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COMPUTERIZED SPILL HAZARD EVALUATION MODELS

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ABSTRACT

Accidents in the transportation or storage and handling of chemicals may result in the release of dangerous chemicals. Rapid prediction of hazard areas are essential so that the necessary remedial actions.

This paper describes a system being developed for the U.S. Coast Guard. The system consists of state-of-the-art mathematical models describing different sources for chemical releases (pressurized storage tanks, bulk storage tanks, barge, rail car and road transports) and hazardous behavior in the environment (two-phase jet flow, instantaneously released vapor cloud, dispersion of heavy gases with liquid aerosols, reactive chemical dispersion in air, jet fires, pool fire thermal radiation, explosion effects, water dispersion in rivers and streams, etc.). The system has a physical and chemical property database (including temperature dependent properties) for over 1200 chemicals which are used in the mathematical models.

This paper discusses the various features of the system. Details of the mathematical models are not given since these have been published before. The questions of how an on-scene commander responding to a chemical spill accident can utilize these models and the level of confidence that can be placed in the model results are discussed.

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INTRODUCTION

A number of hazardous chemicals are produced, stored, handled and transported in industrialized countries by thousands of tons. Many accidental chemical releases have occurred, even in the last decade, resulting in significant loss of life, injury to people and millions of dollars worth of property damage. A conscious effort is being made by industry, local governments, shippers, national governments and the populace in general to reduce both frequency of accidental chemical releases as well as to prepare for effective emergency response with a view to reducing (or eliminating) casualties in a post-accident scenario.

One of the critical pieces of information that a contingency planner or an emergency response official (say, the on-scene coordinator) needs to have is the behavior of the chemical after it is released. There are several thousand chemicals which are considered to be hazardous to the health and safety of the public. Unfortunately, because of the diversity in the physical, chemical and hazard properties, the behavior of each chemical is different. Added to this is the influence of release conditions, atmospheric conditions, and the nature of the substrate onto which the chemical may be released. Given the multitude of release conditions, behavior and environmental effects, it is impossible for those response officials to rapidly determine the potential areas of hazard from the chemical release for evacuation or other purposes.

A computerized hazard evaluation modeling system is an extremely valuable tool in performing the necessary calculations and provide reasonable estimates of hazard areas to the on-scene coordinator or to the risk analyst. The current computer technology with powerful desktop and laptop computers provide the necessary tools to perform complex calculations and display the results on graphic screens. This paper discusses one such computerized system.

There are a number of hazard assessment systems with varying degrees of applicability (chemicals, conditions, etc.), complexity, and cost to operate. Some are government owned and a number of systems are commercially available. A number of reviews are available in the literature (AIPE, 1989; Hanna & Drivas, 1987) on environmental and hazard assessment software.

One of the systems developed under the support of the U.S. Coast Guard in the 1970s is called the "Hazard Assessment Computer System" (Potts, 1981). This system, which is currently being utilized at the U.S. National Response Center, is a VAX mainframe based system. The system consists of two principal elements, namely, (i) a chemical property database consisting of chemical properties (in some cases, as a function of temperature) for over 1,000 chemicals and (ii) a compendium of mathematical models to simulate chemical behavior in or on water. This system is applicable only to the cases of chemical releases on water. The calculation algorithm has a tree structure illustrated in Figure 1. The release of a chemical is simulated first by a source module. This module consists of elementary source models which provide information on the rate of spill or quantity of spill and the conditions of the chemical, after release from the container. In addition, not all properties for all chemicals are available nor has the accuracy of data been checked against experimental values.

The environmental behavior of the chemical released on water depends on the physico-chemical properties of the chemical and, in certain cases, on the conditions of the water body. The behavior path a chemical takes are indicated in Figure 1 and these are simulated in the HACS by pre-assigning possible paths through a series of letter codes in the chemical property database for the particular chemical. Four possible hazard types are simulated, namely (a) thermal radiation from pool fires, (b) unconfined explosion of vapors, (c) dispersion of toxic or flammable vapor clouds in the atmosphere, and (d) dispersion of pollutants in water bodies.

