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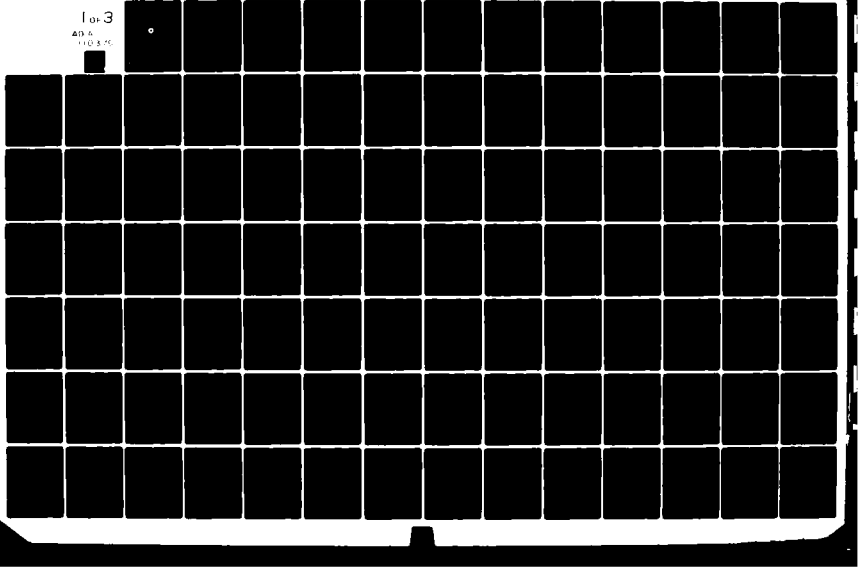

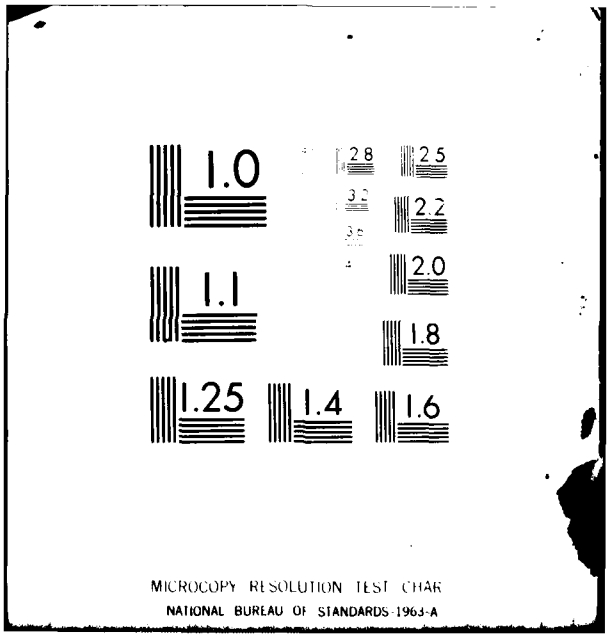
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Report No. CG-D-75-81

LEVEL II

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HAZARD ASSESSMENT COMPUTER SYSTEM

HACS/UIM

USERS' OPERATION MANUAL

VOLUME I

Document is available to the public through the
National Technical Information Service,
Springfield, Virginia 22161

SEPTEMBER 1981

Prepared for

DEPARTMENT OF TRANSPORTATION
UNITED STATES COAST GUARD
Office of Research and Development
Washington, D.C. 20593

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Technical Report Documentation Page

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
CG-D-75-81	AD-A110375	

4. Title and Subtitle	5. Report Date
Hazard Assessment Computer System HACS/UIM Users' Operation Manual, Volume I	September 1981
	6. Performing Organization Code
7. Author's	8. Performing Organization Report No.
Richard G. Potts	
9. Performing Organization Name and Address	10. Work Unit No. (TRAIS)
Arthur D. Little, Inc. Acorn Park Cambridge, MA 02140	4156.3
	11. Contract or Grant No.
	DOT-CG-941999-A
12. Sponsoring Agency Name and Address	13. Type of Report and Period Covered
U. S. Coast Guard Office of Research and Development Washington, D. C. 20593	FINAL REPORT
	14. Sponsoring Agency Code
	G-DMT-1/54

15. Supplementary Notes

Michael Parnarouskis as project officer

16. Abstract

HACS/UIM USERS' OPERATION MANUAL

The Hazard Assessment Computer System (HACS) is one of six major components of the U.S. Coast Guard's Chemical Hazards Response Information System (CHRIS). HACS is a computerized system consisting of chemical spill models and containing all necessary physical and chemical property data to permit hazard assessments to be performed for 900 commonly shipped chemicals.

The User Interface Module (UIM) provides for fully interactive operation of HACS with remote access for users to the central computer facility by means of terminals. User interaction with HACS is controlled by the UIM through a question and answer dialog. The Users' Operation Manual provides HACS/UIM users with information and instructions to run the programs, to select processing sequences, to enter requested or required input data, and then to interpret the output results. This report is primarily a reference manual contains three sections: an overview of HACS/UIM capabilities, detailed description of internal operations, and a detailed guide for making hazard assessment runs. Individual sub-sections for each different assessment procedure are given, each with comprehensive descriptions of the use of HACS data items and assessment model concepts and limitations. Appendices to the user manual contain further detailed reference information.

17. Key Words	18. Distribution Statement
Hazard Assessment, HACS, CHRIS, Hazardous Chemical	Document available through National Technical Information Service Springfield, Virginia 22161

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of Pages	22. Price
Unclassified	Unclassified	228	

Form DOT F 1700.7 (8-72) Reproduction of completed page authorized

HAZARD ASSESSMENT COMPUTER SYSTEM

HACS/UIM USERS' OPERATION MANUAL

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30 September 1981

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DEPARTMENT OF TRANSPORTATION
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WASHINGTON, D.C. 20593

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GENERAL OVERVIEW

CHEMICAL HAZARD RESPONSE INFORMATION SYSTEM (CHRIS)

The Hazard Assessment Computer System (HACS) is one of six major components of the Coast Guard's Chemical Hazard Reponse Information System (CHRIS). CHRIS is designed overall to provide timely information essential for proper decision-making by responsible Coast Guard personnel and others during emergencies involving the water transport of hazardous chemicals. A secondary purpose is the provision of certain basic non-emergency-related information to support the Coast Guard in its efforts to achieve improved levels of safety in the bulk shipment of hazardous chemicals. CHRIS consists of four reference guides or manuals, a regional contingency plan, a hazard-assessment computer system (HACS), and an organizational entity located at Coast Guard headquarters. The four manuals contain chemical data, hazard-assessment methods, and response guides. Regional data for the entire coastline are included in the Coastal Regional Contingency Plans. The headquarters staff operates the hazard-assessment computer system and provides technical assistance on request by field personnel during emergencies. In addition, it is responsible for periodic update and maintenance of CHRIS.

A brief description of each component of CHRIS is provided below.

A Condensed Guide to Chemical Hazards, COMDTINST M16465.11

This handbook, COMDTINST M16465.11 - Condensed Guide to Chemical Hazards, contains information to facilitate "early response decisions" during emergency situations. It is a compact, convenient source of chemical-related information with specific reference to bulk-shipped hazardous materials. The guide is intended primarily for use by port security personnel and others who may be the first to arrive at the site of an incident and need readily available, easily understood, descriptive information about the hazardous nature of the chemical and the situation confronted. It will assist those personnel in quickly determining proper, responsible actions that must be taken immediately to safeguard life and property and to reduce, insofar as possible, further contamination of the environment. The guide contains precautionary advice on the chemical and its characteristic physical and biological hazards so that field personnel can assess the threat as a prerequisite to determining subsequent large-scale action.

Since the Condensed Guide to Chemical Hazards is the only component of CHRIS that will be initially available at the scene of an accident, it includes a list of on-scene information needs that the Hazard-Assessment Handbook (COMDTINST M16465.13) and HACS require as inputs. The on-scene information needs of the Hazard-Assessment Handbook and HACS are listed in the Condensed Guide to Chemical Hazards (COMDTINST M16465.11)

as questions which must be answered and relayed to the user of the handbook or HACS as soon as possible.

Hazardous Chemical Data, COMDTINST M16465.12

The Hazardous Chemical Data Manual, COMDTINST M16465.12, is intended for use primarily by the On-Scene Coordinator's (OSC) office and the Regional and National Response Centers. It contains detailed, largely quantitative chemical, physical, and biological data necessary for formulating, evaluating, and carrying out response plans. The Hazardous Chemical Data Manual contains the hazard-assessment code, which is essential to selecting the appropriate calculation procedures for the hazard assessment, and lists the needed physical and chemical property data which are required to perform the hazard-assessment calculations in COMDTINST M16465.13.

Hazard-Assessment Handbook, COMDTINST M16465.13

The Hazard-Assessment Handbook contains methods of estimating the rate and quantity of hazardous chemicals that may be released under different situations. It also provides the means of predicting the threat that the chemicals present after release. It includes methods for predicting the resulting potential toxic, fire, and explosion effects by providing procedures for estimating the concentration of hazardous chemicals (both in water and in air) as a function of time and distance from the spill.

Response Methods Handbook, COMDTINST M16465.14

The Response Methods Handbook, COMDTINST M16465.14, is a compendium of descriptive information and technical data pertaining to methods of responding to threatened or actual spills of hazardous chemicals. The document has been written specifically for Coast Guard OSC personnel who have had some training or experience in pollution and hazard response. Emphasis has been placed on existing or prospectively available methodology. As new methods become available, the response handbook will be updated to include these new approaches.

In an actual emergency, an assessment of the likely extent of hazard, using the Hazard-Assessment Handbook and/or HACS, will be used in the choice of the appropriate response methods suggested in the Response Methods Handbook.

Data Base For Regional Contingency Plan

The information in this data base is predominantly for use by OSC personnel. It contains data pertinent to a specific region, subregion, or locale. It will provide detailed information on resources that might be threatened and the availability of response equipment. Examples of such information include an inventory of physical resources and personnel;

vulnerable or exposed resources (critical water-use areas); potential pollution sources, geographical and environmental features; cooperating organizations; and recognized experts with identified skills. A good deal of this regional-specific information is in the form of Regional Contingency Plans.

HAZARD ASSESSMENT COMPUTER SYSTEM (HACS)

HACS is perhaps best described as the computerized counterpart of the CHRIS Hazardous Chemical Data Manual (COMDTINST M16465.12) and Hazard Assessment Handbook (COMDTINST M16465.13). It enables personnel at Coast Guard Headquarters to quickly obtain more detailed hazard evaluations than may be possible via COMDTINST M16465.13. Graphic output displays the relationships among spill concentration, thermal radiation, location, and time. This information may then be transmitted to field units and elsewhere by facsimile. Furthermore, HACS can be used for emergency discharge advance planning, and the development and testing of improved hazard assessment methods.

Of concern is the evaluation of and response to any dangerous condition precipitated by accidents involving discharged chemicals which has, as a potential foreseeable consequence, harm or injury to life and/or property. A chemical discharged (or spilled) on water can create a hazard because of its flammability, its toxicity, or both. As the spilled material disperses and/or becomes diluted, the hazard normally decreases and disappears. It is important to know how far and fast the danger of fire or poisoning can spread and at what point the chemical ceases to be hazardous.

The processes of dispersion, evaporation, combustion, and the like, which are associated with the chemicals of concern are quite complex and depend on many variables, not the least of which is the nature of the chemical itself. HACS offers a systematic and convenient approach to estimate the type and extent of hazard. The hazard estimate is given in terms of distance and times over which a toxic or flammable concentration of a given chemical may exist in water and in air, and the minimum safe distance between the spill site and people or combustible materials, should the chemical ignite and a fire ensue. HACS presently contains all necessary physical and chemical property data to permit hazard assessments to be performed for 900 commonly shipped chemicals.

USERS OF HACS

The system is initially intended for use by hazard assessment specialists at Coast Guard Headquarters who possess a fundamental appreciation for the nature of the physical and chemical processes modeled therein. For this reason, it is assumed that users have familiarized themselves with COMDTINST M16465.13 as well as with the report documenting the development of the mathematical models utilized by HACS, Assessment Models in Support of the Hazard Assessment Handbook (COMDTINST M16465.13),

Report No. CG-10-74, U. S. Coast Guard, January 1974.* HACS can be an extremely powerful tool in the hands of an experienced hazard assessment specialist, who can properly formulate a problem for presentation to HACS and then correctly interpret the significance of results obtained. At the same time, however, the system could inadvertently be misused by applying it to situations which were either (1) specifically excluded from consideration by the designers or (2) unanticipated by them. The system designers know of no automatic way to prevent misuse, except to caution users to be "reasonably" familiar with the methodology underlying the assessment models. Several general sections have been included in Section 1 of this manual discussing limitations and accuracy related to physical process modeling, and Section 3 provides further detailed observations pertaining to each assessment model. As the application of HACS progresses to more varied spill conditions, other as yet not anticipated, or discussed, effects of modeling limitations and/or approximations may be encountered.

SYSTEM AVAILABILITY

In view of the above, the system is not directly available to Coast Guard field personnel except through Headquarters' specialists who will operate HACS on their behalf. As experience is gained in using HACS, this policy may be reappraised to permit direct field access, subject to the availability of necessary terminal equipment and computer inquiry processing capability.

USERS'MANUAL

This manual is intended to provide users with information and instructions to run the programs in the Hazard Assessment Computer System and then to assist users in interpreting and understanding the results. It is primarily a reference manual, rather than a tutorial or training document.

The manual contains three sections and a number of appendices. Section 1 is designed to give the user an "instant" overview of HACS capabilities. The second section provides the user with a detailed description of the internal operations, focusing on data operations, and should be referred to for a deeper understanding of the HACS system. Section 3 is a detailed users' guide for making hazard assessment runs, containing individual sub-sections for each different assessment procedure. Comprehensive descriptions of the use of HACS data items, and limitations, for obtain-

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*A later report entitled "Development of Additional Hazard Assessment Models" describes new models installed during 1976.

ing hazard assessments are contained in this section.

Section 3.1 gives an overview of the different hazard assessment models incoporated within HACS, and provides users with the information required to select models appropriate for particular hazard assessment evaluations. Section 3.2 gives a complete guide to the interactive HACS User Interface Module (UIM) procedures which are common to all assessment runs. The material in this section is organized in the sequence that is encountered in a typical HACS/UIM run. Section 3.3 contains detailed descriptions and definitions of individual models, input requirements and output results.

The appendices contained in the HACS user manual provide detailed reference information which will be found useful in the preparation of input to HACS programs and in understanding output print names, codes and messages. Appendix G gives an example HACS assessment run. It is suggested that users unfamiliar with HACS attempt to duplicate this run as an aid in understanding the operation and requirements of the system.

RELATED SYSTEMS

The Hazard Assessment Computer System is comprised of a specific set of assessment models, chemical specific data and an overall system structure to provide data control and output displays. Two separate computer programs are used to define and produce independent displays of the chemical specific data; the use and capabilities of these programs are described in separate reports.

Also to assist in obtaining the compound recognition code used to reference data for a particular chemical, a separate set of indices have been produced and are given in a separate report. These indices enable a user of HACS to obtain a compound recognition code for a chemical given either the compound name or a synonym.

Detailed HACS program code listings and technical documentation are included in a separate report.

1.0 INTRODUCTION

The Hazard Assessment Computer System (HACS) is designed to provide a quick and accurate estimate of hazards presented by a discharge (or potential discharge) of hazardous chemicals, and to display these estimates in a form that is useful to Coast Guard response personnel. HACS is built around the mathematical models that were created for COMDTINST M16465.13, the Hazard Assessment Handbook, and a number of specialized models developed specifically for computer applications. The design and implementation of HACS has focused on providing rapid and quantitative assessments in response to questions such as the following:

- When will the air/water concentration of a discharged material reach a specified level of toxicity at a given location?
- When will the air/water concentration return to a specified safe or nontoxic level?
- What is the concentration of discharged material at a specified location and time?

HACS may be used under emergency conditions involving the accidental discharge of a hazardous chemical into navigable waters and for contingency planning (e.g., preplanned assessments and responses, drills, etc.). To use HACS, the following types of information must first be obtained.

- Discharged chemical characteristics (e.g., name, storage pressure, temperature, quantity).
- Discharge conditions (e.g., tank size, location of discharge opening relative to water's surface and to tank level).
- Environmental conditions (e.g., wind speed, air and water temperatures).
- Marine conditions (e.g., current speed, water depth at spill site, spill geography).

In the interactive operation of HACS, users interface with the computer system by means of a data termainal for input of data and displays of hazard assessment results. HACS contains an internal master data file, and the operation of the system is governed by specific procedures to obtain from the user required data which is then stored in that file. In addition to the information gathered from the field, the user may provide inputs to the computer on options for displaying the information on the estimation of discharge conditions (mainly concentration and/or thermal radiation as functions of spatial and temporal parameters).

When sufficient input data has been obtained from the user, the HACS/UIM will run an assessment model and display the results at the user terminal. Depending on the nature of these results, the user may elect to conduct a number of different runs using the same model with varying input data or proceed to the use of other models. When all assessment calculations to be performed have been obtained and validated by the user, the hazard estimation information can then be communicated to the appropriate personnel.

1.1 GENERAL SYSTEMS FEATURES

The main objective of HACS is to both quickly and accurately provide quantitative estimates of hazards presented by the spill of a hazardous chemical. Such estimates appear in the form of line printer output and plots. To achieve this, the following system features are available.

- The system operates in an interactive mode, using a terminal for input and display of output results.
- The system interfaces with a chemical properties data base which contains chemical and physical properties for 900 hazardous chemical substances.
- The system contains a set of default values which are used for a hazard assessment when the user cannot supply a value.
- The system can plot thermal radiation, concentration, or other variables (e.g., pool radius, temperature of liquid remaining, volume of liquid remaining, etc.) as a function of location and/or time, as appropriate.
- The system can check for the reasonability of estimated hazard levels and input data.
- The system output identifies the spilled chemical, restates the discharge, environmental and marine conditions and reports the hazard assessment. The output information provided will enable the user to validate his input data quickly and accurately.

HACS provides estimates of hazards in the following manner. The system input processor begins a hazard assessment by reading user input data which supply to HACS the name of the chemical substance which was spilled, discharge conditions, marine conditions, environmental conditions, etc. HACS then obtains from the Chemical Properties File, the chemical properties for the specified substance. If HACS needs information that is not supplied by the user or from the Chemical Properties File, it obtains the information from the default file. The default file contains a default quantity for every value needed by HACS. A list of the default values currently contained in HACS is given in Appendix C.

HACS now begins its estimation or assessment. This process is the execution of a sequence of mathematical models to provide information such as what is the concentration of the discharged material at a specified location and time after initial spill.

As each model is executed, HACS controls the required user input process by the type of data items that are stored in an internal file and required for use by a model. If any data item is encountered which currently has only a default value stored, the HACS/UIM will automatically query the user for a specific value to be used in place of the default value. Users may enter these values if available or elect to continue with the run without changing the internal default value.

When the HACS/UIM has obtained sufficient input data from the user, the current assessment model is run and the results obtained are displayed at the user terminal. Users may then modify input data and re-run the model, or proceed to initiate execution of a different model. On completion of each model run, HACS produces summaries of all computed results, and provides options for output tables and plotted displays.

1.2 ESTIMATION MODELS AND ROUTE SELECTION

HACS is built around a set of mathematical models (see Section 3 for more complete rate model descriptions) that are specific computer programs for estimating discharge conditions and chemical behavior, such as flow rates for escaping chemicals (Model A), concentration of water miscible fluids (Model P), and vapor dispersion (Model C). The theoretical basis for these models is described in Assessment Models in Support of the Hazard Assessment Handbook* published by the United States Coast Guard in January 1974. The models contained in HACS are identified by one or two letter codes. The tree structure of the models defined by code is shown in Section 3 in Figure 4.

Each branch (or path) of the tree represents a particular assessment estimation route which describes the behavior of a particular type of chemical under a given set of user specified accident conditions. Since the properties of a chemical may vary with ambient conditions (i.e., temperature), and in some cases, depending upon the chemical spilled, various types of hazards are possible for a given set of accident conditions (e.g., gas or liquid release), some chemicals may follow more than one route down the tree. These alternatives have been reflected in the hazard assessment codes given in COMDTINST M16465.12 and the HACS Chemical Property File. Each "scenario" or possible situation for which an assessment may be desired makes up a sub-set of the total hazard assessment code given. HACS accepts only one sub-set of these alternatives (defining a single branch) at a time, producing the hazard

*A later report entitled "Development of Additional Hazard Assessment Models" describes new models installed during 1976.

assessment for that sub-set. It is important that the user recognize that a number of runs (one for each possible sub-set) may be required to fully assess all the hazards which may be presented by the spill of a given chemical under particular conditions.

A typical estimation route sub-set may be illustrated by the following sequence:

1. Model A - calculate average release flow rate and total quantity released.

2. Model P - compute concentration of water miscible liquid at a downstream point in a river.

If flow rates are known or if other information that normally will be calculated by models is known to the user from a field observation, he can omit a model by submitting user inputs to override (i.e., replace) the information calculated by the model. For example, if a field observer can estimate the amount of liquid released and the other quantities calculated by Model A which are required for execution of Model P, he may input these quantities to override the calculations of Model A and proceed directly to the execution of Model P.

HACS contains an internal decision making capability, done according to a priority scheme described in Section 2.1.1 of this manual, for deciding when and how to utilize user override values of values which are normally calculated outputs of models. This capability also allows the user the option of not omitting the execution of a particular model while at the same time overriding the output of this model which is normally input to a subsequent model. What HACS does is to execute the model for which override values have been provided as if they had not been provided, print out the values it has calculated, and then substitute the override values for the calculated values before proceeding to the next model. This allows the user to compare what HACS calculates as an answer with the answer which he has provided and to decide whether he prefers HACS' answer to his own. If he decides that HACS' answer is more reasonable or accurate, he can then rerun the problem after deleting his override inputs and determine what is predicted when HACS is not interfered with.

1.3 CHEMICAL PROPERTIES FILE

The Chemical Properties File contains the physical and chemical properties necessary to execute HACS for 900 hazardous chemical substances. Some properties, not measured in the laboratory, have been estimated using techniques which have been proven acceptably valid for similar chemicals. The techniques were selected and utilized by R. Reid, co-author of the "standard" reference, "The Properties of Gases and Liquids" by Sherwood and Reid. Properties are arranged in alphabetical order by chemical code (a three letter recognition code assigned to each

chemical) and all properties pertaining to a given chemical are contained in one logical record, automatically available to HACS for conducting a hazard assessment.

The properties for a given chemical are accessed by specifying the recognition code for the desired chemical. This is the only input required by the user to obtain the required physical and chemical properties associated with the discharged chemical.

