Proc. 1992 International Emergency Management and Engineering Conference: Managing Risk with Computer Simulation, Society for Computer Simulation, Orlando, Florida, April 6-9, 1992, pp. 52-56.