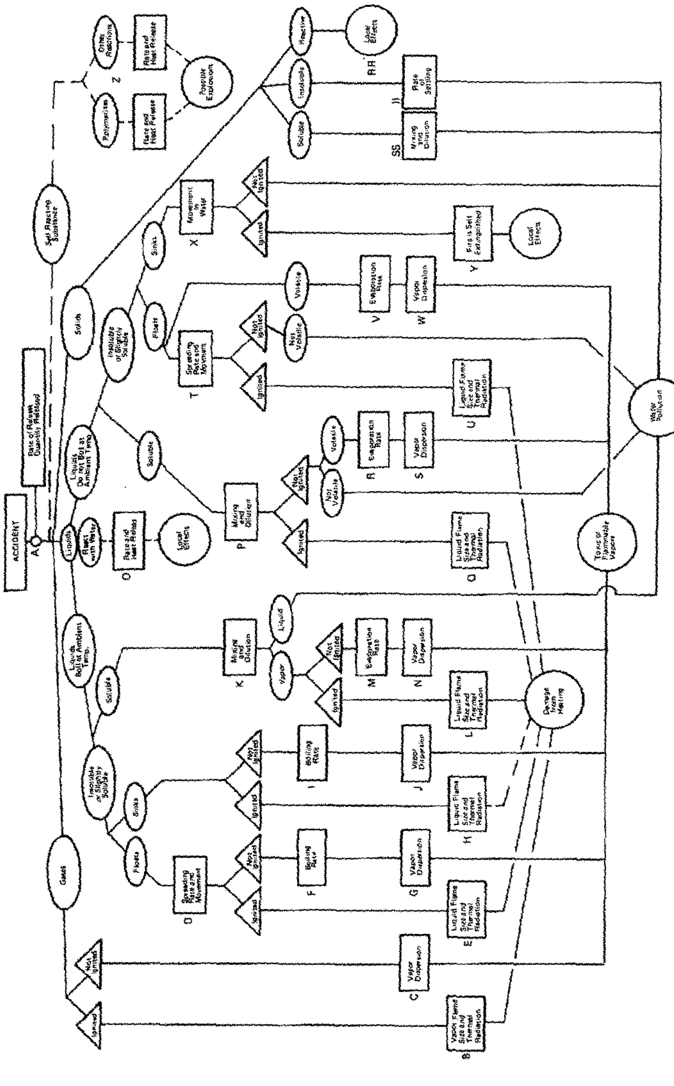

Fig. 1. Hazard assesment tree for chemical release on water (events chart; source: Raj and Kalelkar, 1974).

A new effort was undertaken recently by the authors to develop a new computerized hazard assessment system for use on both IBM-PC compatible platforms and Micro VAX compatible platforms. These systems are called respectively, SAFEMODE™ (Safety Assessment For Effective Management Of Dangerous Events) and MicroHACS. While the overall goal of the two new systems are very similar to the original HACS system of the US Coast Guard, they differ significantly in features, models and the range of applicability.

For example, the HACS was applicable only to the cases of chemical spills onto water. Also, the output of the system was in numerical tables. Finally, the HACS chemical property data base was rigid in its structure and difficult to use. Discussed below are the features of the newer systems, SAFEMODE and MicroHACS. The features of the two systems are similar and differ only in certain details related to the computer platform. Hence, the discussion provided is general.

As with all models, the results have to be viewed with caution and interpreted carefully. Assumptions and simplifications in the models and limited input data will affect the results, sometimes significantly. The results are best viewed as estimates of potential hazards which may be used for planning or response guides.

OVERALL ARCHITECTURE OF THE HAZARD ASSESSMENT SYSTEM

Figure 2 shows the overall structure of the chemical hazard assessment system. The user selects various options through a series of menu driven, easy to use panels. Default data for parameters are presented and these can be changed by the user. Several types of data are input. Intermediate results are presented. The type of hazard to be assessed is selected by the user for the particular chemical. The results of the calculation are displayed graphically, in color. The just performed calculations can be stored in a case file for future use or changes made in the values of one or more parameters and the model rerun.