1.4 PHYSICAL UNITS

HACS performs all internal calculations in CGS (Centimeter-Gram-Second) units. However, for input and output purposes, the user may utilize any or all of four different unit types. Besides CGS units, quantities can be input or output in English, Standard International (SI) or "mixed" units. For example, quantities describing distances may be expressed in units of centimeters, meters, feet, or miles, and velocities may be expressed in units of centimeters per second, meters per second, miles per hour, and knots (nautical miles per hour). Section 3 of this manual describes how the user may utilize or request these various unit systems in running HACS.

1.5 OUTPUT FROM THE HACS SYSTEM

Estimation Route Reports:

For each model that is executed in a HACS run, the system will provide a list of inputs required for the execution of that model and their sources; that is, whether the input quantity used came from a Default File, Chemical Properties File, another estimation model, or from the user. This enables the user to check the validity of the quantities being used by a HACS model and review the sources of input values to determine whether additional observation data can or should be supplied in any given situation. When a model has completed calculation, the system reports the quantities calculated by that model. This continues until all the required models have been executed.

Plotting:

HACS has the capability to plot concentrations and other variables as functions of spatial parameters and time. These plots are produced directly on the user terminal, and are approximately page size to facilitate facimile transmission to field units. The selection of both plots and table output displays is controlled by user options.

Run Summaries:

The HACS/UIM contains a number of options to produce for the user text descriptions or explanations of assessment models and individual data items. At the end of each assessment run, users may request displays

of the values of all data items that were used in the run.

Chemical Properties File Report:

During the execution of each model, an input summary is produced by HACS which lists the current value of each data item required by the model, and identifies the source or origin of each value. The values obtained from the chemical property data file are noted as either estimated or exact values, and the display only includes those values that are actually used by the model. The display which may be produced as part of the overall run summary will, if selected by the user, include all data obtained for the particular chemical from the external file. Alternatively, users may wish to obtain complete data reports via a separate selective retrieval and display program (documented in a separate report).

Using the selective retrieval program the data on the file can be reported in CGS, SI, ENG (English) or MXD (mixed systems of units. A user may specify those chemicals that he wishes to have reported or he may receive a report of all the chemicals on the file. For a given chemical, all of the data or only selected items may be reported.

Some of the data in the properties file consist of coefficients for equations that describe certain properties as a function of temperature (see Section 2.4.3). These coefficients are displayed by the retrieval program in different units, such that the standard form of the equation will give function values in the appropriate units. Conversion among unit systems of the coefficients involves non-linear conversion equations, and since HACS users can provide any coefficient values in any sequence, HACS cannot automatically provide a similar conversion capability of temperature function coefficients. For this reason, user input to HACS of temperature function coefficients is constrained to CGS units only as indicated in Appendices H and I.

1.6 LIMITATIONS AND ACCURACY

HACS is based on the mathematical models presented in Assessment Models in Support of the Hazard Assessment Handbook (COMDTINST M16465.13), Report No. CG-1-74, U.S. Coast Guard, January 1974.* The predictive capability of HACS is directly related to the accuracy of description of real life physical phenomena by these models. Limitations of these models include:

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*A later report entitled "Development of Additional Hazard Assessment Models" describes new models installed during 1976.

1.6.1 Physical Modeling Limitations

Physical modeling limitations are due to the fact that phenomena occurring in nature may be too complicated to describe fully and/or to be amenable to mathematical descriptions. For example, the continuous and large rate of spill of oil from a ship in a heavy sea with gusty winds cannot be modeled completely because the effect of wave action on oil dispersion is not known accurately. HACS assumes for this situation that all of the oil is spilled into a calm sea and predicts that size of the spill as a function of time. Similarly, for vapor dispersion predictions, HACS assumes that the terrain is flat, that the wind velocity and direction are the same at all heights above ground, and that the vapor is neutrally buoyant - a combination which is not particularly common in real life. Similar assumptions are made in modeling the fire and vapor hazard from water miscible, cryogenic liquids. Therefore, it should be noted that though HACS seemingly gives very accurate numerical answers, these are only the best estimates (consistent with presently available models) for the hazards.

The extent to which each of the models in HACS represents a real life situation differs from model to model. For example, the venting rate model (A) represents the actual situation reasonably well, provided that the thermodynamic equilibrium assumption holds. On the other hand, there is no experimental evidence as to what happens when a large quantity of a cryogenic liquid, heavier than water, is dumped into water. The model in HACS for this situation (MODEL I) gives an estimate whose accuracy is at best accurate to within a factor of ten. For example, if Model I computes that all the chemical will evaporate in one minute, the real life case might be that it takes ten minutes. Although a factor of 10 in this particular case may seem excessive, it is important that the user realize it is better to know the evaporation time will be between 0 and 10 minutes than to not know whether 10 minutes, 1 hour, 1 day, or 1 week is required.

1.6.2 Limitations Due to Generalization

HACS is designed to predict the hazards caused by a spill of any of 900 different chemicals on water. Because of the widely varying properties of these chemicals, and the variety of phenomena which each may exhibit under various accidental and environmental conditions, it became necessary to formulate the hazard assessment models in HACS so that they can be useful for general types of chemicals under various general types of accidental and environmental conditions.

Some of the assumptions utilized in making the models non-chemical specific also can affect the accuracy of computed results. For example, development of Model P, the water dispersion model for chemicals spilled onto water, was based upon the assumption that the chemical will completely and immediately dissolve in water. Although this assumption is completely valid for most of the chemicals for which Model P is

applicable, it may lead to inaccuracies for substances which are partially soluble. Substances of this latter type will eventually dissolve completely, but may do so at a rather slow rate.

An additional consequence of generalized models is that unusual hazards such as thermal explosions, vapor explosions, and other such chemical specific phenomena are not addressed by HACS. Thus, the user should not hesitate to carefully review the COMDTINST M16454.12 hazardous chemical data sheets for the substance if its hazard assessment code contains the letters, O, Z, or RR, or if he or she has other cause to suspect unusual hazards.

2.0 HACS INTERNAL OPERATIONS

This section describes in further detail the HACS operations introduced in Section 1. Concepts of the HACS data structure and manipulation are presented in some detail to aid in understanding the operation of the system from a users' viewpoint. Specific technical documentation of the system is provided in a separate report.

2.1 HACS COMPONENTS

HACS consists of several program components:

- Executive System -- to control the overall sequence of operations, and to provide utility functions for data base I/O operations, terminal plotting, output labeling and program overlay and segment loading.

- User Input Processor -- to read, verify and store user input data, and to control the initialization of HACS data files.

- Property Data Processor -- to retrieve requested data from the property file, perform unit conversions to internal HACS CGS units, to compute values of functions of temperature, and to transfer chemical specific property data to the HACS state file.

- Assessment Models -- a series of separate programs retrieving required data from the HACS state file, performing the indicated assessment computations, storing computed values in the state file for subsequent use and generating output to the user terminal.

These components utilize a number of both internal and external files in their operations:

- Program File -- a permanent disk file containing pre-compiled HACS program code in overlay and segment structure. The HACS executive system automatically accesses this file to load portions of the HACS program code into computer memory for execution as required.

- State File -- an internal program file constructed by HACS during an assessment run; provides data base storage for all user input, property, default and computed data items utilizing a data quality priority structure.

- Default File -- a permanent disk file defining the structure of the HACS state file, and containing estimated values for HACS data items to be used only in the absence of any other value.

- Chemical Properties File -- a permanent disk file containing predefined physical property data for 900 hazardous chemical substances.

- Save File -- an internal program file containing a copy of a HACS state file after completion of user input operations. Permits HACS re-runs requiring only new input values to be used.

- Message Files -- three external permanent disk files contain text messages describing the individual hazard assessment models, groupings of models into scenario sequences, and individual data elements. These messages may be requested for display by the user during a run by typing a question mark (?) response at the user terminal.

Figure 1 gives a simplified illustration of the external and internal files used by HACS.

2.1.1 State File

The HACS state file contains all information necessary for the operation of HACS. It provides storage for all input variables for the execution of HACS models and output information (units, values, print names, etc.) for all HACS computed results.

At the start of each new HACS run, the contents of the state file are initially obtained from the HACS default file. This provides basic definitions of each data item (see below) and default values which are only used in the event that no other value is supplied or obtained. The input variables for the execution of HACS models are then obtained by the User Input Processor from the user terminal, and the Property Data Processor from the chemical properties file, and stored in the state file. When a HACS model is executed, the information necessary for the execution of that model is retrieved from the state file, and the results of a model's execution are then stored back into this file. Thus, when another HACS model is to be executed, it has access to input information and the computed results of a previously executed model. For each variable in the state file, the information stored includes:

- Variable number -- a unique four digit number (such as 2015) identifying the input or output quantity; also referred to as field number.

- Type of quantity -- an indicator referencing the permitted units in which values of the variable may be entered, and the conversion factors used to obtain values stored in the state file in CGS units for internal operations.

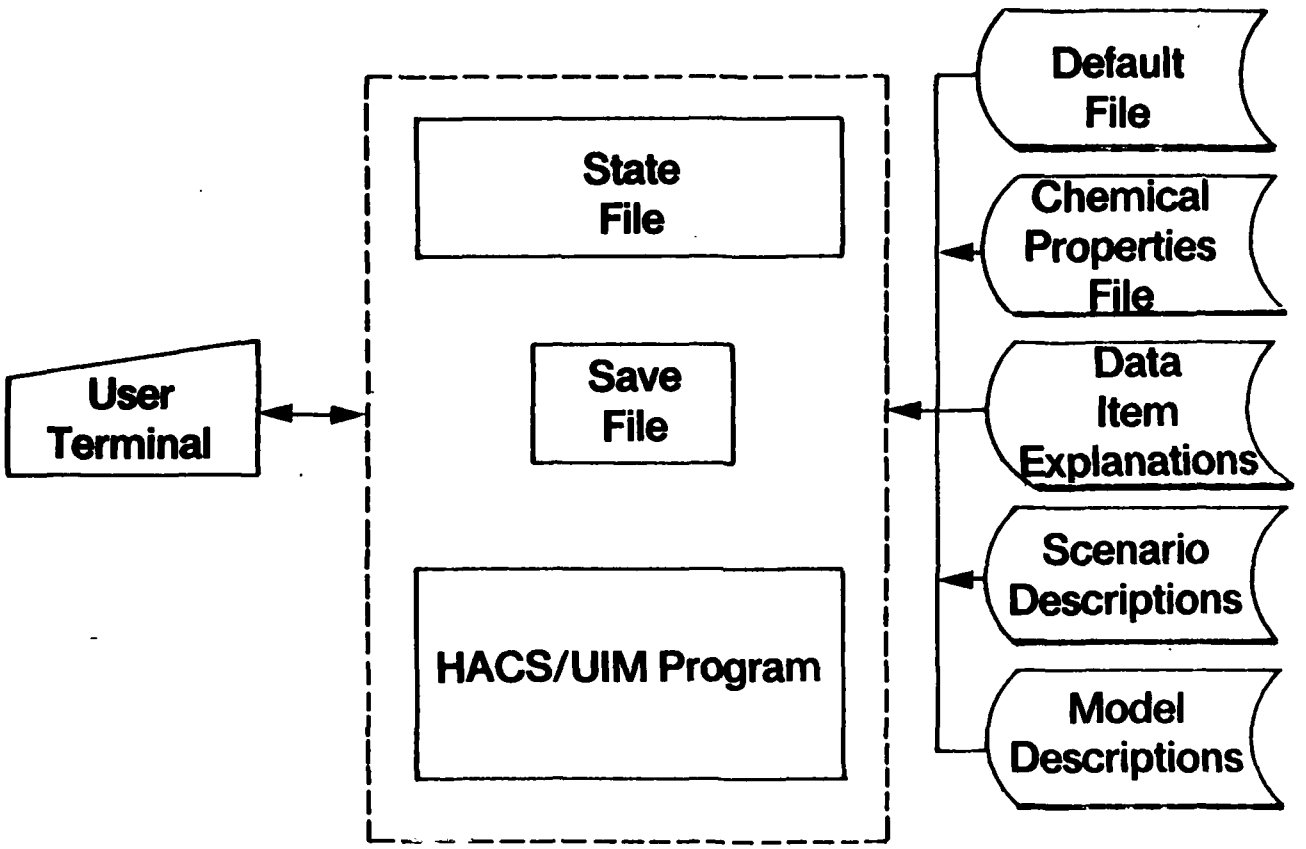

FIGURE 1

HACS/UIM DATA FILES

- A source or priority code -- to indicate the origin of the data item stored in the state file. These priority codes are as follows:

  0 - No value present
  1 - HACS default file value
  2 - Chemical property file estimate
  3 - Chemical property file exact value
  4 - HACS computed value
  5 - User supplied data value
  6 - HACS system value

  For a value of a variable to be used in place of an already existing value of the same variable, it must have a source or priority code that is not numerically lower than the source code of the existing value.

- The value of the input quantity or calculated result.

- The nominal minimum value that the variable is reasonably expected to reach.

- The nominal maximum value that the variable is reasonably expected to attain.

- The display name of the variable for identification of the variable in output reports.

As HACS models are executed, computed values will be stored in the state file and will be available for subsequent model executions. Thus, the sequence in which models are executed has a direct bearing to the information available for a given models' execution.

As the value of any variable is stored in the HACS state file, it is compared to the nominal minimum and maximum limits defined for that variable. If an attempt is made to store a value which does not lie within the nominal range, HACS will produce a warning message but will continue to use the value supplied in subsequent computations.

All values stored in the state file are in CGS units, and all internal HACS computations are done also in CGS units. Unit conversion operations for input and output display are controlled externally to the state file, as governed by the type of quantity indicator stored in the file for each variable.

2.1.2 Default File

The default file contains a value for every input item in the state file, and at the start of each new run the initial contents of the HACS state file are copied from the default file. Thus the default values, having

the lowest source or priority code*, are used only if no value is supplied by either the chemical properties file or the user. The purposes of the default file are (a) to define the structure of the HACS state file, and (b) to supply variable values to HACS so that a model can be executed regardless of whether or not every input item required by that model was specified by the user. This design also permits execution of HACS to continue even if errors are found by the user input processor, and the affected user data values cannot be stored in the state file. An indication in the output that a default value was used should be interpreted as a warning to the user that he has not specified a particular value required by a given model. He may then elect to specify that value and rerun HACS, or he may accept the results of the model based on the default value that has been used if he judges that value acceptable. A list of the default values HACS contains is given in Appendix C.

2.1.3. Chemical Properties File

The chemical properties file contains the physical and chemical properties, currently for 900 hazard chemical substances, stored on an external disk file. The properties of a given chemical are automatically accessed by the Property Data Processor, initiated by a user request specifying the recognition code of the discharged chemical (see Section 3.2 of this manual).

The physical property file is arranged in sequential binary records. The first record on the file is a header record which identifies the version number, creation date and file label. The remaining records are those of chemical properties, appearing in ascending alphabetical sequence by chemical recognition code. All data pertaining to a single chemical are contained in a single record.

HACS users must independently provide instructions to computer system operators to ensure that the appropriate property file version is used for a HACS run. Output is provided with each HACS run to identify the version of the property file that was accessed.

Each binary chemical properties record is arranged in two arrays. The first is a status code array and the second is an array of data values for each of the 74 items recorded for each chemical. Each of these properties has a status code indicating whether the data value associated with it is an exact value (status code = 3), an estimated value (status code = 2), or a missing value (status code = 0). Data values are transferred from the property file to the HACS state file only if the status codes are exact or estimated; missing property values are not transferred.

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*A priority code 0, for no value present, exists only for correspondence with property file status codes, and cannot occur in the present configuration of HACS.

The data array contains the values for each of the properties in either numerical or alphanumerical data. All numeric data is stored on the property file in SI units and conversion to CGS units is performed automatically by HACS on transfer. The properties, and their definitions on the file, are described in a separate report for the property file update and maintenance program. A list of the 900 chemicals currently contained on the file, along with their chemical recognition codes, is given in Appendix A.

2.1.4 Save File

After each initial user input operation, HACS automatically saves the contents of the state file. The state file will contain the initial default values, plus any user input data that has been read and stored. Since the next operation performed is controlled by the property data processor, the save file is assumed not to contain physical properties (logically the user may have specified a different compound, so the property data must be retrieved again). On subsequent runs, the user may elect to provide complete data for an assessment situation, or input values to augment previously entered and saved data. This is particularly useful for investigating the sensitivities of hazards to variations in selected input conditions. The save option is an automatically controlled feature of HACS, initiated by the appearance of user selected options for RUN, RERUN and CONTINUE which are described in Sections 2.2 and 3.1.

2.1.5 Additional System Files

The logical structure of the remaining HACS files identified in Section 2.1 need not be of concern to most users. All external files must however be defined in the computer coded procedures used to invoke the execution of HACS. Prior options to permit HACS operation to exclude the use of the chemical properties file are not contained in the UIM. Section 3.2.1 describes the use of cataloged procedure files for pre-defined control of HACS execution.

2.1.6 User Input Processing

HACS contains an interactive user interface module (UIM) to facilitate use from remote low speed computer terminals. During normal operations HACS displays prompt messages at the terminal, requesting input from the user that controls the overall sequence of operation. These start with the selection of the type of run, identification of the discharged chemical, and specification of the hazard assessment model(s) that are to be run.

The UIM is functionally located between each assessment model and the HACS internal state file. That is, initial user operations control the initialization of the state file, first with default data and then with optional physical property data. At the start of the execution

of any particular model, the required user data is not necessarily contained within the state file. When the model attempts to retrieve a data item from the state file for computational use, the UIM initiates a terminal input sequence for the data item. Users may either accept current values in the state file or enter new values. Once input, the data item is both stored in the state file and returned to the initiating model.

The UIM provides for free-format terminal input, and data entered by the user are validated as received. Diagnostic conditions are displayed, and users may correct errors before proceeding.

Overall, the data input requirements for the assessment models are quite complex. Data items for different models may either be similar or different. Within a single model, different data elements may be required depending on spill conditions or user options. By interfacing directly with each model, the UIM is able to request from the user only those data items that are actually required for the specific computation requested by the user.

2.2 BASIC PROCESSING STEPS OF A HACS RUN

A basic HACS execution involves interfacing with a number of files to collect the input required for HACS estimation models and to present the results of estimation model calculations to the user. Subsection 2.2.1 introduces extended capabilities provided in HACS using options for RERUN and CONTINUE control; the discussion below is limited to basic RUN control only. Figure 2 gives a simplified overview of the HACS internal structure showing the relationship of the UIM Terminal Interface to other components of the system.

(1) Access Default File

HACS begins a basic run sequence by copying the contents of the default file from permanent disk storage to the internal memory space reserved for the state file. This defines a file dictionary for the contents of the state file and enters a value having a source or priority code of 1 for every variable which has been defined in the state file.

(2) Process User Input Control Data

The UIM next conducts a dialog with the user terminal to obtain data which specify run control options, the recognition code of the discharged chemical substance, hazard assessment estimation route codes, and selection of system controlled options.

(3) Copy State File

Following completion of initialization for a single assessment run, the contents of the state file are copied to the internal memory space reserved for the save file. This file may be used to re-start subsequent assessment runs.

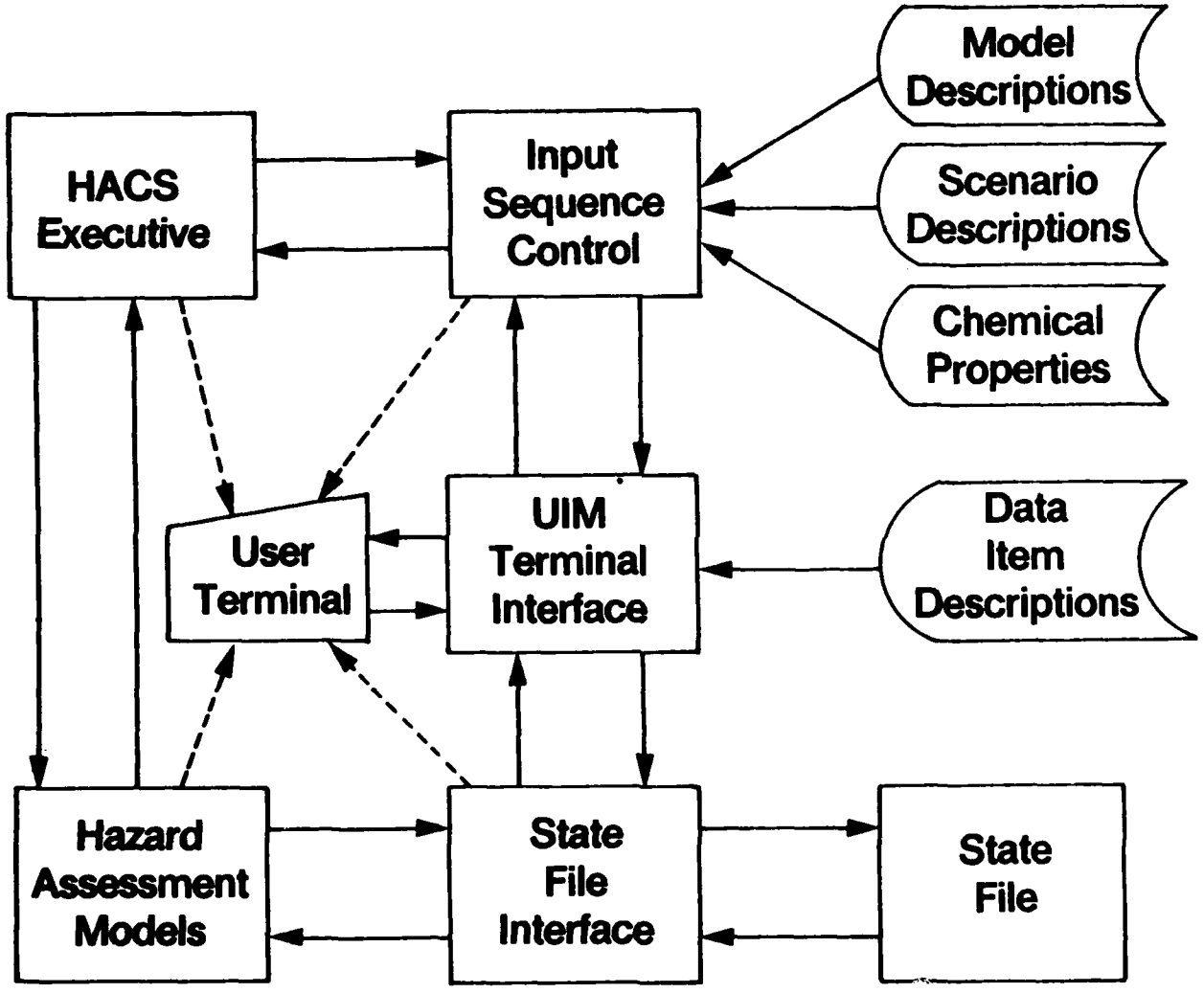

FIGURE 2

SIMPLIFIED OVERVIEW OF HACS/UIM INTERNAL STRUCTURE

(4) Access Property File

Users may enter all necessary physical property data directly, or may elect to have HACS obtain the necessary information by searching the physical property file which presently contains data for 900 hazardous chemical substances. Direct user input is necessary for chemicals not defined on the file and may be advisable if a larger series of runs are to be made using the same chemical. In any case, user values may always be supplied to override any item contained on the property file.

(5) Search Property File

The Property Data Processor takes the user-specified chemical recognition code and controls a sequential search for a matching code on the property file. When found, all data defined (source codes 2 or 3) are read, decoded and converted from SI units to CGS units for transfer to the HACS state file. The Property Data Processor also performs the computation of all properties given as functions of temperature, at both ambient and boiling temperatures.

(6) Property Data Report

The operations performed by the Property Data Processor are summarized by printed outputs produced in an input data listing which can be obtained for each hazard assessment model. Since all defined property values are transferred, the report will reflect the property file content and whether these values are necessary for the user-specified estimation route. The audit reports produced by each assessment model will identify the specific property data used for input to the model. Diagnostic messages are not suppressed.

(7) Transfer Property Data to State File

The Property Data Processor transfers all chemical property values defined (exact or estimated) on the property file, and all functions of temperature which could be computed to the HACS state file. For each item, the status code of the value currently stored for a field is checked before the property value is stored. If present, user data or HACS-computed values will override values obtained from the property file. Users are cautioned that if user-provided chemical property data has been entered, the user values will override the corresponding values from the property file in all following computations.

(8) Initiate Model Executions

Using the model codes specified by the user for the estimation route data, HACS initiates a sequence of model executions. The system routines first locate the appropriate program code on a permanent disk file, load this into memory and then transfer control for execution. Figure 3 gives a conceptual overview of the steps performed in the execution of a single HACS model.

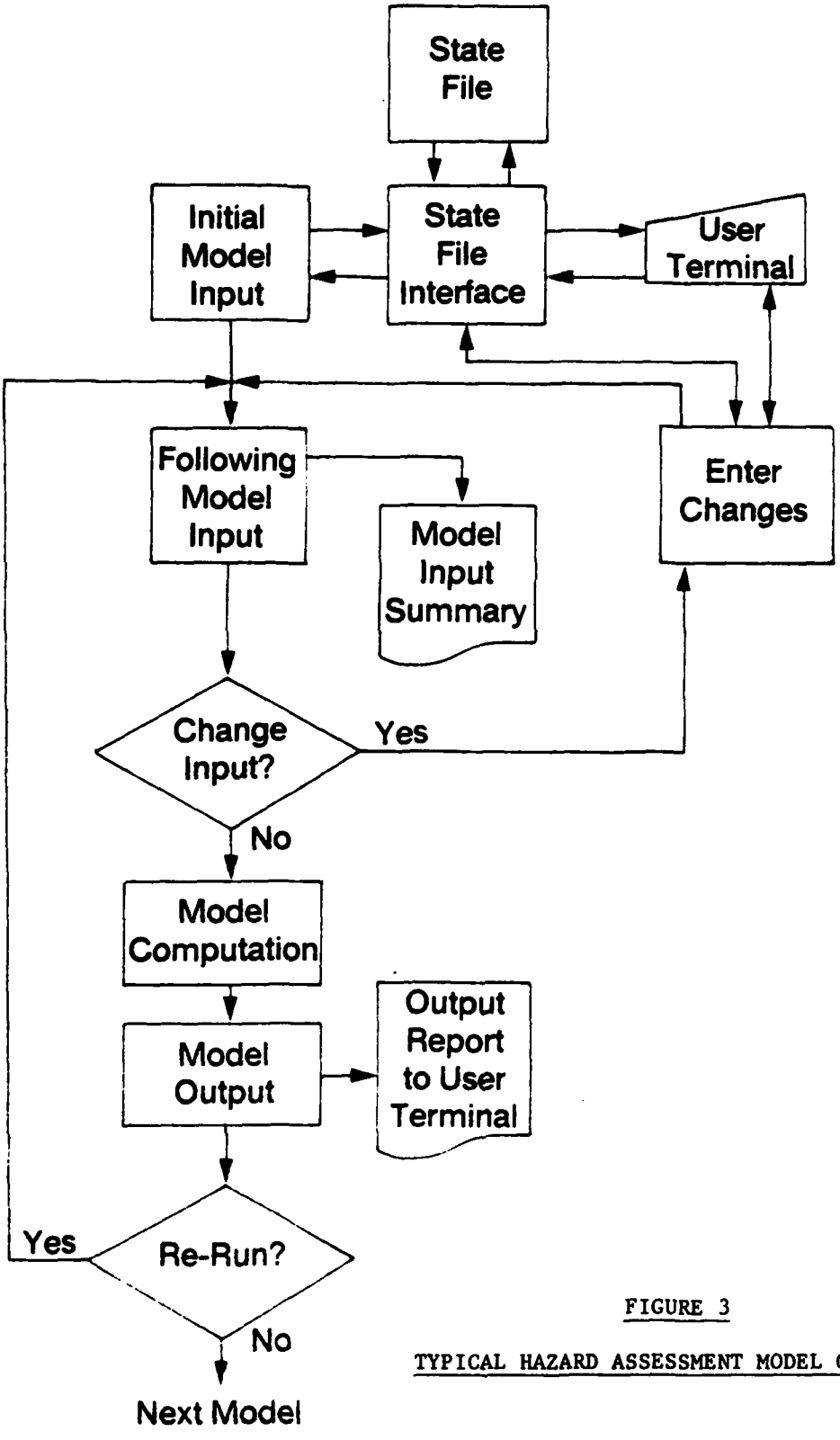

FIGURE 3

TYPICAL HAZARD ASSESSMENT MODEL OPERATION

(9) Initial Model Data Input

As each assessment model is executed, the model retrieves each required data item from the state file. Initially, the current value may be either a default value or a chemical property value. If more than one assessment model is being executed, or HACS is operating under RERUN or CONTINUE control, current values may also be previously computed or user input values. At the time of retrieval from the state file, the UIM detects the transfer of any default data values and, for these, conducts a dialog with the user terminal. Users may either elect to accept the current default value, or enter a new value as may be appropriate. Only input for previously unspecified values are requested.

(10) Model Input Summary

After the initial transfer of data input values from the state file to the model, and UIM queries to the user terminal to obtain values for any previously unspecified data unputs (if any), HACS produces a full printed summary of all input values being used by the model. For each item, the display includes the field number, field name, value and unit, and identification of the origin (or source) of the current value.

(11) Change Model Input

HACS allows a user to change the value of any data item prior to running a model. Generally, these changes will be for one or more items listed in the preceding model input summary; however, actually any data item contained in the internal state file may be changed. Users may wish to change any previously entered value, or internal values (computed results, property data) not previously displayed by the UIM. If any changes are made, the model input summary is automatically repeated to list all input values being used before executing the model.

(12) Assessment Model Execution

On completion of the model input operation, the actual hazard assessment computations are performed and the computed results are displayed. Additional outputs in the form of tables or graphs may also be generated depending on user-specified options. The output of each model is labeled using messages to denote the sequence of operations.

(13) Model Re-Run

On completion of the execution of any hazard assessment model, HACS provides an opportunity to repeat the execution of the model prior to going on to the next model in the selected scenario. This allows users to perform a series of different runs, varying input data as may be desired, until satisfactory results for any particular spill conditions have been obtained. Tables and plotted outputs may be suppressed during initial runs, and only produced on a final run to simplify terminal operations.

(14) Complete Execution of Prescribed Estimation Route

The HACS executive system continues to cycle through steps 9 to 13, executing each of the assessment models specified by the user until all calculations along the hazard estimation path have been performed. Each model obtains in sequence the necessary input data from the HACS state file and stores in the state file its computed results. In general, in the absence of overriding user data, some or all of the output stored in the state file by a rate model will be accessed as input for a model following in the estimation route sequence.

(15) Summary Display

After all the models specified by the user for the hazard assessment estimation path have been run, HACS provides the user with an option to produce a printed summary of the run. Any scenario codes, model codes, user input values, computed values and chemical property values may be selected for display; additional options provide for displays of item values, with or without explanatory discriptions.

(16) Continue User Operations

After all models along the specified estimation route have been executed, the executive system resumes control to begin processing the next user specification for a chemical and hazard assessment path. The state file is initialized depending on the user selection of RUN, RERUN, or CONTINUE options and the above sequence of operations recycles starting with step 2. Computations continue until the user requests termination of the session.

2.2.1 CONTINUE and RERUN Options

Two additional types of basic hazard assessment runs may be performed to provide for interactive analysis, assessments using products of reactive chemicals, and selective control of overriding user data.

The basic RUN option, described above, follows a sequence in which initial default data values are replaced by physical property data; then a series of assessment models are executed to obtain and store computed results in the state file. During these operatations, the sequence of model executions is fixed by the codes entered by the user; user data values in the state file will always override any values computed by rate models.

To illustrate the CONTINUE option, one or more assessment models might be executed using the RUN option to produce an assessment report plus an updated state file containing computed values, as well as the original set of user input data values. The CONTINUE option permits users to immediately follow this run with one or more additional runs starting with the full set of computed values previously obtained but including new or revised user values. This permits selective override control for computed values, allows different portions of an overall hazard assessment situation

to be run with different options for file control, output selections, path codes and even chemicals, and allows different user values to be substituted for the same variables at different locations along the assessment path.

The RERUN option originally provided for repeating a basic assessment RUN while at the same time modifying some of the original input data. In operations with the UIM, however, the use of the CONTINUE operation together with interactive user input directly to each assessment model now provides an equivalent function.

The RUN, RERUN, and CONTINUE options may be repeated indefinitely, within the computer time and line limits set for the HACS job. Users are cautioned, however, to note the sequences that are used to initialize the state file at the start of each type of run so that there is no confusion as to the nature (source) of the data that is used. These options will function even if given in sequences other than intended, and default values will be substituted automatically if necessary. Also, users are cautioned that during the transfer of physical property data items, if a state file already contains either computed or user values for property items, these will not be replaced or re-initialized by values read from the property file.

The HACS executive system controls the state file initialization sequences for all RUN, RERUN and CONTINUE options, and provides on the terminal output a message indicating the file status as EMPTY, DEFAULT, USER, or COMPUTED, referring to the highest source code for any data item in the file.

2.3 CHEMICAL PROPERTY DATA RETRIEVAL AND REPORT GENERATOR

A separate computer program is available to allow HACS users to obtain data from the property file by accepting card input and producing line printer output. Complete descriptions of the use and capabilities of the selective retrieval and report program are contained in a separate manual; a brief overview is given in the following paragraphs.

2.3.1 Read User Input

Control cards (user input) are accepted by the program to specify the system of units (SI, CGS, ENG for English or MXD for mixed) in which the data is to be displayed, options for the specific chemical compounds that are to be selected and within these compounds, options for the particular data items that are to be retrieved. Additional user options provide for line printer page spacing, and copying selected chemical compound data to magnetic tape.

2.3.2 Find the Requested Chemicals on the Property File

For each chemical specified (by chemical recognition code) by the user, the property file is searched until a record containing the same recognition code has been found. All program operations (user input and search) occur in ascending alphabetical order by recognition code. Incorrect user requests for undefined recognition codes will produce diagnostic messages.

2.3.3 Produce the Specified Output

For each specified compound, the selected data items are displayed in the system of units selected by the user. All output is given in only a single system of units. Printed reports are produced using a variable format technique so that only the data items requested are displayed; thus on different reports having different items requested for display values of the same field will in general be given in different positions.

It is suggested that for general reference complete printed reports of the entire contents of the property file should be maintained, and available to HACS users in the commonly used sets of units. Temperature function coefficients, however, may only be entered in HACS using CGS units due to the non-linear form of the unit conversion equations; different units for the coefficients are only allowed directly in the property file report and update programs.

The selective retrieval and report program may also be used to produce abbreviated "directories" of the contents of a property file giving the recognition code, name, and assessment path codes for all, or selected, compounds contained on the property file. This option is useful to obtain a compact guide to the contents of a property file after updates have occurred.

2.4 UPDATING THE CHEMICAL PROPERTY FILE*

A separate computer program is available for use in updating (adding new compounds or replacing previously estimated or missing data items) a chemical properties file. This program operates by accepting card or tape update transaction input, merging the update transactions with an existing property file and producing as output an updated file. The program performs extensive data checking functions to validate each new transaction and to ensure that the process of entering new data does not create any inconsistencies among data previously entered for a compound. Complete des-

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*Use of the physical property file update program must be authorized by the Chief of the Marine Environmental Protection Division.

criptions of the use and capabilities of the property file update and maintenance program are contained in a separate manual; a brief overview is given in the following paragraphs.

The update program automatically indentifies each version of the property file that is produced, and the file identification, creation date, and version number are automatically displayed as part of the HACS output for any assessment run that accesses a property file. HACS users should always be aware of which version of the property file has been accessed, particularly if different versions exist.

2.4.1 Read Update Information

Basic information processed by the update program consists of data cards where each card contains a single data value and unit, and the necessary indicators to associate the value with a particular field position and a particular chemical (specified by recognition code). Each card also contains an indicator to define the type of update operation that is to be performed. Three types of basic update operations are possible -- add a new chemical, delete an existing chemical, and add or change individual values for an existing chemical. A copy function is performed as a special case of these.

Additional data is required for file identification. Input data for chemical properties may be given either on cards or magnetic tape, and options provide for updating or creating a property file.

2.4.2 Process Update Transactions

The update program operates in a sequence of steps, first reading all input data for a single chemical then on completion searching for the appropriate position on the property file. If existing data is to be modified, the program merges the old and new values. Next, if necessary, newly input data items are converted to SI units for file storage, and a completed chemical compound data record is written to the output file. Unit conversions from any of the four systems to SI units for any fields are permitted; these are controlled by a unit conversion specification data deck which must be given at the start of a run.

At each step in this sequence different types of error tests are carried out, and if any errors are found no update for the compound occurs.

2.4.3 Chemical Property Temperature Functions

Certain chemical properties are functions of temperature, and the equations representing these functions lead to chemical specific coefficient values which are stored on the property file. In most, but not all cases, an additional fixed point (value of the function at a specific temperature) is also stored.

The units of the coefficients, and the independent temperature, determine the units in which the function value is obtained. All units are consistently defined in each of the four systems - if the standard form of an equation is used, the units of the function value will be in the same system in which the coefficients are given.

In HACS, however, conversions of temperature function coefficient units are not permitted; all coefficients must appear, if given as user input, in CGS units only.

The temperature functions are defined over a specific temperature range, defined for each function by a lower and an upper temperature bound contained on the property file. Strictly speaking, the equations are only valid within these defined temperature limits. If, during the transfer of temperature function values from the property file to the HACS state file, an attempt is made to obtain a function value at an ambient or boiling temperature which does not lie within the defined bounds of the equation, HACS will generate a diagnostic message and then substitute the appropriate temperature bound as the independent variable for the computation. In this case HACS will also adjust the source code of the function value, if otherwise exact, to estimate.

The equation forms used within HACS for the temperature functions are listed below. The names used are the appropriate field names as defined in the HACS state file.

All computations are performed internally using CGS units, and the independent temperature t is obtained from field 2004, TEMP START or field 1003, BOIL TEM LIQ.

Equation 1: Saturated Liquid Density

$$F(t) = A + Bt + Ct^2$$

$$t_{lo} \leq t \leq t_{up}$$

where the coefficients and bounds from the property file are obtained from the HACS state file as:

- A = field 1038, SLD COF ARHO
- B = field 1039, SLD COF BRHO
- C = field 1040, SLD COF CRHO
- t_{up} = field 1041, SLD UPR BND
- t_{lo} = field 1042, SLD LWR BND

and computed values of the function are stored in the HACS state file as:

field 1004, DENS LIQ AMB, for t = field 2004, TEMP START
field 1021, LIQ DENS BP, for t = field 1003, BOIL TEM LIQ.

Equation 2: Liquid Viscosity

$$F(t) = e^{A + \frac{B}{t + 273.15}}$$

$$t_{lo} \leq t \leq t_{up}$$

where the coefficients and temperature bounds from the property file are obtained from the HACS state file as:

A = field 1045, LQ VIS CF A
B = field 1046, LQ VIS CF B
t_{up} = field 1047, LQVS UPR BND
t_{lo} = field 1048, LQVS LWR BND

and computed values of the function are stored in the HACS state file as:

field 1006, VISCOSITY-AM, for t = field 2004, TEMP START
field 1005, VISCOSITY-BP, for t = field 1003, BOIL TEM LIQ

Note that the equation as written above introduces a third "coefficient", the constant 273.15 is this case, which derives from writing the equation in a form that remains unchanged in any of the systems of units defined for the property file.

Equation 3: Liquid Thermal Conductivity

$$F(t) = A + Bt$$

$$t_{lo} \leq t \leq t_{up}$$

where the coefficients and temperature bounds from the property file are obtained from the HACS state file as:

A = field 1051, L THR CN CFA
B = field 1052, L THR CN CFB
t_{up} = field 1053, LTC UPR BND
t_{lo} = field 1054, LTC LWR BND

and computed values of the function are stored in the HACS state file as:

field 1081, L THR CON-AM, for t = field 2004, TEMP START
field 1082, L THR CON-BP, for t = field 1003, BOIL TEM LIQ

Equation 4: Liquid Heat Capacity

$$F(t) = A + Bt$$

$$t_{lo} \leq t \leq t_{up}$$

where the coefficients and temperature bounds from the property file are obtained from the HACS state file as:

A = field 1057, L HT CAP CFA
B = field 1058, L HT CAP CFB
t_{up} = field 1059, LHC UPR BND
t_{lo} = field 1060, LHC LWR BND

and computed values of the function are stored in the HACS state file as:

field 1007, HT CAP LQ-AM, for t = field 2004, TEMP START
field 1083, HT CAP LQ-BP, for t = field 1003, BOIL TEM LIQ

Equation 5: Solubility

$$F(t) = A + Bt$$

$$0°C \leq t \leq 30°C$$

where the temperature bounds for the equation represented on the property file are fixed for all compounds, and are not stored as data items. Coefficients from the property file are obtained from the HACS state file as:

A = field 1028, SOL EQ COEF1
B = field 1029, SOL EQ COEF2

and computed values of the function are stored in the HACS state file as:

field 1084, SOLUBLTY-AM, for t = field 2004, TEMP START
field 1085, SOLUBLTY-BP, for t = field 1003, BOIL TEM LIQ

Equation 6: Saturated Vapor Pressure

$$F(t) = 10^{A - \frac{B}{t + C}}$$

$$t_{lo} \leq t \leq t_{up}$$

where the coefficients and temperature bounds from the property file are obtained from the HACS state file as:

A = field 1010, VPE COEFF A
B = field 1011, VPE COEFF B
C = field 1012, VPE COEFF C
t_{up} = field 1062, SVP UPR BND
t_{lo} = field 1063, SVP LWR BND

and the computed values of the function are stored in the HACS file as:

field 1086, S VPR PRS-AM, for t = field 2004, TEMP START
field 1087, S VPR PRS-BP, for t = field 1003, BOIL TEM LIQ

Equation 7: Vapor Heat Capacity

$$F(t) = A + Bt + Ct^2 + Dt^3$$

$$t_{lo} \leq t \leq t_{up}$$

where the coefficients and temperature bounds from the property file are obtained from the HACS state file as:

A = field 1064, V HT CAP-CFA
B = field 1065, V HT CAP-CFB
C = field 1066, V HT CAP-CFC
D = field 1067, V HT CAP-CFD
t_{up} = field 1068, VHC UPR BND
t_{lo} = field 1069, VHC LWR BND

and the computed values of the function are stored in the HACS state file as:

field 1013, HT CAP VP-AM, for t = field 2004, TEMP START
field 1088, HT CAP VP-BP, for t = field 1003, BOIL TEM LIQ

2.4.4 Output

At each step of the processing sequence outlined in section 2.4.2, the update program produces a complete audit report of the process. First, individual update transaction cards are read and displayed together with any diagnostic conditions encountered for each card. Next if any unit conversions are required, both the original and converted values are given for all fields converted. The update program does not produce a complete display of the final contents of each updated chemical record as this

function is performed by the selective retrieval and display program. An overall processing summary is generated at the conclusion of each update run, giving total counts of all unit operations which were performed during the run.

2.5 UPDATING THE HACS DEFAULT FILE*

The default file currently used with the HACS/UIM was transferred from the batch version of HACS, and a direct means of updating this file no longer exists in the UIM. If necessary, updates can be accomplished using a combination of display programs and system editors, or regenerating new default files using the batch version of HACS. In future UIM versions, the external default file will likely be replaced by copies of externally saved HACS state files.

Default file updates may be made to change default values, nominal range limits, and even field names. Field numbers, data types (real, integer) and units may not readily be changed without accompanying revisions of HACS internal program code.

Internally, HACS contains several data files for which fixed space has been allocated on the basis of the current size of the default file. The addition of new data fields, or any other expansion beyond the current size of the file, will require internal program revisions.

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*Default file updates must be authorized by the Chief of the Marine Environmental Protection Division.

3.0 DETAILED USERS' GUIDE FOR HAZARD ASSESSMENTS

This section provides all the information necessary for a HACS user, somewhat familiar with the material in the previous two sections, to conduct hazard assessment runs. It consists of three major sections.

Section 3.1 gives an overview of the different hazard assessment models incorporated within HACS, and the rationale used for grouping different models into scenarios for hazard assessment computations.

Section 3.2 contains several sub-sections to describe the different steps or procedures which occur during a typical UIM run. User input data formats are discussed, and the UIM procedures are described using illustrations of the UIM prompt messages. The material covered in Section 3.2 does not depend on the particular hazard assessment models used; the type of dialog and user input covered in this section occurs in every UIM run.

Section 3.3 contains all the essential model specific descriptions for preparing input data and interpreting model output. The material in this sub-section is arranged in alphabetical order by model, describes each model and includes for each model tables of the input and output values.

3.1 HAZARD ASSESSMENT MODELS AND SCENARIOS

HACS is built around a set of mathematical models (see Section 3.3 for more complete rate model descriptions) that are specific computer programs for estimating discharge conditions and chemical behavior, such as flow rates for escaping chemicals (Model A), concentration of water miscible fluids (Model P), and vapor dispersion (Model C). The theoretical basis for these models is described in Assessment Models in Support of the Hazard Assessment Handbook published by the United States Coast Guard in January 1974. A later report entitled "Development of Additional Hazard Assessment Models" describes new models installed during 1976.