Figure 3 shows the initial dialogue menu for invoking the various functions of the system. The user can use the emergency response option

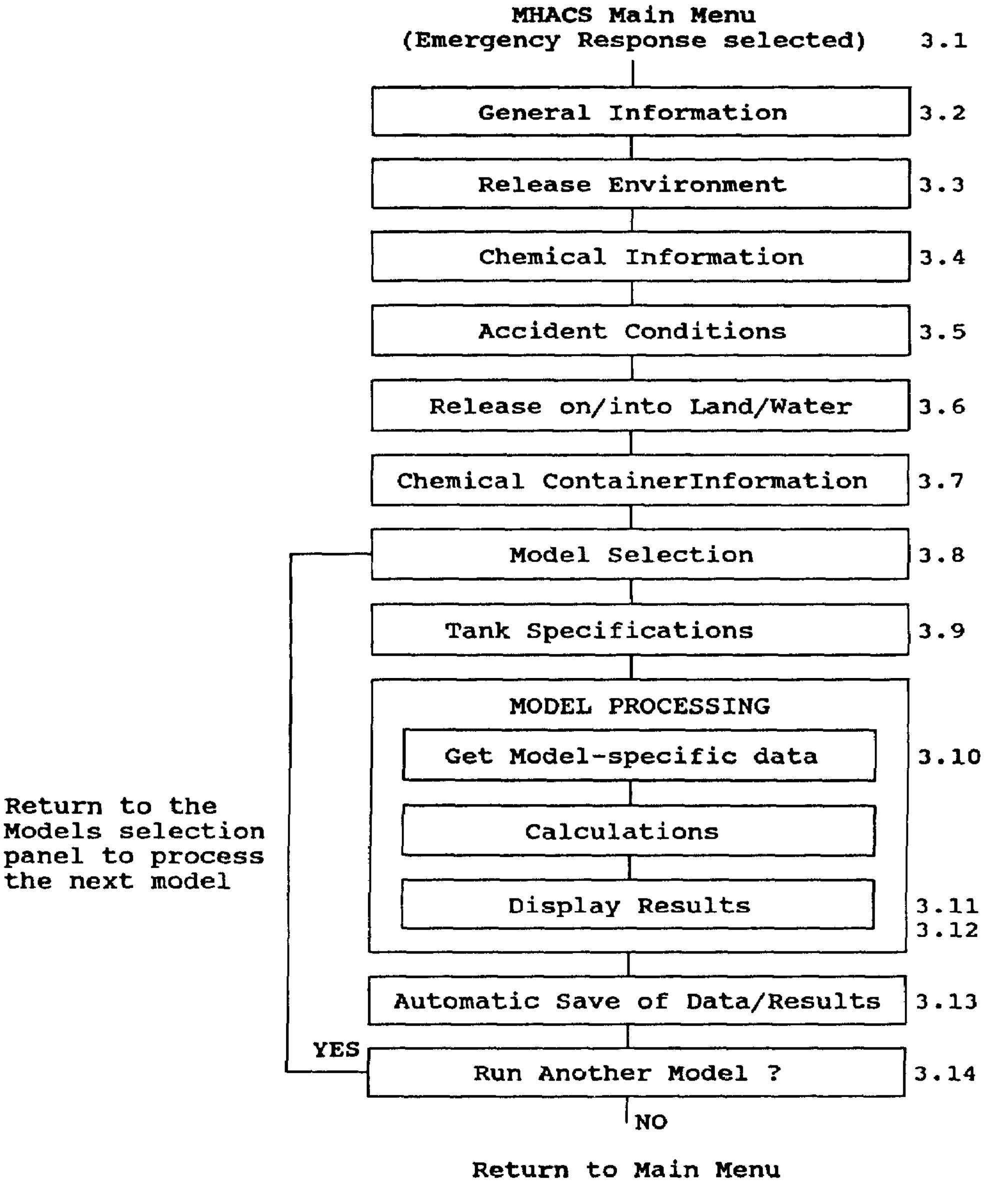

FIGURE 2: Overall Structure of SAFEMODE and MicroHACS Hazard Assessment Systems

or the contingency response option. Also provided is an option to calculate any or all chemical property values for a specified temperature. In the case of emergency response not all information for the execution of the various models are likely to be available and only a quick estimate of the hazard is needed to take any remedial action. The system was designed recognizing this need and has best guess default values built in for all parameters required to run the various models. In the case of contingency planning mode of operation all parameters in all models can be modified.