Each model contained in HACS is identified by a one or two letter code, and is used to estimate a particular type of behavior or hazardous condition resulting from the discharge of a hazardous chemical into water. Since there are a number of different conditions or hazardous phenomena that can arise when different chemicals are discharged, there are a number of different hazard assessment models. These models are logically organized and relate to one another according to specific chemical behavior on discharge; the relationships are defined by a hazard assessment tree which is given in Figure 4.

Individual models, identified by the letter codes in Figure 4, such as P and Q, are located along one or more paths or branches of the tree leading from the accidental release (at the top of the figure) to a possible

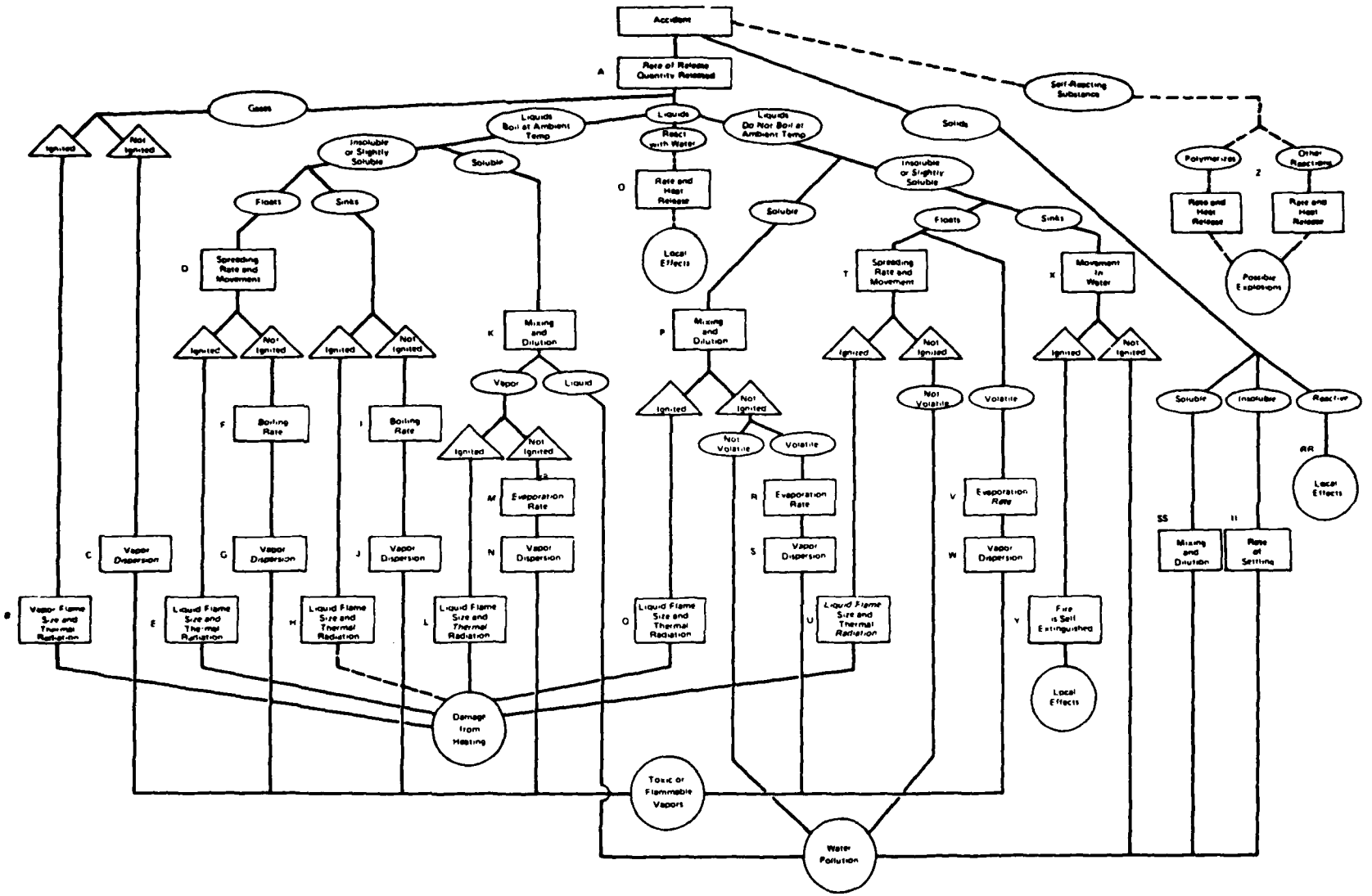


FIGURE 4

HAZARD ASSESSMENT TREE: (EVENTS CHART)

hazardous outcome condition (at the bottom of each branch). In general, each model along a path or branch requires certain input data, some of which may be provided by the user, and some of which may be calculated by a preceding model on the path. Results computed by the models may be displayed to the user as part of the hazard assessment and/or supplied by HACS as input to subsequent models along the path.

The groupings of model codes along single paths, as shown in Figure 4, for example, the group A-D-E, are referred to as hazard assessment scenarios.

Each branch or path of the hazard assessment tree in Figure 4 represents a particular estimation route or scenario which describes the behavior of a particular type of chemical under a given set of user specified accident conditions. Since the properties of a chemical may vary with ambient conditions (i.e., temperature), and, in some cases depending on the chemical spilled, various types of hazards are possible for a given set of accident conditions (e.g., gas or liquid release), some chemicals may follow more than one path down the tree. These alternatives are reflected in the hazard assessment codes (model letters) assigned to each chemical in CHRIS Manual II and on the chemical properties data file which is accessed by HACS/UIM. Each scenario or possible situation for which an assessment may be desired makes up a sub-set of the total hazard assessment code given in Manual II or the HACS data file.

Hazard assessment computations performed by the HACS/UIM are governed by the user selection of the hazard assessment models to be run, and the UIM contains extensive tutorial information to aid in the selection. Models may be specified individually, in groups of two or more for portions of a complete path through the tree, in groups representing complete scenarios, and in some cases in groups representing more than one scenario.

In most cases, however, the user model selection will specify a single sub-set (scenario) of the possible alternatives at a time, producing the hazard assessment for that sub-set. It is important that the user recognize that a number of runs, one for each possible sub-set or scenario may be required to fully assess all the hazards which may be presented by the spill of a given chemical under particular conditions.

A typical estimation route sub-set may be illustrated by the following sequence:

1. Model A - calculate average release flow rate and total quantity released.

2. Model P - compute concentration of water miscible liquid at a downstream point in a river.

If flow rates are known or if other information that normally will be calculated by models is known to the user from a field observation, he

can omit a model by providing user inputs to override (i.e., replace) the information calculated by the model. For example, if a field observer can estimate the amount of liquid released and the other quantities calculated by Model A which are required for execution of Model P, the HACS user may input these quantities to override the calculations of Model A and proceed directly to the execution of Model P.

HACS contains an internal decision making capability, done according to a priority scheme described in Section 2.1.1 of this manual, for deciding when and how to utilize user override values of values which are normally calculated outputs of models. This capability also allows the user the option of not omitting the execution of a particular model while at the same time overriding the output of this model which is normally input to a subsequent model. What HACS does is to execute the model for which override values have been provided as if they had not been provided, print out the values it has calculated, and then substitute the override values for the calculated values before proceeding to the next model. This allows the user to compare what HACS calculates as an answer with the answer which he has provided and to decide whether he prefers HACS' answer to his own. If he decides that HACS' answer is more reasonable or accurate, he can then rerun the problem after deleting his override inputs and determine what is predicted when HACS is not interfered with.

Additional information is contained in sub-section 3.2 of this manual regarding the user specification of hazard assessment models. Briefly, the models are specified by entering one or more of the one or two letter model codes. The models requested are then subsequently executed by the HACS/UIM in the sequence entered by the user. This is controlled by saving the user specified model letter codes in memory, and the current system limits the maximum number of codes that can be used in a single run to 15. This limit is substantially larger than any scenario currently required.

Since, for a variety of reasons, users may elect to run individual models, scenario sub-sets, complete scenarios or scenario groupings, the HACS/UIM does not limit the models that can be combined in a single run. Instead, prompts and text descriptions are provided to display appropriate selections to the user, but the user must exercise caution to insure that the model selections specified are compatible and appropriate. For this reason, a thorough understanding of both the individual models and scenario groupings is extremely important.

In Section 3.1.1 following, a brief overview is given for each of the individual hazard assessment models. These descriptions are actually the displays that are produced by the HACS/UIM in response to a user query for model explanation. (Section 3.3 gives detailed descriptions of the individual models and the specific input requirements.) Section 3.1.2 then following gives the detailed rationale of appropriate combinations for scenario formation. For further reference, Appendices J and

K contain tabulations of the current 900 chemical recognition codes by individual assessment models and complete sets of hazard assessment path codes.

3.1.1 Overview of Assessment Models

The following paragraphs give the text which is displayed by the UIM in response to a user query for a description of an individual model (refer to query-request procedure in Section 3.2). In referring to individual model descriptions, users should also reference the hazard assessment tree in Figure 4 to identify related models.

MODEL A

Model A is the venting rate model for discharges of liquids or gases from ruptured tanks. It estimates total amount of liquid and/or gas released, elapsed times for discharge, average flowrates and other characteristics of the discharge. Input requirements include the dimensions of the tank, the size and location of the hole from which the chemical discharges, and characteristics of the cargo contained within the tank (e.g., amount, temperature or pressure). The model provides two options for the tank venting process: adiabatic for well-insulated tanks, and isothermal for tanks which are not insulated. These represent extreme conditions and users should realize that actual release conditions will lie between these extremes, tending more toward one or the other depending on actual tank wall construction.

Model A should not be used if the hole is underwater, if the hole is very large compared to the size of the tank, or if there is more than one hole in the tank. The model assumes that the tank is an upright cylinder or a rectangular box shape, and is not currently applicable to horizontal cylinders or spherical tanks. Its accuracy for release of vapors is limited when venting liquids with low boiling points flash vaporize upon exiting a tank.

MODEL B

Model B is used when a flammable gas vents under pressure, may become ignited and form a flame jet. Potential thermal radiation hazards are obtained as minimum safe separation distances. It can also be used to assess whether an intact tank holding a compressed liquefied gas will rupture if exposed to the flame.

Model B is comprised of three modules: Model B1, Model B2, and Model B3. Model B1 estimates the length and diameter of the flame jet. Model B2 estimates separation distances from the flame that are safe for people and combustible materials. Model B3 (optional) addresses the effect on an intact tank subjected to fire, and requires detailed tank construction data as input. HACS default data for B3 specifies a propylene barge; use of default values may produce inaccurate results for other

types of tanks or vessels. The pressure relief valve setting and the tank wall thickness are particularly important input data for B3. If the tank from which the gas is discharging has a low internal pressure, or if the ignited gas produces a sooty flame, the results estimated by model B can be very conservative.

MODEL C

Model C is the primary model for assessing vapor dispersion hazards. For either instantaneous or continuous releases of gases or vapors evolved from holes in tanks, evaporating pools of spilled liquid, or both, the model estimates the size and characteristics of the resulting flammable and/or toxic cloud or plume.

Model C is comprised of two modules: Model C1 and Model C2. Model C1 estimates the downwind distance over which the cloud or plume may be hazardous. Model C2 computes the time of arrival, duration, and width of the cloud or plume (for given concentrations) at user specified downwind locations. These models are intended for use with gases or vapors only and may provide excessively conservative results for chemical fumes, mists, or dusts that may become airborne. The model assumes that the vapor cloud is neutrally buoyant, that it moves downwind over a flat terrain with no obstructions, and that the wind remains constant in direction and intensity.

MODEL D

Model D addresses discharged liquids that are lighter-than-water, insoluble or slightly soluble in water, and have boiling points below ambient temperatures. For discharges onto the surface of a water body, it computes the size of the floating, boiling pool and the elapsed time for all the liquid to evaporate.

Model D is applicable to either instantaneous or continuous discharges of a liquid onto water. It is not applicable to underwater discharges or spills onto land. The model assumes the spilled chemical is not depleted by dissolution in water (i.e., it assumes the chemical is completely insoluble in water), and that the chemical spills onto calm water.

MODEL E

Model E is the primary model for assessing the hazards from a burning pool of liquid on either land or water. It is used in situations where a pool of flammable liquid has been ignited or has the potential to be ignited. The model estimates size characteristics of the fire and safe separation distances for people and combustible materials, and can be used to assess whether an intact tank holding a compressed liquefied gas will rupture if exposed to the fire.

Model E is comprised of four modules: Models E1, E2, B2, and B3. Model E1 computes the height of the flame and Model E2 computes the angle the flame will bend due to the wind. Model B2 estimates safe separation distances from the flame while Model B3 (optional) addresses the effect on an intact tank subjected to fire. Model B3 requires detailed tank construction data as input. HACS default data for B3 specifies a propylene barge; use of default values may produce inaccurate results for other types of tanks or vessels. The pressure relief valve setting and the tank wall thickness are particularly important input data for B3. If the ignited liquid burns with a sooty flame, the estimates produced by these models can be very conservative. For spills onto water, the chemical may burn for only a short period of time if the pool is very thin or has become diluted with water.

MODEL F

The path code F appears on the hazard assessment tree for the boiling rate of spilled liquids which are lighter-than-water, boil at ambient temperature, and are slightly soluble or insoluble. This function has been implemented within HACS Model D, and Model F does not exist as a separate model. If called, it simply states that model F has been functionally incorporated into Model D.

MODEL G

Model G is the vapor dispersion model for insoluble or slightly soluble liquids which are lighter-than-water and have boiling points lower than the ambient temperature. Depending on the release conditions, the model adjusts the total amount of vapor released, then uses Model C, the primary vapor dispersion model, for assessment of hazards.

For instantaneous releases, the model sums the amount of gas vented from the tank or pipe with the amount of boiling liquid that is discharged. For continuous releases, it calls Model C without intermediate calculations. The model does not account for any gas or vapor that may discharge after liquid discharge ceases. If Model A output indicates that gas or vapor discharge is significant, the user may wish to appropriately adjust the flow rate and time for vapor evolution that enters Model C. This may be particularly necessary when isothermal venting is specified in Model A and the hole in the tank is below the liquid level but higher than the tank bottom.

MODEL H

Model H is the pool fire hazard assessment model for insoluble or slightly soluble flammable liquids that are heavier than water and have boiling points below ambient temperature. Model H estimates the diameter of the base of the flame, then calls Model E for estimates of the size characteristics of the fire, safe separation distances for people and combustible materials, and an assessment of whether an intact tnak containing a

compressed liquefied gas will rupture if exposed to the fire.

MODEL I

Model I is an evaporation rate model for insoluble or slightly soluble liquids that are heavier-than-water and have boiling points below ambient temperatures. It computes the elapsed time for complete evaporation of a liquid discharged instantaneously into water and computes the critical depth in water at which the liquid will not boil due to hydrostatic pressure effects. The critical depth can be important if a barge or other tank vessel has sunk in fairly deep water. The vapor dispersion Model J which generally follows Model I will assume that all the liquid released will vaporize; these vapor dispersion hazards in Model J assume that the chemical has not been released below its critical depth and that some of the chemical does not sink beneath its critical depth before vaporizing. Model I is not applicable for spills onto land.

Model I assumes that the discharged liquid breaks up into small drops that boil as they sink into water. In consequence, the elapsed time for complete evaporation is not a function of the total amount of liquid discharged. If the release occurs underwater, Model A should not be used preceding Model I since the release model, A, is valid only when the hole discharging the chemical from a tank is at or above the surface of the water. Model I assumes the discharge occurs at or above the surface of the water, or below the surface at a depth which is considerably less than the critical depth.

MODEL J

Model J is the vapor dispersion model for insoluble or slightly soluble liquids which are heavier-than-water and have boiling points lower than the ambient temperature. Depending on the release conditions, the model adjusts the total amount of vapor released, then uses Model C, the primary vapor dispersion model, for assessment of hazards.

For instantaneous releases, the model sums the amount of gas vented from the tank or pipe with the amount of boiling liquid that is discharged. For continuous releases, it calls Model C without intermediate calculations. The model does not account for any gas or vapor that may discharge after liquid discharge ceases. If Model A output indicates that gas or vapor discharge is significant, the user may wish to appropriately adjust the flow rate and time for vapor evolution that enters Model C. This may be particularly necessary when isothermal venting is specified in Model A and the hole in the tank is below the liquid level but higher than the tank bottom. Model J assumes that all the liquid discharged will vaporize; the effect of the critical depth computed in Model I is not modelled.

MODEL K

Model K addresses liquids that are fully or partially soluble in water and that have boiling points below ambient temperature. For releases more than 10 feet underwater, it can estimate the weight fraction of chemical that dissolves in water and the fraction that evolves from the surface as gas or vapor. It also estimates the critical depth in water at which the chemical will not boil due to hydrostatic pressure effects, and calls Model P for an assessment of water dispersion hazards. For releases near the surface of the water, it does all of the above except for estimating the fraction of chemical that dissolves in water and the fraction that evolves as gas or vapor. If the release occurs underwater, Model A should not be used preceding Model K since the release model, A, is valid only when the hole discharging the chemical from a tank is at or above the surface of the water.

Model K is based on complex logic with numerous limitations. If unable to determine the specific fraction of spilled liquid that dissolves in water, the model will simply assume that all of it dissolves leading to very conservative results produced by Model P for water pollution hazards. If the chemical is released at a depth greater than its critical depth, is heavier-than-water and, in addition, is not considerably soluble in water (e.g., 5-10% soluble), then there may be advantage to executing Model X instead of Model P for water pollution hazards.

MODEL L

Model L is the pool fire hazard assessment model for soluble liquids which have a boiling point less than the ambient temperature. It very roughly estimates the diameter of the base of the flame and then calls Model E, the primary pool fire hazard assessment model.

MODEL M

Model M is first in a sequence of models for assessment of vapor dispersion hazards when a liquid addressed by Model K is discharged. Due to limitations in Model K, it simply informs the user that HACS assumes that all vapor is evolved instantaneously. (Execution of Model M must be followed by Model N.)

MODEL N

Model N is part of the sequence of models for assessment of vapor dispersion hazards when a liquid addressed by Model K is discharged. If Model K has been able to determine the specific amount of gas or vapor that is generated at the spill site, Model N provides rough estimates of the size and shape of the vapor source and calls Model C, the primary vapor dispersion model. Otherwise, Model N asks the user to estimate the fraction of discharged liquid that vaporizes and proceeds from there to estimate the total amount of gas released before calling Model C.

MODEL O

Model code O indicates that the substance is a liquid which, when discharged from a container into a body of water, reacts with the water to form other substances. Model O in HACS simply states that the liquid is water reactive and refers the user to the HACS User Manual for a description of the reaction process. (See Page 119 and Table 1 starting on Page 120.) If the reaction is slow, the path code will include other scenarios for the substance discharged. If the reaction is fast, HACS can only be executed for hazardous products of the reaction after the Users' Manual is consulted.

MODEL P

Model P is the primary model for assessing water dispersion hazards of chemicals which do not boil at ambient temperature. For either instantaneous or continuous releases of soluble liquids or solids into water, the model computes concentrations in water as a function of location and time. All the chemical discharged is assumed to go into solution with water. The model can address spills into lakes, rivers, or estuaries.

Model P may be only approximately correct when the discharged chemical is significantly heavier- or lighter-than-water, or if the chemical is not fully soluble in water. It assumes that the discharge occurs near or on the surface of the water body and may provide somewhat inaccurate results for locations near the spill site when the spill is deep underwater. Model P cannot be accurately used for spills in offshore coastal regions.

MODEL Q

Model Q is the pool fire hazard assessment model for flammable liquids addressed by Model P. After estimating the diameter of the base of the flame, it calls Model E for estimates of the size characteristics of the fire, safe separation distances for people and combustible materials, and an assessment of whether an intact tank containing a compressed liquefied gas will rupture if exposed to the fire.

MODEL R

Model R is used for instantaneous spills of liquids that are soluble in water and evaporate easily. The model computes the amount of vapor evolved from the surface of the water body and the downstream distances over which the water body can liberate vapors that are toxic or flammable. It can be used for still water (lakes or ponds) and non-tidal rivers. Spills into estuaries can only be addressed approximately by assuming they are into non-tidal rivers.

Model R may produce excessively conservative results when the discharge takes place over a long period of time. There may also be inaccuracies

if the spilled chemical is significantly heavier- or lighter-than-water or the chemical is not fully soluble in water. The model is not applicable to spills on land.

MODEL S

Model S appears in a hazard assessment path code to address vapor dispersion hazards from spills of liquids that are soluble in water and evaporate easily. Since the amount of vapor released is obtained from Model R, Model S performs no additional computations, and, instead, directly calls Model C, the primary vapor dispersion model.

Caution: The model assumes that all vapor is generated at the spill site. This is not entirely valid in this case because some vapor will be generated from contaminated water traveling downstream. Populated areas immediately adjacent to the travel path of the chemical/water solution might be subjected to toxic and/or flammable vapor concentrations for distances downstream estimated by Model R.

MODEL T

Model T contains spreading and dispersion models for spills into water of liquid chemicals that are insoluble or slightly soluble in water, have a boiling point greater than the ambient temperature, and are lighter-than-water. It can provide the size of the liquid spill pool as a function of time and can be used to find the concentration of the chemical in water that results from the dissolution (mixing with water) of the floating pool.

Model T assumes that the chemical does not evaporate and has been spilled onto calm water. The spreading model can only handle instantaneous spills onto the surface of the water or underwater, and continuous discharges onto the surface of the water. The dispersion calculation procedure is only for instantaneous spills into still water or non-tidal rivers. If the release occurs underwater, Model A should not be used preceding Model T since the release model, A, is valid only when the hole discharging the chemical from a tank is at or above the surface of the water.

MODEL U

Model U is the pool fire hazard assessment model for flammable liquids addressed by Model T. It calls Model E, the primary pool fire model, for estimates of the size characteristics of the fire, safe separation distances for people and combustible materials, and an assessment of whether an intact tank containing a compressed liquefied gas will rupture if exposed to the fire.

MODEL V

Model V addresses liquid substances that are insoluble in water, lighter-than-water, have boiling points greater than ambient temperature, and are volatile. The model computes the size of the floating pool as a function of time as well as the elapsed time it will take for all the liquid to evaporate. Only instantaneous spills onto calm water are treated.

Model V assumes that the liquid spilled is completely insoluble in water and has a density less than water at all times after the discharge. Its execution is usually followed by execution of Model W for vapor dispersion hazards. If pool fires are of concern, the user should utilize Models T and U.

MODEL W

Model W initiates an automatic model execution sequence for assessing vapor dispersion hazards for liquids addressed by Model V. After a few initial computations, it calls Model C, the primary vapor dispersion model.