Once the mode is selected, the user is prompted to indicate the type of accident by identifying the chemical storage type which includes, leaks from barge or ship, rail car, road tanker, fixed storage tank, bullet tank on land, or a pipeline. Figure 4 shows the various icons presented. Subsequent to selecting the release mode, the user selects the chemical spilled or released by identifying it with one of several chemical identification designators. Figure 5 shows the possible options for chemical identification.

Information on the nature of the accident (i.e., the size of hole, location of hole on the container, size of the container or its geometric description, etc.) are input. Also input are the environmental conditions such as wind speed, temperature, relative humidity, type of substrate, the local topography, atmospheric stability (this may also be calculated from other input data) and other parameter values. The user is then presented with the different modes of hazardous behavior of the chemical upon release. One or more options can be chosen for evaluation.

Based on the data input, including the chemical chosen, its physical and thermodynamic properties, and the location of the hole, different source strength calculation models are executed. These source models include releases of (i) liquid, (ii) pressurized liquefied gas, (iii) cryogenic liquid , (iv) gas or vapor only release, (iv) two phase jet release, etc. Instantaneous and continuous releases of chemicals are modeled. Spills of liquid, spreading of the pool, evaporation/boiling of pool and entrainment of vapor into the prevailing wind are modeled. Results of source strength calculations, including the rates of release, quality of the released

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HAZARD ASSESSMENT COMPUTER SYSTEM

Welcome to MicroHACS

Selection
  Number                       Selection

   1 ............ Emergency Response
   2 ............ Contingency Planning
   3 ............ Chemical Property Value Calculations
   4 ............ Default Data Modification
   5 ............ Exit MicroHACS

Enter a Selection Number : 3
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FIGURE 3: Main Selection Menu Panel

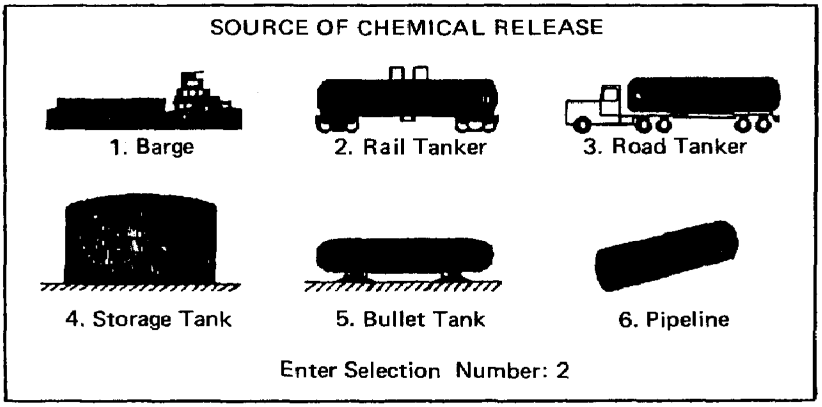

FIGURE 4: Icon Based Selection of Type of Container From Which Chemical Release Occurs

chemical immediately upon release (temperature, density, liquid aerosol fraction, velocity, etc.), geometrical results (pool diameter, boiling rate, etc.) and results after any initial mixing with air are presented to the user for possible modifications of any and all calculated parameters. This provides a means of inputting any data available from the field to override values calculated by the source models.