MODEL X

Model X primarily addresses liquids that are insoluble or slightly soluble in water, are heavier-than-water, and have boiling points greater than ambient temperatures. The model describes how the chemical sinks in water, how it spreads and then dissolves on the bottom of the water body (if slightly soluble), and how the dissolved chemical disperses. Portions of the model may also be used for similar materials with low boiling points when they are discharged at depths that preclude their boiling due to hydrostatic pressure effects.

Model X assumes that the spill occurs instantaneously into the center of a non-tidal river. In addition, it assumes that the density of the discharged liquid is always greater than that of water. Model A should not be used preceding Model X if the release takes place underwater.

MODEL Y

Model Y does not exist in HACS because the flammability hazard of low vapor pressure substances that sink in water is limited if the substance is spilled into water. Flammability hazards for spills on land can be treated by using Model E.

MODEL Z

Any substance that is somehow self-reacting under certain circumstances is assigned the path code Z. A Model Z for self-reaction hazards is not available in HACS and the user is referred to the data provided in CG-446-2, CHRIS Hazardous Chemical Data, for a description of self-reaction hazards.

MODEL II

This model code indicates that the substance is a solid that does not dissolve in water. A model for the actions of these substances on discharge into water is not currently available in HACS.

MODEL RR

Model code RR indicates that the substance released is a solid that somehow reacts with water. Model RR in HACS simply states that the substance is water-reactive. Refer to the sections of the HACS User Manual dealing with water-reactive solids before addressing hazards. (See Page 184 and Table RR.1 starting on Page 185.)

MODEL SS

Model code SS indicates that the substance released is a solid that dissolves in water (like sugar or salt). A specific model for such substances is not available in HACS. The user should realize, however, that once a soluble solid dissolves in water, the resulting solution behaves similarly to the solution resulting from a spill of soluble liquid into water. Hence, water pollution hazards for such spills can generally be assessed by straight-forward application of Model P.

3.1.2 Scenario Definitions

The one or two letter codes (A to Z, II, RR and SS) each identifies a specific type of chemical behavior on release, and identifies an appropriate assessment model. The codes, for each chemical, are listed in both CHRIS Manual II and contained on the HACS physical property data file. All codes that may apply to a particular chemical are listed and these generally are given in alphabetical order.

The hazard assessment tree, shown in Figure 4, defines the groupings of letter codes into scenarios to describe a complete assessment path through the tree. Since more than one scenario will often occur, the list of letter codes appearing with the chemical contains elements of different scenarios mixed within a single list.

The UIM provides a means via user requests to produce displays of the full set of model letter codes, and to automatically display the appropriate scenario groupings together with text descriptions of each scenario. The minimum user requirement for model selection is to simply request the display, identify a scenario of interest, and enter the model letter codes for that scenario. Table 1 lists the complete set of valid hazard assessment scenarios, and Section 3.1.2.1 contains brief summary descriptions of each. The information contained in Table 1 and Section 3.1.2.1 is sufficient for users to identify and select appropriate valid scenarios for hazard assessment computations. Additional detailed information pertaining to scenario formation and model relationships given in Section 3.1.2.2 identifies the specific logic used

TABLE 1

VALID HAZARD ASSESSMENT SCENARIOS

Scenario	Primary Hazard	Scenario	Primary Hazard
AB	T	APQ	T
AC	V	APRS	V
ABC	M	APQRS	M
ADE	T	AT	W
ADFG	V	ATU	T
ADEFG	M	AVW	V
AH	T	ATUVW	M
AIJ	V	AX	W
AHIJ	M	AXY	L
AKL	T	Z	L
AKMN	V	II	W
AKLMN	M	RR	L
AO	L	RR-C	M
AP	W	SS	W

NOTES:

1. Explanation of primary hazard:
   - T = Damage from heating
   - V = Toxic or flammable vapor
   - L = Local effects
   - W = Water pollution
   - M = Multiple hazards
2. Any model can be executed by itself if the user has sufficient input data.
3. Model A execution need not be performed if the user has sufficient input data for subsequent models.
4. Models O, Y, Z, II, RR and SS are not currently available in HACS. The user can, however, use Model P in place of Model SS under most circumstances.

for the translation of the collections of path codes contained on the current file for the 900 chemicals.

3.1.2.1 UIM Scenario Displays

Individual scenario descriptions produced by the UIM in response to a user request are listed below. A particular request will cause a display of only those scenario descriptions that apply for the specified chemical. The complete display includes a header and trailing footnotes that are discribed in Section 3.2.

SCENARIO A B

The hazardous material is a compressed gas stored under pressure. A hole in its container permits venting to the atmosphere where the gas quickly ignites and forms a jet of flame. It is desired to determine characteristics of the venting process (Model A) and of the flame jet hazards (Model B).

SCENARIO A C

The hazardous material is a compressed gas. A hole in its container permits venting to the atmosphere where the gas forms a cloud or plume with toxicity and/or flammability hazards. It is desired to determine characteristics of the venting process (Model A) and of the cloud or plume of gas that travels downwind (Model C). This path code is not appropriate when any of the hazardous material is released in the liquid state.

SCENARIO A B C

This path code permits consideration of both scenarios A B and A C in a single HACS run.

SCENARIO A D E

A liquefied compressed gas like LNG discharges onto water and forms a floating, boiling pool of liquid that does not mix with water. It is desired to determine characteristics of the venting process (Model A), of the pool spreading and evaporation processes (Model D), and of the resulting flammability hazards (Model E) if the pool is ignited.

SCENARIO A D F G

This sequence recognizes that a liquid like LNG spilling on water may vaporize to form a hazardous vapor cloud or plume. It is desired to determine characteristics of the venting process (Model A), of the pool spreading and evaporating process (Model D), and of the resulting vapor toxicity and/or flammability hazards (Models F and G).

SCENARIO A D E F G

This path code permits consideration of both scenarios A D E and A D F G in a single HACS run.

SCENARIO A H

A relatively insoluble, heavier-than-water, liquefied compressed gas discharges from a container into a body of water. The boiling liquid ignites to form one type of pool fire. It is desired to determine characteristics of the venting process (Model A), and of the resulting flammability hazards (Model H).

SCENARIO A I J

A relatively insoluble, heavier-than-water, liquefied compressed gas like chlorine discharges from a container into a body of water. The boiling liquid vaporizes to form a vapor cloud with toxicity and/or flammability hazards. It is desired to determine characteristics of the venting process (Model A), of the liquid vaporization process (Model I), and of the hazardous cloud that forms and travels downwind (Model J).

SCENARIO A H I J

This path code permits consideration of both scenarios A H and A I J in a single HACS run.

SCENARIO A K L

A soluble, liquefied compressed gas is discharged into water. Part of the liquid mixes with water while the rest vaporizes. It is desired to determine characteristics of the venting process (Model A); of the mixing, vaporization, and dispersion (in water) processes that take place (Model K); and of the flammability hazards (Model L) that will result if the substance ignites and forms a pool fire.

SCENARIO A K M N

A soluble, liquefied compressed gas is discharged into water. Part of the liquid mixes with water while the rest vaporizes. It is desired to determine characteristics of the venting process (Model A); of the mixing, vaporization, and dispersion (in water) processes that take place (Model K); and of the toxicity and/or flammability hazards of the vapors that may be released to the atmosphere (Models M and N).

SCENARIO A K L M N

This path code permits consideration of both scenarios A K L and A K M N in a single HACS run.

SCENARIO A O

A liquid discharges from a container into a body of water and reacts with the water to form other substances. Model A addresses venting process characteristics. Model O in HACS simply states that the liquid is water-reactive and refers the user to the HACS User Manual for a description of the reaction process. (See Page 159 and Table 1 starting on Page 160.) If the reaction is slow, the path code will include other scenarios for the substance discharged. If it is fast, HACS can only be executed for hazardous products of the reaction after the User's Manual is consulted.

SCENARIO A P

A water-soluble liquid with low to moderate volatility is discharged into water and causes a water pollution hazard. It is desired to determine the characteristics of the venting process (Model A), and of the manner in which the pollutant disperses in water (Model P).

SCENARIO A P Q

A water-soluble liquid with low to moderate volatility is discharged into water. It is desired to determine characteristics of the venting process (Model A), of the manner in which the pollutant disperses in water (Model P), and of the hazards involved if the liquid ignites and forms a pool fire (Model Q).

SCENARIO A P R S

A water-soluble liquid with moderate volatility is discharged into water. It is desired to determine characteristics of the venting process (Model A), of the manner in which the pollutant disperses in water (Model P), of the processes by which chemical vapors are evolved from the surface of the water body (Model R), and of how the toxic and/or flammable vapors disperse in air (Model S).

SCENARIO A P Q R S

This path code permits consideration of both scenarios A P Q and A P R S in a single HACS run.

SCENARIO A T

A relatively insoluble, lighter-than-water liquid of low to moderate volatility (like fuel oil) is discharged from a container into a body of

water. It is desired to determine characteristics of the venting process (Model A), and of the pool spreading, dissolution, and dispersion processes that take place (Model T).

SCENARIO A T U

A relatively insoluble, lighter-than-water liquid of low to moderate volatility (like fuel oil) is discharged from a container into a body of water. It is desired to determine characteristics of the venting process (Model A), of the pool spreading, dissolution, and dispersion processes that take place (Model T), and of the flammability hazards (Model U) that would result if the hazardous material ignites and forms a pool fire.

SCENARIO A V W

A relatively insoluble, lighter-than-water liquid of moderate volatility (such as gasoline) is discharged from a container into a body of water. It is desired to determine characteristics of the venting process (Model A), of the pool spreading and evaporation processes that may take place (Model V), and of the hazards associated with dispersion of the vapors generated from the pool (Model W).

SCENARIO A T U V W

This path code permits consideration of both scenarios A T U and A V W in a single HACS run.

SCENARIO A X

A relatively insoluble, heavier-than-water liquid is discharged from a container into water. It is desired to determine the characteristics of the venting process (Model A), and of the manner in which the liquid sinks in water, forms a spreading pool on the bottom of the water body, slowly dissolves, and disperses in water (Model X).

SCENARIO A X Y

A relatively insoluble, heavier-than-water liquid is discharged from a container into water. It is desired to determine the characteristics of the venting process (Model A), and of the manner in which the liquid sinks in water, forms a spreading pool on the bottom of the water body, slowly dissolves, and disperses in water (Model X). In addition, the presence of a potential flammability hazard is indicated (Model Y). However, since flammability is not a problem with liquids under water, HACS will inform the user that model Y is unavailable.

SCENARIO Z

Any substance that is somehow self-reacting under certain circumstances is assigned to path code Z. A Model Z for self-reaction hazards is not available in HACS and the user is referred to the data provided in COMDTINST M16465.12, CHRIS Hazardous Chemical Data, for a description of self-reaction hazards.

SCENARIO II

This path code refers to spills of insoluble solids into water. A model for the actions of these substances is not currently available in HACS.

SCENARIO RR

This code indicates that the substance released is a solid that somehow reacts with water. Model RR in HACS simply states that the substance is water-reactive and refers the user to the User's Manual. (See Page 223 and Table RR.1 starting on Page 224.)

SCENARIO RR C

This code sequence indicates that the substance discharged is a solid that reacts with water to generate a toxic and/or flammable gas. Model RR in HACS simply states that the substance is water-reactive and refers the user to the HACS User Manual. (See Page 223 and Table RR.1 starting on Page 224.) Use Model C to determine dispersion hazards for the specific gas that is generated after consulting the User's Manual.

SCENARIO SS

This code indicates that the substance released is a solid that dissolves in water (like sugar or salt). A specific model for such substances is not available in HACS. The user should realize, however, that once a soluble solid dissolves in water, the resulting solution behaves similarly to the solution resulting from a spill of soluble liquid into water. Hence, water pollution hazards for such spills can generally be assessed by straight-forward application of Model P.

GENERAL NOTES:

1. Any model can be executed by itself if the user has sufficient input data.

2. Model A execution need not be performed if the user has sufficient input data for subsequent models.

3. There are many substances that exhibit borderline behavior when released into the environment. Depending on air and water temperatures, they may sink or float in water, dissolve or not dissolve, boil or not boil, and so on. The path codes for such substances can therefore represent scenarios that at first appear to be contradictory, but which are individually valid under certain environmental conditions.

As noted earlier, the hazard assessment model letter codes from which the preceding displays are derived are contained in both CHRIS Manual II and the HACS property file, thus the UIM displays will be consistent in nearly all cases with Manual II (COMDTINST M16465.12). For five chemicals, however, different path codes are recommended for use with HACS than are given in COMDTINST M16465.12. The appropriate codes for use with HACS are:

Ethyl Ether:	Recognition Code	EET
	HACS path codes	APQRS
Isopropyl Acetate:	Recognition Code	IAC
	HACS path codes	APQRS
Methyl Acrylate:	Recognition Code	MAM
	HACS path codes	APQRSZ
Methyl Methacrylate:	Recognition Code	MMM
	HACS path codes	APQRS
Vinyl Acetate:	Recognition Code	VAM
	HACS path codes	APQRSZ

These codes are already entered on the HACS property file, so no additional user action is required.

3.1.2.2 Detailed Logic for Path Code Interpretation

The hazard assessment tree given in Figure 4 contains a few minor changes from the previous version, principally regarding the use of Model A with Models Z, II, RR and SS. Also, the tree structure as shown does not quite conform to the current capabilities of Model K, that is, the water pollution hazard is incorporated directly within Model K, and the path A-K does not represent a separate scenario.

Table 1 gives the final list of valid scenarios that was tabulated according to the relationships shown in the hazard assessment tree, and the additional criteria that the scenarios presented for display should give as complete a representation of the potential hazards as possible. That is, although users may elect to select individual models to partially evaluate a particular set of hazards, the scenario lists do not separately identify possible sub-sets of model codes. For example, the scenario A-P-Q contains

the legitimate path A-P which would apply if the liquid were not ignited. It was decided in this and all other similar cases that the path A-P-Q provides a more complete definition. In this example, path A-P will be given as a scenario only if model codes Q, R and S are not present for the chemical.

The logic for the translation of the collections of path codes contained on the file for the 900 chemicals to valid scenarios listed in Table 1 is described in the paragraphs below. This documentation is important to provide standardization for new chemicals which may be added to the file in the future, and to identify possible need for program revisions should any of these new chemicals not conform to this interpretation.

1) Model RR - is a special case which may appear alone, with model C only or with other model codes.

   If both RR and C appear, then RR-C is a special scenario and the only one which may appear.

   If RR appears with any other model codes, then RR alone is a valid single scenario, and other scenarios may also be indicated.

   RR-C is the only exception for which no other scenarios are permitted. In all other cases described below, all path codes are examined to identify each applicable scenario.

2) Models Z, II, SS - are each special case situations for which no models presently exist. These may be given as single model codes, or included with model A and/or other model codes which indicate other applicable scenarios. The appearance of models Z, II, and SS in the list of codes each translates to scenarios Z, II and SS, respectively.

3) Model O - is also a special case similar to the above, and may also appear with other scenarios or models, and with or without model A. If model O does appear, the appropriate scenario is A-O however.

4) Models B, C - indicate gas venting of flammable (B) and/or toxic (C) vapor.

   Valid scenarios are A-B (if B appears), A-C (if C appears) and, in addition to these, A-B-C if both B and C appear.

   Model C is also used in a special case with model RR as described in (1) above.

5) Model D - is used for volatile liquids which are insoluble or slightly soluble and float on water. If the liquid is not ignited, then a vapor dispersion hazard is present; thus model D always appears with models E, and/or F and G.

If models D and E appear, the scenario is A-D-E. If models D and F appear, the scenario is A-D-F-G. If models D, E and F all appear, then, in addition to these, scenario A-D-E-F-G is also listed.

6) Models H, I, J - apply to volatile chemicals that sink in water and are slightly soluble or insoluble. With one exception, model codes are listed as A, H; A, I, J; or A, H, I, J.

Scenarios are defined to be A-H (if model H appears); A-I-J if model I appears; and, in addition, A-H-I-J if both models H and I appear.

The exception occurs with oxygen which is listed on the chemical property file with model letters A, I only. The scenario listed for oxygen determined as above is A-I-J, not A-I.

7) Model K - is the mixing and dilution model for soluble liquids which boil at ambient temperature. A-K would be a valid scenario only if models L, M or N were not indicated. However the absence of L, M or N implies that the liquid does not boil at ambient temperature in which case model P instead of K applies. Thus A-K alone is not a valid scenario, and K can only appear in combination with L, and/or M and N.

Scenarios are defined to be A-K-L if both K and L appear; A-K-M-N if both K and M appear; and, in addition to these, A-K-L-M-N if K, L and M all appear.

8) Model P - is the mixing and dilution model for soluble liquids with low to moderate volatility. For liquids with moderate volatility, the dispersion in water may also be accompanied by vapor evolution from the surface of the water body, and models R and S apply as well as possibly Q for liquid burning. Thus A-P is a valid scenario only for non-volatile, non-flammable liquids (for which models Q, R and S do not apply).

If model P appears without Q, R and S, then only a single scenario A-P is given. If model P does appear with Q, R and S, scenario A-P is not given. Instead, scenarios are A-P-Q if both P and Q are given, and A-P-R-S if both P and R are given. If P, Q and R all appear, then, in addition to these, scenario A-P-Q-R-S is also indicated.

9) Models T and V - apply to liquids of low to moderate volatility which float on water and which are insoluble or slightly soluble. These two models are used separately: T for non-volatile liquids which may or may not be flammable, and V for volatile liquids if the liquid is not ignited.

If the liquid is flammable but non-volatile, then only model codes T and U appear and the scenario is A-T-U. If the liquid is volatile, but non-flammable, then only V and W appear but not T or U and the scenario is A-V-W.

If the liquid is both flammable and volatile, then the codes U, V, W all appear, and valid scenarios are: A-T-U, A-V-W, and, in addition, A-T-U-V-W.

If the liquid is both non-flammable and non-volatile, then only T appears without U, V or W and the scenario is A-T.

Note that this logic does not permit defining a scenario for A-T-V-W (which would imply a chemical which is both volatile and non-volatile).

10) Model X - is the dispersion model for insoluble or slightly soluble non-volatile liquids which are heavier than water. Model Y may or may not be listed with X, and indicates that a flammability hazard may also be present (although no hazard assessment model is available.

Scenarios are defined to be A-X-Y if both X and Y are present, and A-X if X is present, but Y is not.

Using the definition of scenarios by groupings of model letter codes, Table 2 identifies the translation from the unique set of path codes currently contained on the file for the 900 chemicals to the appropriate scenarios.

For the 900 chemicals, there are 70 different sets of path codes on the property file representing different groupings of 28 different scenarios.

The distribution of these 900 chemicals by number of scenarios is given below:

TABLE 2

TRANSLATION FROM
ACTUAL PATH CODES TO SCENARIOS

PATH CODES		=	SCENARIOS	COUNT
1	APQ	=	APQ	88
2	ABCKLMNZ	=	AB	1
			ABC	1
			AC	1
			AKL	1
			AKLMN	1
			AKMN	1
			Z	1
3	APZ	=	AP	2
			Z	2
4	APQTU	=	APQ	16
			ATU	16
5	SS	=	SS	162
6	AO	=	AO	40
7	AXY	=	AXY	32
8	AP	=	AP	41
9	II	=	II	100
10	ABC	=	AB	1
			ABC	1
			AC	1
11	AOXY	=	AO	10
			AXY	10
12	RR-C	=	RR-C	7
13	APQRSZ	=	APQ	6
			APQRS	6
			APRS	6
			Z	6
14	ATUXY	=	ATU	21
			AXY	21
15	APQZ	=	APQ	5
			Z	5
16	APQRS	=	APQ	31
			APQRS	31
			APRS	31
17	SS II	=	SS	2
			II	2

TABLE 2 (Continued)

TRANSLATION FROM
ACTUAL PATH CODES TO SCENARIOS

PATH CODES		=	SCENARIOS	COUNT
18	ATU	=	ATU	144
19	ATUVW	=	AVW	37
			ATUVW	37
			ATU	37
20	ABCKLMNO	=	AB	1
			ABC	1
			AC	1
			AKL	1
			AKLMN	1
			AKMN	1
			AO	1
21	SS Z	=	SS	1
			Z	1
22	APRS	=	APRS	1
23	AP SS	=	AP	3
			SS	3
24	APQTUXY	=	APQ	5
			ATU	5
			AXY	5
25	AOX	=	AO	3
			AX	3
26	RR	=	RR	13
27	II SS	=	II	13
			SS	13
28	ATUZ	=	ATU	7
			Z	7
29	APTX	=	AP	1
			AT	1
			AX	1
30	AX	=	AX	11
31	ABCDEFGZ	=	AB	4
			ABC	4
			AC	4
			ADE	4
			ADEFG	4
			ADFG	4
			Z	4
32	AOZ	=	AO	7
			Z	7

TABLE 2 (Continued)

TRANSLATION FROM
ACTUAL PATH CODES TO SCENARIOS

PATH CODES		=	SCENARIOS	COUNT
33	ACO	=	AC	3
			AO	3
34	APX	=	AP	2
			AX	2
35	ABCDEFG	=	AB	20
			ABC	20
			AC	20
			ADE	20
			ADEFG	20
			ADFG	20
36	AXYO	=	AXY	1
			AO	1
37	ATX	=	AT	2
			AX	2
38	II RR	=	II	4
			RR	4
39	ACIJX	=	AC	1
			AIJ	1
			AX	1
40	AC II	=	AC	1
			II	1
41	ACIJ	=	AC	5
			AIJ	5
42	AOTUVWXY	=	AO	1
			AVW	1
			ATUVW	1
			ATU	1
			AXY	1
43	ABCKLMN	=	AB	9
			ABC	9
			AC	9
			AKL	9
			AKLMN	9
			AKMN	9
44	ATU II	=	ATU	1
			II	1
45	APQXY	=	APQ	2
			AXY	2

TABLE 2 (Continued)

TRANSLATION FROM
ACTUAL PATH CODES TO SCENARIOS

PATH CODES	=	SCENARIOS	COUNT
46 ATUXY II	=	ATU	1
		AXY	1
		II	1
47 APQTUVW	=	APQ	3
		AVW	3
		ATUVW	3
		ATU	3
48 AXY II	=	AXY	1
		II	1
49 APQTUZ	=	APQ	1
		ATU	1
		Z	1
50 AOTUXY	=	AO	2
		ATU	2
		AXY	2
51 AC	=	AC	2
52 ATUXYZ	=	ATU	1
		AXY	1
		Z	1
53 ACKMNO	=	AC	3
		AKMN	3
		AO	3
54 II Z	=	II	1
		Z	1
55 ABCIJ	=	AB	1
		ABC	1
		AC	1
		AIJ	1
56 AIJO	=	AIJ	1
		AO	1
57 ATUX	=	ATU	1
		AX	1
58 ACDFG	=	AC	1
		ADFG	1
59 AOP	=	AO	1
		AP	1
60 AI	=	AIJ	1

TABLE 2 (Continued)

TRANSLATION FROM
ACTUAL PATH CODES TO SCENARIOS

PATH CODES	=	SCENARIOS	COUNT
61 II AXY	=	II	1
		AXY	1
62 ACIJO	=	AC	1
		AIJ	1
		AO	1
63 AOPQRSZ	=	AO	1
		APQ	1
		APQRS	1
		APRS	1
		Z	1
64 APO	=	AP	2
		AO	2
65 AOTUVW	=	AO	1
		AVW	1
		ATUVW	1
		ATU	1
66 ACKMN	=	AC	1
		AKMN	1
67 ABCHIJ	=	AB	1
		ABC	1
		AC	1
		AH	1
		AHIJ	1
		AIJ	1
68 ABCZ	=	AB	1
		ABC	1
		AC	1
		Z	1
69 II ATU	=	II	1
		ATU	1
70 AXYZ	=	AXY	1
		Z	1

Number of Chemicals		Number of Scenarios		Sub-total
642	x	1	=	642
123	x	2	=	246
85	x	3	=	255
12	x	4	=	48
2	x	5	=	10
30	x	6	=	180
6	x	7	=	42
900				1,423

There are 1,423 scenarios contained on the file for the 900 chemicals, and these are distributed over the 28 different scenarios as follows:

AB	39
AC	57
ABC	39
ADE	24
ADFG	25
ADEFG	24
AH	1
AIJ	11
AHIJ	1
AKL	11
AKMN	15
AKLMN	11
AO	78
AP	52
APQ	158
APRS	39
APQRS	38
AT	3
ATU	243
AVW	42
ATUVW	42
AX	21
AXY	79
Z	39
II	126
RR	17
RR-C	7
SS	181
	1,423

Note: The path codes for oxygen, A-I, are translated to scenario A-I-J.