The execution of the hazard model results in the calculation of potential hazard areas for prescribed hazard limits. In general, the hazard areas are plotted to user specified scale as isopleths or contours. The graphical display results may be printed on a graphics printer. The scale, orientation and color of the display on the screen can be changed by the user. The numerical results are presented on the screen and stored as tabular information in data files. Finally, after each execution of the software the data input and the results generated can be stored en mass as a case for future analysis or modification.

DESCRIPTION OF TYPES OF HAZARDS EVALUATED BY THE SYSTEM

Four principal types of chemical hazards are considered. These include (i) thermal radiation from pool fires, (ii) explosion, (iii) dispersion of toxic or flammable vapors generated by the release of the chemical, and (iv) dispersion of soluble chemicals in streams, rivers and other water bodies.

FIRE RADIATION MODEL: This model calculates the thermal (heat) radiation hazard distance arising from the radiative plume of a burning liquid chemical pool. The model is based on the results from a number of field tests with such chemicals as LNG, LPG, jet fuel, etc. (Raj, 1983; Raj, et al., 1979). In this model the fire geometry is assumed to be a cylinder with axis tilted by wind, if the wind is strong. The plume is assumed to be a grey emitter with an emissivity dependent on the diameter and the characteristics of the chemical. The irradiance of the fire depends on the chemical. The latter is based on field test data where available. The geometric size and the angle of tilt are modeled using experimental correlations.

The radiation to a specified location outside the fire is determined by calculating the geometric view factor between the fire and the object and taking into account any atmospheric absorption of the radiant heat. Contours of constant heat flux levels are calculated and displayed. The hazard heat flux levels can be input by the user.

EXPLOSION MODEL: The unconfined detonation of a mixture of the chemical vapor (susceptible to explosion) and air can result in serious damage far removed from the source of ignition. Damage in such cases is a result of significant over pressures created by the blast wave. Injury to humans and structural damage can result from the over pressures. This model calculates the over pressure field surrounding a vapor cloud assuming that a certain fraction of the mass of vapor detonates. The model calculates the distances to various user specified or default hazard over pressures. Typically, the areas of hazard for such damages as lung puncture, ear drum rupture, glass breakage, and severe structural damage are determined. These areas are plotted.

MODELS FOR THE DISPERSION OF VAPORS IN THE ATMOSPHERE: This model calculates the concentrations at various locations due to the release and dispersion of vapors, heavy gases and vapors containing liquid aerosols. Both instantaneous releases and continuous releases are handled. For certain reactive chemicals (ammonia, nitrogen tetroxide, hydrogen fluoride, etc.) thermodynamic sub-models are exercised to determine the equilibrium state of the chemical for various dilutions with humid air. This also determines the density of the cloud for further dispersion. Several sub modules calculate the atmospheric stability parameters, air entrainment rates and other parameters. While topography is taken into account in the form of the aerodynamic roughness over the field of dispersion, the dispersion calculations in the current version of the model do not follow the topographic undulations.

The dispersion of heavy vapors and clouds containing liquid aerosols is based on the heavy gas box model modified by the super posed finite source size gaussian model. The results of this model, called ADAM (Raj and Morris, 1987), have been tested against field test data from a number of experiments involving the release of different chemicals both on land and on water. The model is applicable to continuous dispersion of heavy vapors produced by a jet flow (say, from a hole in a liquefied pressurized gas tank) or generated by the evaporation of a pool of liquid. It is also applicable to the dispersion of a cloud of vapor generated, say, by the sudden release of a vaporizable chemical.

The results of the calculations are stored in a file and presented graphically as contour plots for user specified toxic/flammable concentrations. In the case of the plume, steady state chemical release is assumed. The meander of the plume due to wind direction changes can also be displayed on the screen. In the case of cloud dispersion, the path of the cloud and the size of the cloud to specified concentration boundary are displayed. The facility to replot the hazard area contours and display other concentration contours are also provided.

WATER DISPERSION MODELS: The spill of soluble hazardous chemicals into water bodies and their subsequent dispersion poses toxic threat to humans and aquatic animals. This model calculates the down stream concentrations of a soluble chemical dispersed in a flowing stream, river or other water bodies whose turbulence characteristics can be defined. The model provides output in the form of peak concentrations at specified down stream positions from the spill point, the arrival time and the persistent time for concentrations above a certain specified threat limit. Also, provided, in the case of an instantaneous release, is the distance from the spill point beyond which the concentration is below the hazard threshold.

SAMPLE RESULTS FROM THE HAZARD ASSESSMENT MODELS

Figure 6 shows the result of a run involving the determination of the hazard area arising from the release of anhydrous ammonia leaking from a road tanker. As can be seen the continuous release plume extends up to 3.5 km, for the threshold limit value toxic concentration of 25 ppm under the weather conditions specified in the figure.

RELEASED CHEMICAL INFORMATION

Selection Number	Selection
1	CHRIS Chemical Code
2	Chemical Name
3	CAS #
4	UN / DOT #
5	STCC #

Enter a Selection Number .... : 1

Enter Chemical Identification : EOX

FIGURE 5: Selection of Chemical By One of a Number of Identification Standards

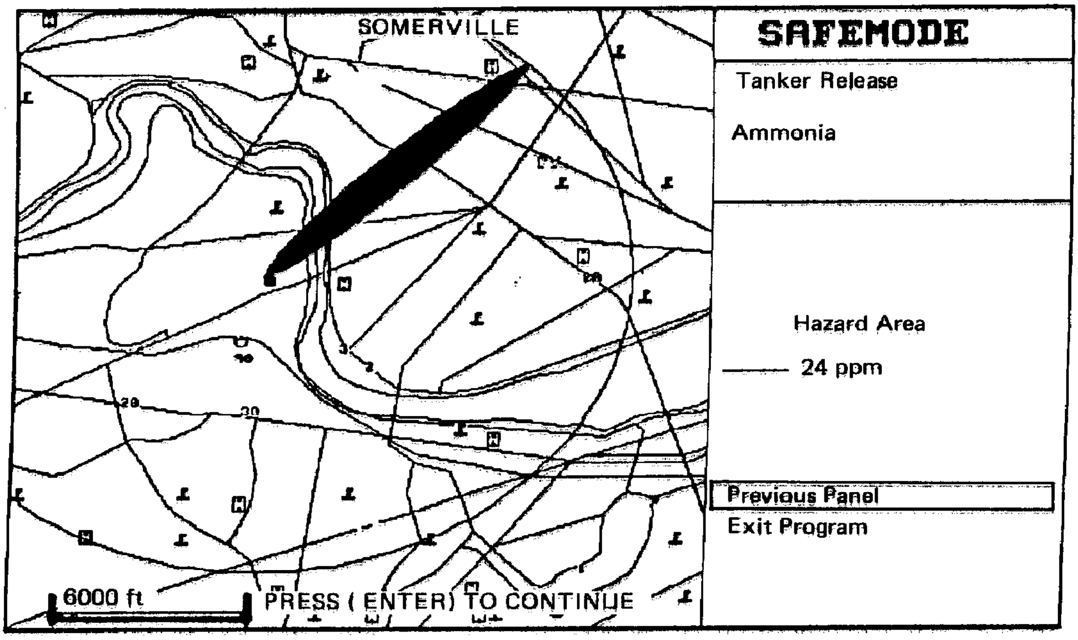

FIGURE 6: Sample Output of Calculations: Toxic Gas Dispersion Hazard Area Shown Superposed on a Map

The results of the contour calculations are superposed on a map of a specified scale. The total area under the plume is also calculated and displayed.

The results from calculations involving other types of hazard are also presented in a manner similar to that shown in Figure 6.