3.2 USER OPERATIONS WITH THE UIM

This section contains several sub-sections to describe the different steps or procedures which occur during a typical UIM run, more or less independently of the actual hazard assessment models which are selected.

Sub-section 3.2.2 contains general information describing the types of input data, provided by the user, that are processed by the UIM, and gives the rules that must be followed for current input. Sub-sections 3.2.3 to 3.2.5 then describe the major steps in a typical run which are:

- Chemical and scenario selection
- Typical model execution sequence
- Output summary

For each of these, the UIM operation is illustrated using the actual HACS messages that are displayed as user prompts, and the manual then describes the resulting action which is taken by HACS for each possible user response.

Section 3.2.1 has been reserved for documentation of specific terminal access procedures used by National Response Center and other Coast Guard personnel. Specific confidential access information such as system passwords and charge account numbers has been intentionally omitted from this section; interested users should obtain access information and authorization from the National Response Center.

3.2.1 Terminal Access

The HACS/UIM as described in this Users' Reference Manual was originally developed using Control Data Corporations Cybernet Service under the NOS operating system to provide for interactive access by low speed (300 baud, 1200 baud) terminals. The Cybernet operation is currently available to users within the National Response Center (NRC). Also, HACS is being converted to operate on the Prime 750 equipment for NRC use at the Operational Computer Center (OCC). Specific log-on procedures, access commands, and similar operating system interfaces are not yet available for that version of HACS.

For the Cybernet version of the system, authorized Coast Guard users follow a standard sign-on procedure provided by the NRC to access the Cybernet system. After signing on, the only necessary step is to start execution of the HACS/UIM which is done by typing:

```
-UIMRUN (CR)
```

where (CR) denotes a carriage return. The UIMRUN is a procedure file stored on Cybernet which contains the necessary instructions to link the

external HACS data files that are used, and to start the execution of the program. The first user input to be entered is described in Section 3.2.3 which follows. Basic information describing the rules for UIM input formatting is first covered in Section 3.2.2.

On normal completion of a HACS/UIM run, HACS responds by displaying an end-of-run message. System control then reverts to the NOS system. Users may then continue with non-HACS tasks, or sign-off the system by typing BYE followed by a carriage return.

3.2.2 UIM Input Rules

User input to HACS under the UIM is given by different combinations of only six types of input data items. These are identified as:

- Integer values
- Decimal values
- Names
- Yes/No responses
- Query
- Blank

Each type of input is described individually in sub-sections which follow below.

All user input processed by the UIM is read by the computer in a "free-format" mode, that is, there are no restrictions on the location in the input line where a data item may be placed.

Blank spaces are used by the UIM to identify separate data items. If a user input line contains, for example, two different data entries, at least one space must be typed between the entries. Data items may be typed starting at the first typing position, or after any number of initial spaces have been keyed. Data items may be typed so that they end anywhere on the input line, up to the end of the input line. The last data item on an input line is completed either by a following blank, or automatically by the end of the line (it is not necessary to type a space after the last item). Single data items may not be continued from one input line to the next.

Virtually all the UIM requests for user input are programmed to expect the complete user input data items for the request in a single input line. Typing a carriage return after typing the requested data items completes the input line, and the UIM interpretation of the user input is initiated. If required input has not been entered, a diagnostic message will be printed and the UIM will expect the user to re-enter complete information in response to the request; additional input lines are not searched for the missing input elements.

Although the input is typed by the user in "free-format," if a UIM input request requires more than one input item to be provided, these inputs must be typed by the user in the sequence indicated by the request.

3.2.2.1 Integer Values

Integer values are used primarily by the UIM for plot or table option selections, and for field number references. The required integer format for user entry is defined for the most general purposes as:

$$b\left(\frac{+}{b}\right)d(d\ldots d)^{b}_{CR}$$

where the symbols used denote characters that might be keyed by the user. Characters not enclosed by parentheses are mandatory, characters enclosed in parentheses are optional:

b	=	blank; at least one blank must be keyed before entering the integer to separate it from a previous entry. If the integer is the first item typed on a line, then the initial space does not need to be keyed.
$\left(\frac{+}{b}\right)$	=	+ for plus sign, - for minus sign or b for blank or skip; preceding the integer value, an optional plus or minus sign may be keyed, or the sign may be omitted (+ is assumed).
d	=	decimal digit (a number from 0 to 9). An integer value may contain one or more decimal digits, but at least one decimal digit is mandatory.
(d...d)	=	denotes optional decimal digits that might be entered following the first digit as in 123.
$^{b}_{CR}$	=	denotes the end of the integer value to be input by either a space typed by the user (one or more spaces) or a carriage return typed to enter the entire line.

A valid integer value consists of an optional + or - sign, followed immediately by one or more decimal digits, for example:

+10 103 -5

are all acceptable integer values to the UIM input processor. Note that since the input scan stops when blanks are encountered, inputs such as +b10 or +1b0 will not be read as "10."

It should also be noted that there are two types of input checks performed. First, the UIM processes the user input to determine if a valid integer format has been used, such as -5. Second, a test is performed on the resulting integer using range limits stored in the HACS state file. If these limits are exceeded, a warning diagnostic message will be displayed. For example, the valid integer -5 is not an acceptable table selection option.

Error conditions which can be detected by the UIM when reading integer value inputs are:

(1) an input line in which the requested integer input is missing;

(2) an incomplete integer value in which a plus or minus sign is not followed by a decimal digit; and,

(3) any characters other than +, -, 0 to 9 typed within the integer value, or + or - positioned incorrectly.

For any of these error conditions, scanning of the remainder of the integer input value stops and an error message is displayed:

WHAT? INTEGER SYNTAX ERROR

The UIM will then repeat the original prompting display and the user will be required to re-enter the complete input line.

Note that an integer value followed by a decimal point is an illegal integer input for the UIM.

An error condition which cannot be detected by the current version of the UIM consists of typing more digits than the computer being used has the capacity to store as a single integer value. Generally, errors of this type will be flagged by the operating system, not the UIM, and it may or may not be possible to continue with the UIM run. Since integer values used for field numbers and output options are relatively quite small, under normal HACS operations, users should not encounter errors of this type.

3.2.2.2 Decimal Values

Decimal values are used by the UIM for specification of most spill conditions, environmental data, chemical data and other non-integer type quantities. The required decimal format for user entry is defined for the most general purposes as:

$$b\left(\frac{+}{b}\right)(d...d)\ (.)\ (d...d)\ (EI)^{b}_{CR}$$

where the symbols used denote characters that might be keyed by the user. Characters not enclosed by parentheses are mandatory, characters enclosed in parentheses are mandatory, characters enclosed in parentheses are optional except that at least one of the optional entries shown above must be given. Individual portions of the input are:

b = blank; at least one blank must be keyed before entering a decimal value to separate it from a previous entry. If the decimal value is the first item to be typed on a line, then the initial space does not need to be keyed.

$\left(\frac{+}{b}\right)$ = + for plus sign, - for minus sign or b for blank or skip; preceding the decimal value, an optional plus or minus sign may be keyed, or the sign may be omitted (+ is assumed).

(d...d) = denotes optional decimal digits that might be entered before the decimal point. None, one, or more, digits may be entered. Each character keyed must be a valid digit, 0 to 9. The decimal point is always assumed to be located immediately to the right of the last digit entered. For example, a user entry of -5 keyed without the decimal point will be correctly stored as -5.0.

(.) = optional decimal point which may be entered with or without preceding decimal digits, and optionally followed by decimal digits. If no decimal digits are given either before or after the decimal point, a value of 0.0 is assumed.

(d...d) = denotes optional decimal digits that might be entered following the decimal point. None, one or more digits may be entered. Each character, if entered, must be a valid digit, 0 to 9.

(EI) = optional exponent, specified by typing the letter E followed by a signed or unsigned integer value; this is a scale factor where the integer value gives the power of 10 by which the decimal value to the left is to be multiplied. If the E is typed, the integer value following must not be omitted. The sign of the integer exponent may be omitted if the exponent is positive, but it must be present if the exponent is negative. Note that the letter E must be typed immediately after the value to the left. Although blanks between the letter E and the following integer exponent value will not cause an error, they should not be used.

$^{b}_{CR}$ = denotes the end of the decimal value to be entered by either a space typed by the user (one or more spaces) or a carriage return typed to enter the entire line.

Examples of valid decimal values include:

+5.0	+5E2 (=500.)
5	+5E-2 (=0.05)
-4	-0.003
-4.3	-3.E-3 (=-0.003)

Note that since if no decimal digits are entered both before and after the decimal point, a value of 0.0 results, then forms such as -E5, or +.E-2 will be accepted by the UIM but give a value of 0.0. A single decimal point will also give a value of 0.0.

As with integer input values, there are two types of input checks performed. First, the UIM processes the user input to determine if a valid decimal format has been used, such as +6.32. Second, a test is performed on the resulting decimal value using range limits stored in the HACS state file. If these limits are exceeded, a warning diagnostic message will be displayed, but the value entered by the user will continue to be used.

Error conditions which can be detected by the UIM when reading decimal value inputs are:

(1) an input line in which the required decimal value input is missing;

(2) an incomplete decimal value in which a plus or minus sign is not followed by a decimal digit, a decimal point or an exponent;

(3) any characters other than +, -, 0 to 9, and E typed within the decimal value, or any otherwise acceptable characters positioned incorrectly; and,

(4) an exponent in which the letter E is followed by a user entry which does not conform to the required integer format.

For any of these error conditions, scanning of the remainder of the decimal value input stops and an error message is displayed:

WHAT? DECIMAL SYNTAX ERROR

If the error was detected while interpreting the integer exponent then the integer syntax error message will also be given. After an error occurs, the UIM will repeat the original prompting display and the user will be required to re-enter the complete input line.

An error condition which cannot be detected by the current version of the UIM consists of typing more digits, or a larger exponent, than the computer being used has the capacity to store as a single decimal value. Generally, errors of this type will be flagged by the operating system, not the UIM, and it may or may not be possible to continue with the UIM run. However, during normal use of the UIM, users should not encounter errors of this type.

3.2.2.3 Names or Labels

Certain UIM inputs are read by the UIM as names or labels; these include the chemical recognition code, model path codes, and data item unit labels. Inputs of this type are stored as character data and any characters may be used. Only up to the first 8 (or 10) characters of any input are actually used; any excess characters are ignored.

Reading of name input by the UIM starts with the first non-blank character typed for the name entry and stops at the next blank or carriage return typed by the user. If the position expected in the user input line by the UIM contains only blanks, the name value used by the UIM will also be blank.

Processing of name or label information in the UIM occurs in two steps: first, reading the name information as user input, and second, using the name(s) read to perform requested operations in HACS. Since names containing any characters, or all blanks, can be accepted by the UIM, the step to read the value cannot test for any error conditions. However, diagnostic messages are produced at the time the UIM attempts to use a name input which is invalid for that use. For example, user entry of a chemical recognition code which does not correspond exactly to one of the recognition codes on the HACS chemical properties file will cause an error condition. Similarly, mis-typed data item unit labels will cause an error when the UIM attempts to match the user input to the stored lists of acceptable unit labels. Errors of this type will cause the UIM to ignore the entire preceding user input line, and repeat the original prompt message.

Users should note that since these internal operations are performed by matching the user input to pre-stored lists, user entries for items such as unit labels must correspond exactly to the labels given in the prompt message. Also, the circumstances under which name input may be skipped are variable, depending on the type of UIM request. Name entries for data item unit labels do not need to be given by the user if the first unit in the prompt message is to be assumed. Name entries for the chemical recognition code and hazard assessment models must be given correctly and cannot be omitted.

3.2.2.4 YES/NO Responses

Some of the UIM interaction takes place in the form of questions asked the user, and the UIM expects to interpret the resulting user response in the form of a yes or no answer.

Correct user responses are any input in which the first non-blank character is either a Y or an N, followed by a carriage return. Any of the following correspond to a 'yes' input: Y YES or YXXX. Any of these are acceptable 'no' responses: N NO NXXX.

If the user enters an input line which is completely blank, or if the first non-blank character typed by the user is not Y or N, then the UIM will display a message:

```
WHAT?
ENTER YES OR NO (Y/N):
```

Processing will not proceed until a valid response has been read.

3.2.2.5 Query and Display

In response to UIM prompts, two standard alternate user responses are provided.

User queries for information in response to a UIM prompt are issued by typing a question mark (?) followed by a carriage return. The question mark may be preceded by any number of blank characters, and followed by any number of blank or non-blank characters. Only the first non-blank character must be a question mark. The UIM response is to display available or pre-stored information, then to repeat the original prompt for specific user values.

If the user responds to a UIM prompt by typing a carriage return, the convention has been adopted that this user response is a request for the current value of the requested information and a UIM display is produced. For some, but not all input items, the user is then given a choice of either using the current value or entering a different value. Note that a blank response is accepted as a request to display a current value only if no other user input on the current line has been previously processed. For example, when entering model letter codes, blanks following any non-blank model code are only skipped and do not produce a display of current values.

3.2.3 Chemical and Scenario Selection

The initial steps of a HACS run involve the user selection of the chemical of concern and the models to be used to form the hazard assessment scenario. The UIM provides prompts to request this information from the user, and the dialog that follows depends on user input or requests for optional displays. The paragraphs below describe the dialog by first illustrating the UIM prompt or display, followed by a description of the action taken under different conditions. In this and other following sections, message numbers enclosed in parentheses at the left margin are used for reference when the UIM may branch to different sections of the dialog.

Following terminal log-on and accessing the HACS execution procedure, execution of the HACS/UIM starts with the system display of the message:

(3.1) HAZARD ASSESSMENT COMPUTER SYSTEM
EXECUTION STARTED ON date AT time

where the values of the current date and time are written with the message. This message simply indicates that the HACS/UIM is now running and the UIM-user dialog starts with the following prompt message:

(3.2) ENTER RUN REQUEST, OPTIONS ARE RUN/RERUN/CONTINUE/END

The system requests that the user enter a code word to describe the type of run to be performed. A correct response is for the user to type one of the words RUN RERUN CONTINUE or END followed by a carriage return. Spaces may precede or follow the control word typed.

If the input line typed at the terminal is blank (only blanks and/or a carriage return was typed), no additional display is necessary and the prompt message (3.2) is repeated. If the user response to message (3.2) cannot be correctly interpreted by the system as a valid code word, then the following message is displayed:

(3.3) WHAT? (RUN REQUEST ERROR)

and message (3.2) is repeated.

If the user response for the run request is END, further execution of HACS/UIM is terminated, and the system responds with the message:

(3.4) **********
END OF HACS RUN
****

Further control for the terminal operation then returns to the computer operating system, and the user might normally log-off the system.

If the user response to the run request prompt (3.2) is one of RUN RERUN or CONTINUE, internal parameters are automatically set to control initialization of state file values, and then the state file is initialized. Processing proceeds to subsequent specification of output display units:

(3.5) ENTER OUTPUT UNITS SELECTION (0-4):

Appropriate user responses are an integer value (one of the values 0, 1, 2, 3, or 4) or a question mark, followed by a carriage return, or a carriage return with no preceding input.

If a question mark followed by a carriage return is entered, the UIM displays a definition of the allowed output units selection:

(3.6) THE AVAILABLE OPTIONS ARE -
0 FOR ALL UNITS
1 FOR CGS UNITS
2 FOR SI UNITS
3 FOR ENGLISH UNITS
4 FOR MIXED UNITS

Following this display the input prompt message (3.5) is repeated.

If the user response to the prompt (3.5) is a carriage return, or blanks followed by a carriage return, the UIM displays the current value of the output unit selector with the display:

(3.7) CURRENT SELECTION IS n

where n is displayed as an integer value 0 to 4. In this case, after the display of the current value the UIM repeats prompt message (3.5) and the user is expected to enter a value.

Values entered by the user in response to the prompt (3.5) for unit selection must be valid integers. If not, an integer syntax error message is displayed and prompt (3.5) is repeated until a valid response has been given. Currently, the value of the user input is stored by the UIM and cannot be

changed during a run until prompt message (3.5) is again encountered; also, since the unit conversion occurs separately from the storage of values in the HACS state file, the input is not range-checked in the usual manner. If values other than 0 to 4 are entered, output results will not be correct.

The unit selection option is used to control the units or dimensions in which other data items will be displayed during the remainder of the run. A value of 1, 2, 3 or 4 will cause only a single display to be produced, with the value given in the display in units appropriate for the specified system. A value of 0 will cause each display of data items (real or decimal values) to consist of up to four lines, one for the value in each system of units. Displays of values in duplicate dimensions are omitted. Since all integer data items are treated as non-dimensional quantities, these items are always displayed in a single line independently of the value selected for this option.

(3.8) ENTER CHEMICAL RECOGNITION CODE:

The expected user response is to type the three-letter chemical recognition code for the chemical of interest. The complete set of 900 codes which can be used with the current version of the system are listed with the chemical names in Appendix A. The allowable codes are defined by entries in the external file of chemical property data which is accessed by HACS. Since from time to time additions may be made to this file, additional codes may become available which are not listed in Appendix A.

Acceptable user responses to prompt message (3.8), in addition to a chemical recognition code, are a carriage return, or a question mark (?) followed by a carriage return.

The question mark causes a descriptive display to be produced:

(3.9) THE CHEMICAL RECOGNITION CODE IS A THREE-LETTER ALPHABETIC CODE USED TO SELECT THE CHEMICAL FOR HAZARD ASSESSMENT. REFER TO CHRIS MANUAL II FOR CROSS-REFERENCE LISTS OF CHEMICAL NAMES, SYNONYMS, AND RECOGNITION CODES.

Following this display the chemical recognition code input prompt (3.8) is repeated.

A carriage return response causes the current value of the recognition code to be displayed:

(3.10) CURRENT CODE = code

where the actual value is inserted as code. This is included simply to provide a reminder to the user, but not for actual use. The display is followed by repeating the input prompt message (3.8). Note that if this display is requested before any code has been entered by the user, the value to be displayed will be undefined.

Once typed in response to (3.8), the chemical recognition code entered by the user is saved and used to control accessing the external chemical properties file. The search of the properties file has four possible outcomes: (a) the file cannot be accessed by HACS, (b) the file is searched completely and the requested chemical is not found, (c) the position on the file where the requested chemical should exist has been passed, or (d) the requested chemical is found.

Condition (a) cannot currently be controlled by the UIM, and indicates that the procedure used to initiate execution of HACS/UIM has accessed an incorrect or faulty file. Depending on the type of error that has occurred, the UIM will either not be able to proceed and a system diagnostic message will be given, or, the UIM will become locked in a loop requesting the user to input a chemical recognition code or proceed to hazard assessment model input without reading the chemical property data.

If either condition (b) or (c) occurs, the user-specified chemical recognition code is in error (that is, a chemical record having the user-specified code does not exist on the file), and one of the following messages is displayed:

(3.11) *****ERROR - UNABLE TO FIND CHEMICAL
SEARCH TERMINATED BY END OF FILE

or

(3.12) *****ERROR - UNABLE TO FIND CHEMICAL
SEARCH TERMINATED AFTER PASSING EXPECTED ALPHABETICAL POSITION

Following either of these error conditions, the UIM expects the user to re-enter an acceptable chemical recognition code, and control returns to prompt message (3.8). Note that in contrast to the prior batch mode of operation, the HACS/UIM does not provide an option to suppress access of the chemical property file, and a valid recognition code must be entered before any further operations can be performed.

When the search of the chemical property file is successfully completed, the data contained on the file for the requested

chemical is read, decoded and converted for storage in the internal HACS state file. Only the values actually defined on the file are transferred; storage of these values in the HACS state file as estimated or exact property values will then cause the UIM to later suppress interactive prompts to the user to supply input values. For data items which are not available on the property file, corresponding entries in the HACS state file will remain as default values, and, if subsequently accessed by a hazard assessment model, these will cause the UIM to request input values from the user for these items. (This situation cannot be avoided until the work to update the property file with "data gap" values has been completed.)

Completion of the property file retrieval step is noted by the UIM by the brief display:

(3.13) PHYSICAL PROPERTY DATA RETRIEVED FOR CHEMICAL code
NAME = name
SHIPPING STATE = s

where the entries (code, name, s) in the display are obtained from the file.

The chemical data file record transferred to HACS in the above step contains information describing appropriate hazard assessment models for the user specified chemical, and the UIM next requests user input for the models to be selected:

(3.14) ENTER ASSESSMENT MODEL LETTER CODES (A-Z/II/RR/SS):

The expected user response is to type one or more of the model letter codes: A to Z, II, RR and/or SS. The letter codes entered must be separated by at least one space. Any valid codes may be entered, and, once accepted by HACS, these are stored and used to control subsequent execution of the models, in the sequence the codes have been entered by the user, until all models requested by the user have been run. Note that individual model runs can also be selected by entering a single model code in response to message (3.14), then on completion of that model run, responding to message (3.2) for run control with a CONTINUE response; this second pass run can then be used for executing the second model, and so forth, allowing all prior user input values to be available for these following runs.

Acceptable user responses to prompt message (3.14) are, in addition to a list of hazard assessment model code letters, a carriage return or a question mark (?) followed by a carriage return. Both of these responses are designed to allow the UIM

to generate additional displays to assist the user in the selection of model codes.

The question mark causes the UIM to produce a display describing the appropriate hazard assessment scenarios for the specified chemical:

(3.15) HAZARD ASSESSMENT MODEL CODES ARE ALPHABETIC LETTERS DESIGNATING DIFFERENT MODELS. MODEL CODES MAY BE ENTERED ONE-AT-A-TIME, OR IN A SERIES OF CODES, EACH SEPARATED BY ONE OR MORE BLANKS, TO SELECT A COMPLETE HAZARD ASSESSMENT SCENARIO FOR EVALUATION.

SCENARIOS APPROPRIATE FOR CHEMICAL code ARE DESCRIBED BELOW -

- The scenario codes and descriptions applicable to the selected chemical are displayed. The complete set of scenarios and descriptions are given in Section 3.1.2.1 of this manual. The chemical recognition code for the selected chemical is automatically inserted in the above message.

GENERAL NOTES:

1. ANY MODEL CAN BE EXECUTED BY ITSELF IF THE USER HAS SUFFICIENT INPUT DATA.

2. MODEL A EXECUTION NEED NOT BE PERFORMED IF THE USER HAS SUFFICIENT INPUT DATA FOR SUBSEQUENT MODELS.

3. THERE ARE MANY SUBSTANCES THAT EXHIBIT BORDERLINE BEHAVIOR WHEN RELEASED INTO THE ENVIRONMENT. DEPENDING ON AIR AND WATER TEMPERATURES, THEY MAY SINK OR FLOAT IN WATER, DISSOLVE OR NOT DISSOLVE, BOIL OR NOT BOIL, AND SO ON. THE PATH CODES FOR SUCH SUBSTANCES CAN THEREFORE REPRESENT SCENARIOS THAT AT FIRST APPEAR TO BE CONTRADICTORY, BUT WHICH ARE INDIVIDUALLY VALID UNDER CERTAIN ENVIRONMENTAL CONDITIONS.

Following the display of the appropriate scenarios and general notes, the UIM branches to determine if the user requires descriptions of individual models (see prompt message 3.19).

If the user response to the UIM request for hazard assessment model code input is a carriage return, the UIM produces a display identifying the path codes stored on the chemical property file for the specified chemical:

(3.16) APPROPRIATE HAZARD ASSESSMENT MODELS ARE: list

where list represents the actual codes from the property file which are displayed with the message. Again, the UIM will

branch to determine if the user requires descriptions of individual models (see prompt message 3.19).

If the user response to the UIM request (3.14) for model code input is not a question mark or a carriage return, the UIM expects the user input to give the model letter codes for the run, and the user input is displayed at the terminal for verification. At present, the UIM allows a maximum of 15 codes to be entered, and any additional codes, if entered, are ignored. This limit is ample for any scenarios of practical interest. No model code may be given more than once, and, except for O, Z, II, RR and SS, the different codes specified must be given in alphabetical order from left to right.

The user should exercise caution in specifying the model codes to insure that HACS is being requested to execute the models representing one scenario or branch of the hazard assessment tree at a time, and should be familiar with the model and scenario selection description in Section 3.1 of this manual. Evaluation of alternative scenarios requires repeated executions of HACS with each scenario specified separately. Table 1 lists individual scenarios. For example, if the hazard assessment code for a chemical is ABCDEFG, the user must realize the sub-sets AB, AC, and ABC are applicable when a gas is venting from a ruptured tank, and that sub-sets AD, ADE, ADFG, and ADEFG are applicable when liquid is being vented from the tank. These various sub-sets of the code obviously represent two radically different conditions under which the chemical is being released. HACS cannot in a single run first assume that only gas is venting and then attempt to execute models which pertain only to liquid releases. Thus, the user must perform at least two separate runs if he wishes to assess each possibility. If he does so, he must then review all output to decide which set more fully represents the actual discharge situation (i.e., if Model A indicates that liquid has been released, the user must realize that the output of Model G is more accurate than that of Model C for determining vapor dispersion hazards).

After reading the user input to specify model codes for the assessment run, several tests are then performed to partially validate the user entered codes. An error identified by the UIM will cause one of error messages (3.17) or (3.18) to be displayed. Whether an error condtion is detected or not, the UIM provides an option to the user to obtain a printed display describing any of the available models (see prompt message 3.19).

(3.17) *****INPUT CONTAINS UNRECOGNIZABLE RATE MODEL CODE

One or possibly more of the model codes entered by the user is not one of the codes A to Z, II, RR or SS. Since this test is performed by comparing the user input to an internal list of codes, the user should check the UIM display of user entered codes to determine whether the UIM has stored these codes as intended. The most likely cause of this error will be the omission on user input of a space separating two or more codes which the UIM will attempt to treat as a single code. Following this error message, the UIM will first branch to determine if the user requires an explanation of the models (see message 3.19) before returning to (3.14) to request corrected user input.

(3.18) *****MODEL CODES NOT IN CORRECT ASSESSMENT SEQUENCE

Referring to the hazard assessment tree in Figure 4, it can be seen that the sequence of model operations in any scenario (along any branch or path of the tree), occurs such that the models are to be used in an alphabetical sequence (e.g., A T U V W) when two or more models are to be linked to form a path. Single model paths (i.e., O, Z, II, RR and SS) are automatically omitted from this requirement. Also, along a valid path or scenario, any single model letter may appear only once. The error message indicates that one of these conditions has not been satisfied by the user input. The UIM will first branch to determine if the user requires an explanation of the models (see message 3.19 below) before returning to (3.14) to request corrected user input.

(3.19) DO YOU NEED DESCRIPTIONS OF THE MODELS?

where acceptable user responses are Y (or YES) or N (or NO). Responses other than YES or NO will produce a UIM diagnostic. If the user response is no, the UIM checks for completion of input of the hazard assessment model codes. If the codes have been entered by the user and no errors detected, then the UIM proceeds to the model execution steps (a typical model execution sequence is described in Section 3.2.4). If the user has not previously selected assessment models, or if an error was found in the user input, then the UIM will repeat prompt message (3.14) to request user input of these codes.

If the user response to (3.19) is Y or YES, the UIM enters a cycle to produce for the user descriptions of as many models as desired:

(3.20) ENTER MODEL LETTER:

Acceptable responses to the initial model description request are a one or two letter model code or a question mark followed by a carriage return, a carriage return, or the label EXIT followed by a carriage return.

If the user specifies a model code which is not one of the defined codes, the UIM will respond with:

(3.21) code IS INVALID

where code is displayed as the user entered value.

This condition, or a carriage return or question mark response to (3.20) will cause the UIM to display:

(3.22) VALID LETTER CODES ARE A TO Z, II, RR, OR SS

followed by:

(3.23) TYPE MODEL LETTER OR
TYPE EXIT TO CANCEL REPORT

In response to each valid model code entered by the user for prompt (3.20), the UIM will produce the desired text display (reproduced in Section 3.1.1) followed by message (3.23). The user may continue this cycle for as long as desired and obtained printed descriptions of any of the models, not just those entered for the particular HACS run. The cycle is stopped when the user responds to either (3.20) or (3.23) by typing EXIT. The UIM then responds as if the user had not requested the model displays (see 3.19 above).

3.2.4 Typical Model Execution Sequence

On completion of the user input for the chemical recognition code, hazard assessment scenario codes and any associated displays requested by the user, the UIM initiates a sequence of operations to execute in turn each assessment model specified by the user in the scenario input. Each model is different, and the input requirements, output displays and results obtained are also different. Section 3.3 contains detailed descriptions of each individual model, including definitions of all required model inputs which may be entered by the user.

However, within the HACS/UIM, each of the hazard assessment models is executed in the same manner, according to a set of standard procedures in the UIM which are described as follows.

Initially, prior to the execution of any hazard assessment models and the input of any user data items, the internal state file contains only the chemical property data available from the external HACS property file. For all other variables only default values are available at this stage for use by any of the assessment models. The UIM uses the user specified models to request from the user only those data items which are required to run a model requested by the user. This input is obtained in the form of a UIM query -- user response dialog until all the required input for the model has been obtained. The UIM will automatically suppress requests for user input of chemical property data which is already available. When all the input data for a single model run has been entered, the UIM automatically prints a display of these values. The user at this point may either request the UIM to run the model with these values, or may elect to change previously entered values. The user may change the value of any data item defined in the HACS state file, not just those listed as inputs for the particular model. When the user has entered as many changes as desired, the UIM again displays the summary of input values for the model and the user can again elect to make further changes or to run the model.

Following the model execution, the UIM allows the user to either proceed to the next model in the scenario sequence or to repeat the execution of the current model. At the time the current model is re-executed, the internal HACS state file contains all the user input values entered previously, that is, sufficient data is now available for re-execution, and the UIM dialog to request user input values is suppressed. Instead, the UIM continues to provide displays of current model input values, and provides a means for the user to selectively enter changes if desired.

This approach continues for each of the models requested in the user's scenario list. The UIM requests specific required input values on the first execution of a model only if they have not previously been entered, and stores these values in the HACS state file. Thereafter, the user may change any value if desired otherwise the previously stored user input value is used and the input prompt is suppressed.

Since the UIM-user input dialog is governed by the hazard assessment models themselves, the input requirements for a single model are not always the same. For example, if a model provides for both instantaneous and continuous discharge situations and the user specifies an instantaneous release, the UIM will automatically request from the user input regarding the total mass of the discharge. If in a later run, the user switches to a continuous release situation, the UIM will require user input values for the mass rate of release and the duration of release. These requirements will be noted by the appearance of default values in the model input summary. All other input values entered for the instantaneous spill condition will remain the same and, if also used for the continuous release case, will not be requested by the UIM a second time. These values may however be changed by the user if desired.

Users may also elect to perform a similar type of query control for different runs using different hazard assessment scenarios. (Refer to Section 2.0.) Under RUN control, the HACS/UIM is automatically initialized to the default state. Any input data required to execute a model is initially requested from the user via a prompt dialog. If a second scenario is then executed in a new RUN sequence, the UIM will return to the prompt mode, and request from the user the full set of input values required for the second scenario. If instead the second scenario is executed in the CONTINUE mode, the HACS state file is not re-initialized and the current contents, including user values, remains unchanged. Thus, for the second scenario, only the additional data items not previously entered will need to be entered by the user.

The general procedures, common to all assessment models, by which the UIM performs these operations, start with the execution of a model, and the associated UIM display is:

(3.24) FOR EXECUTION OF MODEL code,

where code is inserted in the display as the appropriate one or two letter model code. If the model has been previously executed during the assessment run, then user input values have already been entered and the UIM proceeds directly to print a summary of model input values (see message 3.29). For the first time each assessment model is executed, the UIM initiates the input dialog with the display:

(3.25) PREVIOUSLY UNSPECIFIED INPUT DATA, IF ANY, ARE REQUESTED BELOW...

The UIM begins to process each data item required for input to the model which is being run. For each input item, the value currently stored in the HACS state file is retrieved, and the source or status code associated with the value is examined. If the current value is not a default value, then the current value is saved for use with the model and the UIM skips to examine the next input item.

If the current value of a data item is a default, then the UIM initiates a query to obtain a value from the user:

(3.26) ENTER REAL VALUE FOR name IN $unit_1$, $unit_2$, $unit_3$, $unit_4$

or

(3.27) ENTER INTEGER VALUE FOR name

where (3.26) is used if the data item required is a decimal value, and (3.27) if the data item is an integer. The name of the HACS data field is inserted in the prompt, and for decimal values, the defined units are displayed in message (3.26).

Acceptable user responses to (3.26) or (3.27) are a carriage return, a question mark followed by a carriage return, or the requested input value. If the user types a question mark, the UIM automatically prints a description of the field (refer to Appendix L) then repeats the prompt (3.26) or (3.27).

If the user types a carriage return, the UIM interprets this response as a request for a display of the current value of the field. The current value is displayed and followed by:

(3.28) DO YOU WISH TO USE THIS VALUE?

If the user responds NO, then the UIM returns to (3.26) or (3.27) to permit the user to enter a value. If the response is YES, the displayed value is first compared to pre-stored upper and lower range limits; and if a limit is exceeded, a warning message is displayed to the user. The stored value is used as requested however and the UIM proceeds to obtain the user input for the next data item required by the model. Later in the run when the model input summary is displayed the user may elect to revise any input values if desired.

When the user responds to the input prompts (3.26) or (3.27) by entering a value and optional unit labels, the UIM first interprets the value typed as either a decimal value or an integer. Input rules for these quantities are given in Section 3.2.2. If an error occurs, a diagnostic message is given by the UIM which then returns to the input prompts (3.26) or (3.27)

If a decimal value is being entered, the UIM expects the value to be followed by an optional unit label, which, if present, must be typed exactly as shown in message (3.26). Refer to Section 3.2.2 for additional rules governing input of name quantities. If the unit label is omitted, the UIM assumes that the unit appearing first in the list is implied. If a unit label is given, the UIM will compare the user typed label to the labels given in the list. If an error occurs, the UIM issues a diagnostic then repeats message (3.26). For correctly entered unit labels, the decimal value is appropriately converted to internal units for further use. Note that unit labels may be typed for integer quantities; however, they are not used by the UIM since all integers are assumed to be non-dimensional.

After a user value has been successfully input, it is compared to the internal range limits, and a warning message is displayed by the UIM if either the lower or upper bounds has been exceeded. The value is stored for further use as entered, and may be changed later by the user if desired. Note that values directly entered by the user in response to (3.26) and (3.27) are stored in the HACS state file as "user" values. Existing default values retained by responding "YES" to (3.28) remain as default values.

The UIM continues to process the prompts for user input values, (3.26) and (3.27), and the corresponding user responses, until all input values required for the particular model run have been obtained.

After the initial prompt input cycle for a model, and each additional time a model is executed, the UIM initiates a display of the current values of all model input data items:

(3.29) THE SUMMARY OF INPUT DATA FOLLOWS...

Each input item required by the model is displayed; included are the field number, value, field name, and source code. The display of decimal values uses units according to the user specified option. Note that the values displayed may in general include a mix of user input values, chemical property data, computed results and default data items. As each value is displayed, it is also automatically compared to the range limits stored in HACS and a warning message is printed if the current value of a data item exceeds one of the corresponding limits.

As the display is produced, the UIM tracks the status or source codes of each data item, and if any default values were encountered the UIM completes the display of input values with:

(3.30) WARNING - MODEL code IS USING DEFAULT VALUES

where the model letter code is inserted in the message. This condition is displayed as a warning only since users may elect to run a model with default value input data in the absence of other data, or if the default value is known not to significantly affect model results, or if the default value is completely acceptable (e.g., as in a table or plot option).

However, the printed model input summary should be carefully reviewed, and the occurrence of any default values specifically checked to ensure that the desired model input has been obtained. Since the user specification of model input data items is controlled by each model itself, it is possible for a

user to change a value of one input data item which in turn will cause the model to require additional data not anticipated by the user. When this occurs on the initial execution of a model, the UIM will automatically request these additional values from the user by means of the input prompt dialog. When this occurs after the initial input has been entered, the current version of the UIM cannot repeat the prompt messages, and instead any additional data input requirements are identified by the appearance of default values in the model input summary.

Following the display of current model input values, and the diagnostic message for the default value condition if appropriate, the UIM provides an opportunity for the user to correct or change any data item prior to executing the model:

(3.31) DO YOU WISH TO CHANGE ANY MODEL INPUTS?

Appropriate user responses are either YES (or Y), or NO (or N). Responses other than yes or no will produce a diagnostic message, and a repeated request.

If the user response is no, the UIM proceeds to execute the particular model, and subsequent output displays of the model results are governed by the model as well as any optional output requests entered by the user. Appendix G contains a sample HACS/UIM run for illustration. Following the model run, the UIM provides an opportunity for the user to repeat the run with revised input values if desired before proceeding to the next model in the scenario list (refer to message 3.35 which follows below).

If the user response to (3.31) is yes, the UIM responds with:

(3.32) ENTER FIELD NUMBER:

The field number is a standard four digit (integer) data item reference used by HACS, and the field numbers for each data item used by the current model are all listed in the model input summary displayed prior to this prompt by the UIM. The full set of data item field numbers for all models in HACS are identified in Section 3.3 and the appendicies of this manual.

The expected user response to (3.32) is a valid four digit integer. If an invalid integer is typed, the UIM will respond with an integer syntax error message, followed by prompt (3.34). A question mark response, or any other non-integer input will be treated as an invalid integer.

The field number entered by the user is first tested for a value of 9999 which is used to terminate this user input procedure. If the value is not 9999, then the field number typed by the user is used to access the appropriate data item value in the HACS state file.

If the field number typed by the user does not correspond to an entry in the HACS state file, the UIM displays:

(3.33) FIELD NUMBER nnnn IS UNDEFINED.

where nnnn is replaced in the message by the value entered by the user. The UIM then displays message (3.34) to request corrected input.

If the field number entered by the user is accepted, the UIM enters the prompt mode for user input of a data value for that field; prompt messages (3.26) or (3.27) are displayed for input of decimal or integer values. Acceptable user responses are the same as for the initial data input step, that is,

(a) enter a value with optional units for decimal values

(b) enter a carriage return to display the current value

(c) enter a question mark and carriage return to obtain a description of the data item.

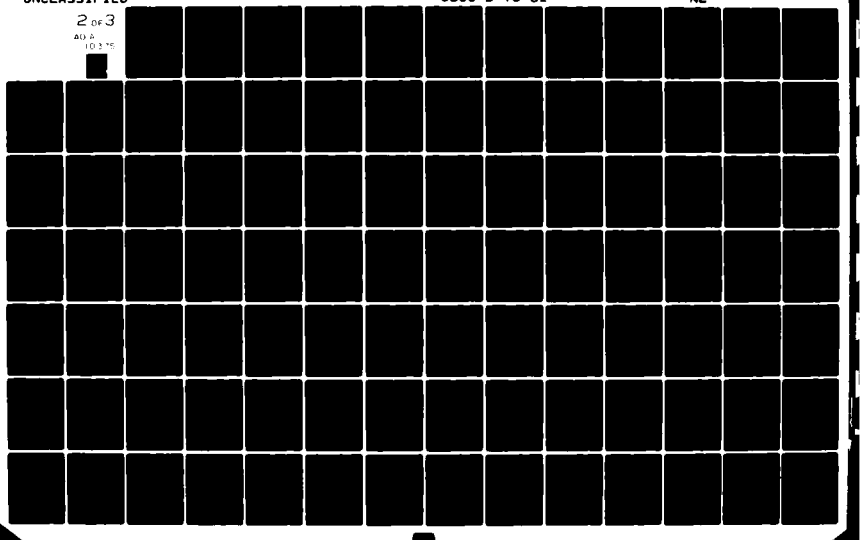
Refer to the description of messages (3.26) and (3.27) and following to review the operation of the UIM in response to these alternatives. As before, if the user elects to leave the current value unchanged, or enters a new value, the value stored is compared to range limits prior to continuing for the next input.

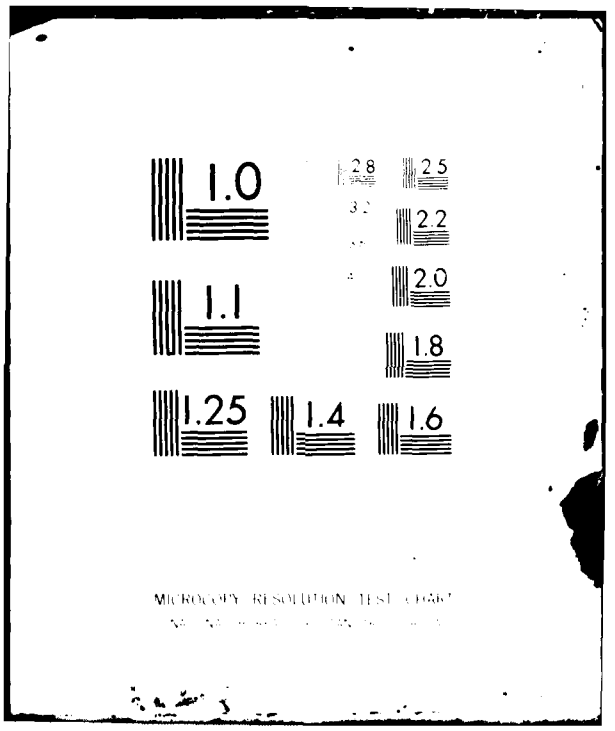
Although the model input display produced by the UIM prior to message (3.32) lists only those data fields required for the particular model being run, this user update procedure can accept any valid HACS field number whether or not listed in the preceding summary. Thus, if desired, users may at this stage enter data not only for the particular model, but also for any other model as well.

Once an acceptable user response has been obtained to the input prompts (3.26) or (3.27), the UIM continues the cycle for the next user value, if any, by:

AD-A110 375 LITTLE (ARTHUR D) INC CAMBRIDGE MA F/6 7/1
HAZARD ASSESSMENT COMPUTER SYSTEM HACS/UIM USERS' OPERATION MAN--ETC(U)
SEP 81 R G POTTS DOT-CG-941999-A
UNCLASSIFIED USCG-D-75-81 NL

2 OF 3
AD A
110375




1.0
1.1
1.25
1.4
1.6
2.0
1.8
2.2
2.5
MICROCOPY RESOLUTION TEST CHART

(3.34) ENTER FIELD NUMBER OR 9999 TO EXIT

If the user types another field number, input prompts (3.26) or (3.27) are repeated for the new field, and this cycle continues for as many field numbers as the user wishes to enter until a value of 9999 is entered.

Since the user has appeared to have changed at least one data item, when the changes are completed by responding to either (3.32) or (3.34) with 9999, the UIM will automatically repeat the summary of model input values, followed by (3.31) to determine if any further changes are desired. At this point, users should carefully review the model input display before proceeding since the effect of user entered changes may be to produce additional, unanticipated, input requirements, and the model input summary may, after the changes have been made, include default values which were not present before the changes were entered.

The process of producing an input summary, followed by entering changes may be continued for an indefinite number of cycles, continuing until the user response to (3.31) is no (i.e., no changes to model inputs are to be made). The model is then executed, and the model output results are displayed.