DISCUSSIONS: INTERPRETATION OF MODEL RESULTS

The models described in this paper are applicable to a variety of accidental chemical release situations. A number of different types of release scenarios, chemicals, soil conditions, atmospheric conditions and chemical behaviors can be simulated. The input of data into the computerized systems is simple and the user need not be an expert in either hazardous material properties or in computers to run the simulations. The output is graphical giving the decision maker a pictorial view of the hazard so that quick decisions can be taken. The number of situations considered in this system will probably encompass over 90% of accident situations involving chemicals. The mathematical models used are the state-of-the-art models. However, in the use of these computerized hazard assessment systems, the user must be aware of limitations. These are discussed below. Like all mathematical models simulating natural phenomena and the behavior of chemical systems there are limitations to these models. While the results are reasonable estimates of the potential hazard zones, one needs to exercise caution and certain amount of skepticism in using the results of these or similar models. The computerized hazard assessment models should be treated as only tools and should not be a substitute to experience or actual observational information.

The model result uncertainties arise from a number of causes. First is the accuracy of data from an accident scene. The second is due to the inherent approximations made in the models. Third is due to the in ability of the models to handle the particular situation of the accident and therefore use of a wrong type of model to simulate an event. We discuss below the implications of each of these uncertainties on the overall outcome of the hazard assessment.

In many cases not only are the environmental conditions not known precisely but the exact type of damage to the containment vessel may not be known either. For example, if the size of the hole is wrongly estimated by, say, a factor of 2 the calculated mass flow rate from the tank will be off by a factor of 4 if all other input data are correct. Similarly, the soil condition may be wrongly described. Take for example the case of a soil that is porous (which, therefore, can absorb a considerable volume of a liquid spilled) but is described to the model as "ground". In such a case the evaporation rate is calculated wrongly and to this extent the hazard distances calculated will be erroneous.

The second type of inaccuracy arises due to the inherent model limitations. In the case of the vapor dispersion model, considerable simplification of the atmospheric dynamics (especially the turbulence mixing) has been made. Similarly, in the case of fire radiation the irregularities of radiant emission and the non uniformity of the temperature in a fire over its plume length have been ignored and average emission values are used. For many chemicals the fire irradiance values are not available at all! In such cases the best guess values are used - these may or may not be close to the real values. In the case of explosion models all irregularities (stratifications) in the vapor cloud before its detonation are ignored. Also ignored are the multiple reflections of shock waves by structures, collimating effects of atmospheric stratifications and other important "collimating or reflecting" phenomena.

The third type of uncertainties in the models arise when the models are used for situations for which they were not intended to be used. For example, it is impossible to describe, in a system such as the one described in this paper, all possible types of topography in which accidents can happen. Consider a road accident involving a tanker which releases its hazardous material content onto the ground. If the ground happens to be sloping and drains into a gully, then the liquid ignited will form a channel fire. This is not described in the system of models described above. The use of the fire model in the system described for this case will give not only erroneous distance but also will not give the overall extent of the actual hazard area (which may be long and narrow instead of being circular or elliptical).

Finally, there are a number of chemical properties of interest and required by the models that are either not available or are inaccurate to a considerable extent. Therefore, the hazard assessment model results could be inaccurate under these circumstances.

Therefore, in the use of any computerized hazard assessment model the user should be aware of its limitation and the range of applicability. While computer models are useful and provide a very valuable tool to the first responder or the on scene coordinator they should not be afforded too lofty a position in decision making regarding the appropriate response. A computerized spill hazard assessment tool should not be a substitute for human expertise based on experience and sound technical assessment with due considerations to a number of physical, economics and political factors.

CONCLUSIONS

The behavior of chemicals in the atmosphere depends on so many chemical dependent and environmental factors. The complexity of calculations require the use of computerized models to assess quickly the potential areas and types of hazards. Described in this paper is a system which provides important results that can be useful to the on scene coordinator or a planner. The computerized system can provide a useful, effective, and rapid means of estimating the potential hazard areas without too much effort.

The models, on the other hand, cannot form a panacea; their limitations have to be fully understood before they are used and their results considered in any decision making. This paper has discussed both the wide range of hazards modeled as well as limitations of these models due to input errors, inherent model limitations or wrong applications. Not withstanding the limitations, the computerized models serve a very important role in reducing the effects of accidental releases and their impact on populations by providing estimates of hazard areas due to chemical releases.

ACKNOWLEDGEMENT

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