After completion of the individual model run, the UIM displays:

(3.35) DO YOU WANT TO RE-RUN THIS MODEL?

where only YES (or Y), or NO (or N) responses are acceptable. If the user response is yes, the UIM responds by displaying the model input summary and requesting changes from the user. Each model may be re-run as many times as necessary until the desired results have been produced. If a large number of repeated runs are anticipated, users might want to omit any table or plot options for all except the last model run to minimize the amount of output which will be generated.

If the user response to (3.35) is no, the UIM will proceed to the next model (if any) specified by the user in the scenario codes (refer to message 3.14). Each model requested is executed in turn, and for each the UIM operation consists of the steps from message (3.24) to (3.35).

After all the requested models have been run, the UIM processes run summary options (refer to Section 3.2.5) which may be selected by the user, and then returns to determine if any new chemicals or scenarios are to be run (refer to Section 3.2.3).

3.2.5 Output Summary

As the UIM steps of user input and model execution proceed, values of the HACS data fields are collected in the HACS state file as user input values, chemical property values, and computed values. Any items not otherwise referenced during a hazard assessment run remain as default values in the state file.

After all models specified for a single hazard assessment scenario have been run, the UIM provides an option to obtain displays of the values stored in the state file, together with descriptions of the models and hazard assessment scenarios applicable to the specific chemical:

(3.36) DO YOU WANT TO PRINT A SUMMARY OF THESE RESULTS?

If the user response is NO (or N), the output summary is omitted and the UIM begins to process the next user run request. If the user types YES (or Y) in response to (3.36), the UIM proceeds to ask a series of questions to obtain the selection of user options for the requested report. For each option requested, for example, computed field values, the user is also given an option to include or omit text descriptions with the output. For options that are not selected, the UIM prompt to select text descriptions is omitted.

The UIM prompts to obtain user selections for the display are:

WHICH OF THE FOLLOWING DO YOU WANT?

(3.37) SCENARIO CODES?

(3.38) MODEL CODES?

(3.39) USER FIELD VALUES?

(3.40) COMPUTED FIELD VALUES?

(3.41) CHEMICAL PROPERTY FIELDS?

If the user response to any of (3.37) to (3.41) is yes, the UIM replies for each YES response with:

(3.42) WITH TEXT DESCRIPTIONS?

and appropriate user responses are yes or no. After the response to (3.41) has been entered, the UIM produces the requested report. An example output report is included with the sample UIM run in Appendix G of this manual. After printing the report, the UIM begins to process the next user run request as if the response to (3.36) had been no.

3.2.6 Methodology Behind Input Preparation

When preparing input data for a HACS run, it should be kept in mind that HACS will substitute default values (i.e., nominal values that in general cannot be expected to represent all discharge situations, environmental conditions, or particular chemicals discharged) for any information that is necessary for the execution of the specified estimation route but has not been supplied by the user or the Chemical Properties File. For this reason, no run that uses default values should be considered as an "accurate" run unless the default values can be considered representative or of no consequence to the validity of the results (e.g., optional output specifications may be omitted without affecting calculations). In any event, all default values that have been reported to have been used for a model execution should be examined carefully before the results of that model are accepted. The default values are included in HACS solely for the purpose of allowing a full execution of all mdoels during the first run for a given discharge incident. By allowing this execution the user is able to check out input information and can get an indication of expected results under default conditions when environmental and discharge conditions are not fully known. A list of the default values in HACS is given in Appendix C.

For the complete assessment of the hazards associated with the discharge situation, it is anticipated that a series of HACS runs will have to be made. When the hazard situation is extremely well understood and defined and the user is very familiar with HACS, it might be possible to analyze any discharge with only one run. In general, however, the user should anticipate a series of steps similar to the sequence presented below.

- Initial Information Verification Run. On this run the user will input for the first time current data on the discharge situation to verify (1) that all input information is presented correctly to HACS and (2) that all relevant information required by HACS for the particular discharge incident is provided by the user or obtained from the Chemical Properties Files. Any default values that are reported to be used by HACS during this run should be analyzed carefully for possible replacement by user inputs.

- First Production Run. Given the proper information in terms of user input to HACS, this will be the first run to assess the effects from the discharge condition for specific spatial and temporal parameters.

- Subsequent Hazard Assessment Analyses. Additional runs can be made to analyze the hazardous effects (i.e., toxicity and thermal radiation exposure, etc.) for different time periods or for different distances from the discharge.

Further, alternative environmental conditions (e.g., changes in wind velocity, current velocity, etc.) may be analyzed to prepare for a possible change in the environment of the discharge.

Multiple assessments, selective replacements of HACS computed values by on-scene observations, and evaluation of hazard sensitivities to selected parameters may be performed utilizing the assessment run control options described in Section 2.

3.3 MODEL DESCRIPTIONS AND USAGE SPECIFICATIONS

This section contains descriptions and usage specifications for each of the hazard assessment models as designated in Figure 4, the hazard assessment tree of possible events. The part for each model contains a description of the model followed generally by four tables.

The first table in each case describes the on-scene and operational data input the model requires. The second table lists the chemical property data the model will obtain from the Chemical Property Data File unless user overridden. The next table defines the output of the model and the last tables contains descriptions of the specifications necessary for optional output of plots or tables.

MODEL A

Purpose

Model A computes the rates and times of release, and total quantities released, of gases or liquids which are discharging from a punctured tank or container. It is, in general, the first model which is executed in a given hazard analysis.

Insufficient Data Problems

Execution of Model A requires that the user provide detailed data which describe the size and location of the hole in the tank, the dimensions of the tank, and the cargo contained within the tank (i.e. amount, temperature or pressure, etc.). It can be expected, therefore, that the user will not always have sufficient data from on-scene to properly execute this model.

In such cases, the user can still fully utilize the resources of HACS by providing subsequent models those required input data which would normally be output from Model A. For example, if the user only knows that a certain amount of gas has been released, he may execute the vapor dispersion models (e.g. C) by inputting the amount of gas released by use of data field number 4001, the field number which describes the total mass of gas released into the atmosphere. He would, of course, have to also specify that the release has taken place instantaneously (by setting field number 2061 to "0"). Alternatively, if he knows the total amount of gas which has been released, and the time span over which the release has taken place, he may wish to use field numbers 2061, 4044, and 4045 to execute the vapor dispersion models for a continuous release of gas.

Restrictions and Cautions on Model Use

The model cannot be used if the hole from which the discharge is taking place is underwater. It can be used when the hole is at or above the surface of land or water.

The hole size input should not be very large compared to the size of the tank. In such a case, the tank contents will discharge so rapidly that use of the model will be unwarranted and may, indeed, lead to inaccurate results. For example, the user should not specify that the hole in the bottom of a tank is the same size as the bottom of the tank!

The model only works for liquids or gases which are discharging from a tank. It will not work for solids.

Important Assumptions of the Model

The model assumes that the tank or container is of uniform cross-sectional area from top to bottom (e.g. an upright cylinder or a

rectangular box shape). It will not work correctly for spherical tanks.

The model assumes there is only one hole in the tank, i.e. that there is not one hole on the bottom or the side through which liquid is being released and another on or near the top through which air is entering or gas escaping, etc.

Important User Decision

The user must select whether he wishes the venting (discharge) process to be assumed by the model as being adiabatic or isothermal in nature. The adiabatic option is best suited when a well-insulated tank which will not allow much heat to pass through its walls is involved. The isothermal option is best for tanks which are not insulated.

If a liquid is being released, the differences in answers produced by the two options will not be very significant. It is when gas is discharged that the differences can be great. For example, if discharge is due to gas escaping the top of a tank containing a compressed, liquefied gas, the adiabatic option will allow the liquid to cool down due to gas expansion effects whereas the isothermal option will keep the liquid at a constant temperature. In the former case, venting may stop of its own accord when the temperature of the liquid becomes low enough. In the latter case, the venting may continue until all the liquid has evaporated. Depending upon the given conditions of the release, therefore, one choice may show that much more gas has been released than the other.

The choices of adiabatic or isothermal venting represent the two extreme conditions under which venting can take place. The user should be aware that no tank is perfectly insulated, or vice versa, and that the most realistic case will be somewhere between the two conditions, tending more towards one than the other depending upon tank wall construction.

Input Data Considerations

Input to the model requires the diameter of a circular hole through which discharge is taking place. If the hole in the actual tank is not circular, but enough is known that its cross-sectional area may be estimated, the user must calculate and input the diameter of a hole which is of equivalent area to the actual hole. This is done using the formula:

$$\text{Hole diameter} = 2 \times \sqrt{\text{hole area}/3.14}$$

Model A does not require both the initial temperature of the cargo and the initial pressure in the tank as input. However, the HACS operating system requires the initial temperature in order to determine the values of certain data items which are a function of temperature. Since uncertainties in the initial temperature can be tolerated better than uncertainties in the pressure for Model A, and the pressure is estimated from

the temperature if it is not given, the user is given the option of which of these two data items he wishes Model A to use. If he specifies the pressure, it will be used. If he does not specify the pressure, either his value for temperature or the default file value for temperature will be used.

Output of the Model

Output of the model consists of the total mass of gas which discharges from the tank, the average gas discharge rate, and the time span over which gas discharge takes place. It also includes similar output for any liquid which vents and the total volume of liquid released. Following these data, the model then gives estimates of which spill duration flags are appropriate for use in subsequent models.

A time span of 10 minutes was chosen as the criterion for spill duration flag estimates. If discharge times are less than 10 minutes, HACS assumes that the discharge has been "instantaneous." If the time is greater than 10 minutes, the discharge is considered to represent a continuous spill. The user can, of course, override these flags as he desires. To be noted is that some subsequent models may change these initial spill duration estimates if their computed output indicates a change is appropriate.

Optional output for this model includes tables giving the total mass flowrate, the amount of gas released, the total amount of liquid released, the temperature of the cargo, and the pressure in the cargo tank as a function of time. Two tables are printed out. In one, the units of output quantities are given in SI units. In the other, the units used are English.

Data Specification

Table A1 defines the on-scene and operational data which the model requires.

Table A2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table A3 defines the output of the model. The user may override any computed output data with his own values.

Table A4 defines the data necessary for production of the optional tables.

TABLE A1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2001	TANK VOLUME	CM3 M3 FT3 GALS	Volume or capacity of tank which is venting	
2002	TANK HEIGHT	CM M FT MI	Tank height or overall depth	
2003	HOLE HEIGHT	CM M FT MI	Height of bottom of hole above the bottom of the tank	
2004	TEMP START	C K F	Temperature of liquid before discharge starts	
2005	TANK PRESS	D/CM2 N/M2 PSI MM HG	Pressure (absolute) in the tank before discharge starts. This is an optional input if 2004 TEMP START is known.	
2006	ADBT OR ISO	ND (Integer)	Flag indicating whether venting is to be assumed adiabatic or isothermal.	0 = isothermal 1 = adiabatic
2007	INITIAL MASS	G KG LB TN	Initial weight of chemical in tank	
2008	HOLE DIAM	CM M FT MI	Diameter of hole in tank-hole is assumed to be circular	See model description if hole is not circular.
2009	NUMB MASS INC	ND (Integer)	Number of mass increments the model is to use for integration	Any integer from 10-150 is allowed. 50 is minimum for accurate results. 100 is the default value.

TABLE A2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	
1004	DENS LIQ AMB*	G/CM3 KG/M3 LB/FT3	Density of liquid at ambient temperature	Required only if 2004 TEMP START is greater than or equal to 15 deg. C (59 Deg F)
1007	HT CAP LQ-AM*	CL/GC J/KGK BT/LBF	Heat capacity of liquid chemical at its initial temperature	
1010	VPE COEFF A	LOG FCN	Coefficients of a vapor pressure equation in the form of the one in Section 2.4.3 but which gives an answer in mm Hg.	
1011	VPE COEFF B	C		
1012	VPE COEFF C	C		
1013	HT CAP VP-AM*	CL/GMC J/KGMK BT/LBMF	Heat capacity of chemical vapor at its initial temperature	
1014	HEAT OF VPR	CL/G J/KG BT/LB	Heat of vaporization of chemical	
1021	LIQ DENS BP	G/CM3 KG/M3 LB/FT3	Density of the liquid at its boiling point	Required only if 2004 TEMP START is less than 15 deg C (59 deg F)

* These data items are automatically computed at temperature 2004 TEMP START.

TABLE A3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4001	TOT MAS GAS	G KG LB TN	Total weight of gas which will escape from the tank	
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid which will escape from the tank	
4003	TOT VOL LIQ	CM3 M3 FT3 GALS	Total volume of liquid which will escape from the tank	
4047	GAS FLWRATE	G/S KG/S LB/S TN/HR	Average discharge rate of gas while it vents	
4048	GAS FLW TIME	S MIN HR	Time span over which gas will vent	
4049	LIQ FLW RATE	G/S KG/S LB/S TN/HR	Average discharge rate of liquid while it vents	
4050	LIQ FLW TIME	S MIN HR	Time span over which liquid will vent	
4044	AVG VAP RATE	G/S KG/S LB/S TN/HR	Average flow rate at which gas discharges from tank. Value is same as given by 4047 GAS FLW RATE	Value is stored as an ESTIMATED value in case Model C directly follows. This allows subsequent models to override this value with better COMPUTED data.
4045	EVOLVE TIME	S MIN HR	Time span over which gas discharge takes place.	Same as above
4068	AVG GAS TEMP	C K F	Average temperature of discharging gas. Stored as an estimated value.	Answer may be refined by subsequent models.

TABLE A3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS (CONT'D)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
Data Estimated For Use By Subsequent Models				
2029	SPILL TYPE P	ND (Integer)	Duration flags indicating whether discharge is continuous or instantaneous	0 = Instantaneous discharge 1 = Continuous discharge
2058	SPILL TYPE T	ND (Integer)	Estimated for use by subsequent models. See model description for discussion	
2060	SPILL TYPE D	ND (Integer)		
2061	SPILL TYPE C	ND (Integer)		

TABLE A4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3001	TABLE FLAG A	ND (Integer)	Flag for indicating whether tables are desired. See model description for description of tables.	0 = Tables not desired 1 = Tables are desired

MODEL B

Purpose

Model B is utilized in situations where a gas is venting under pressure from a hole in a tank and the gas is flammable. It computes the length of the flame jet, the average diameter of the flame, and the distances from the flame which are "safe" for people and combustible materials. It can also determine whether or not an intact tank containing a compressed liquefied gas will rupture if exposed to the flame, and how long the tank must be exposed before it does rupture.

Modules Which Constitute Model B

The model is comprised of three modules (i.e., parts) which are designated Model B1, Model B2, and Model B3. Model B1 calculates the length and diameter of the flame jet. Model B2 calculates the safe separation distances from the flame, and Model B3 computes whether or not an intact tank containing compressed liquefied gas will rupture if exposed to the flame and how long it will take before rupture occurs.

Restrictions and Cautions on Model Use

If the tank from which the gas is discharging has a low internal pressure (i.e., relatively close to 1 atmosphere), the flame jet might be much smaller than that estimated by the model.

If the ignited gas produces a sooty flame, the answers given by the model can be very conservative.

If the construction specifications for a tank of compressed liquefied gas exposed to the flame are not known precisely, Model B3 may provide answers which are substantially in error.

See the sections below for more details on the above cautions for use.

Important Assumptions of the Model

The model assumes that the flow in the gas jet is turbulent, i.e, that the gas discharges from the hole at a high speed. Under these conditions, the size of the flame jet which is computed has been found to be reasonably accurate. When the gas discharges at a slow rate, however, this model provides conservative answers.

Thermal radiation flux is a measure of the heat energy from the flame which reaches an object near the flame. The model outputs safe separation distances from the flame for people exposed for a very short period of time, people exposed for a long period of time, and wooden structures. These distances are computed using three corresponding radiation flux levels. These levels are:

0.0339 cal/cm^2-sec: Causes burns to people exposed to the flame for a long period of time. It is about 1.5 times the energy flux that the sun can generate on earth on a very hot, bright, sunny day.

0.113 cal/cm^2-sec: Causes light burns to people almost instantantiously.

0.753 cal/cm^2-sec: Eventually causes wooden structures to ignite.

The model assumes that the flame is "clean" and radiates the maximum possible amount of energy. Many gases, however, generate sooty flames. Since substantially less heat is generated from sooty flames, the answers of the model represent *conservative estimates* of the hazard in such cases.

Input Data Considerations for Flame Size and Safe Separation Distance Computations

Input to the model requires the diameter of a circular hole through which gas discharge is taking place. If the hole in the actual tank is not circular, but enough is known that its cross-sectional area may be estimated, the user must calculate and input the diameter of a hole which is of equivalent area to the actual hole. This is done using the formula:

$$\text{Hole diameter} = 2 \times \sqrt{\frac{\text{Hole Area}}{3.14}}$$

The shape of the hole is not important to the manner in which this model operates. Hence, it is less complicated to input just a hole diameter than to provide complete specifications of the hole size and shape.

An optional input to the model is a thermal radiation flux for which a safe separation distance will be calculated. The model will not accept as input any value which is less than 0.0226 cal/cm^2-sec, a flux which corresponds to that generated by the sun on a hot, sunny day. If the user does not provide a value for this data item, he should ignore the default data warning message which appears for it.

Input Data Considerations for Tank Heating Model

Models B1 and B2, as noted above, respectively compute flame size parameters and safe separation distances from the flame. Chemical property data these models require, therefore, are those for the gas which is burning. Model B3 determines what will happen to an intact tank which contains a compressed, liquefied gas and which is exposed to thermal radiation from the flame. Model B3 utilizes certain data, therefore, for the substance within the intact tank. When Model B3 is requested for execution, the user must input chemical property data required by the model. These data, represented by field numbers 1010, 1011 and 1012, are listed for each pertinent chemical in a table following Table B1b.

A considerable amount of tank construction data is also required if Model B3 is desired to be executed. These data will be extremely difficult for a user to provide unless he has access to the blueprints and specifications of the tank which is exposed to the fire. To enable the user to execute this model in emergency situations, the HACS default file has been provided actual data from a pressurized propylene barge used by the Union Carbide Corporation and built by the Bethleham Steel Corporation. If the user utilizes these data, he must be aware that the reliability of the answers given is only as good as the degree to which these "typical" data apply to the actual tank in question. He is urged, therefore, to provide as much actual data as he possibly can. The relief valve setting and the wall thickness are of particular importance.

Input 2066 HEAT FLUX is an optional input value by which the user may specify the thermal radiation flux to which a tank is exposed. HACS computes a value for this flux and uses it if the user does not provide a value.

Output of the Model

Output of Model B consists of the safe separation distances from the flame for people exposed for a very short period of time, people exposed for a long period of time, and wooden structures. If the user desires, the model will also compute a safe separation distance for a thermal radiation flux level which he specifies. The minimum safe separation distance which can be computed in any case is 5 feet, with an accuracy of $\pm$ 5 feet. At longer distances, the accuracy of the model is $\pm$ 10 feet.

If execution of Model B3 is requested, the model will also determine if and how rupture of the tank occurs, how long it will take for rupture to occur, what the temperature of the tank wall is, and what stress is placed on the wall at failure.

Optional output from the model consists of a plot of radiation flux versus distance from the flame.

Data Specification

Table B1a defines the on-scene and operational data which the model requires for execution of modules B1 and B2.

Table B1b defines the tank construction specification data required for execution of Model B3. These data have been placed in a separate table because it is not expected that the tank heating model will be used as often as other parts of Model B.

Table B2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table B3 defines the output of the model.

Table B4 defines the data necessary for production of the optional plot.

TABLE B1a: ON-SCENE AND OPERATIONAL DATA
(EXCEPT THOSE SPECIFICALLY REQUIRED FOR TANK HEATING MODEL)

FIELD NUMBERS	FIELD NAME*	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2082	TNK HEAT FLG	ND (Integer)	Flag telling HACS which parts of the model to use. The input data for execution of the tank heating model are described in Table B1b. The data in this table are required for execution of either or both models.	0 = Compute flame size and safe separation distances 1 = Execute tank heating Model B 3 2 = Do both of the above
4008	FLAME ANGLE	RAD DEG	Angle of flame from plumb vertical (straight up = 0)	Flame is assumed to be vertical if value is not provided.
2008	HOLE DIAM	CM M FT MI	Diameter of hole in tank - hole is assumed to be circular	See model description if hole is not circular
2010	RAD FLUX	CL/CM2S W/M2 BT/FT2H KC/M2H	Thermal radiation flux for which a safe separation distance from the flame will be calculated	This is an optional user input. Ignore the default data warning message if it is not provided.

* Note: All data items on this page must be provided, with the exception of optional data item 2010, under all circumstances. The chemical recognition code specified for field 1001 should be for the substance which is burning.

TABLE B1b: ON-SCENE AND OPERATIONAL DATA
(FOR TANK HEATING MODEL)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2062	TANK DIAM	CM M FT MI	Internal diameter of the tank exposed to fire	
2063	WALL THICKNS	CM M FT MI	Wall thickness of the tank exposed to fire	
2064	ULLAGE FRCTN	ND	Fraction of the tank volume which does not contain liquid	
2065	RLF VALV SET	D/CM2 N/M2 PSI MM HG	Pressure setting (gauge) for the relief valve on the tank	
2066	HEAT FLUX	CL/CM2S W/M2 BT/FT2H KC/M2H	Radiation flux to which the tank is exposed (optional input)	Will be computed by HACS if user does not provide a value
2067 2068 2069 2070 2071	THR CND 0 DG THR CND 400 THR CND 800 THR CND 1200 THR CND 1600	CL/CMSC W/MK BT/FTHF KC/MHK	Thermal conductivity of the tank wall at 0,400,800,1200, and 1600 degrees F respectively	Default data is for a typical propylene barge. See model description
2072 2073 2074 2075 2076	SPEC HT 0 DG SPEC HT 400 SPEC HT 800 SPEC HT 1200 SPEC HT 1600	CL/GC J/KGK BT/LBF	Specific heat of the tank wall at 0, 400, 800, 1200, and 1600 degrees F respectively	*Same as above*

TABLE B1b: ON-SCENE AND OPERATIONAL DATA (Cont.)
(FOR TANK HEATING MODEL)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2077 2078 2079 2080 2081	TNS STR 0 DG TNS STR 400 TNS STR 800 TNS STR 1200 TNS STR 1600	MM HG N/M2 PSI D/CM2	Ultimate tensile strength of the tank wall at 0, 400, 800, 1200, 1600 degrees F respectively	Same as above
2083	TNK-FIRE DIS	CM M FT MI	Distance from the flame to the tank exposed to the fire.	
1010 1011 1012	VPE COEFF A VPE COEFF B VPE COEFF C	LOG FCN C C	Coefficients of a vapor pressure equation in the form of the one in Section 2.4.3 but which gives an answer in mm Hg. A list of coefficients for pertinent chemicals is given on the next page for the user's convenience.	These coefficients must be for the compressed, liquefied gas in the tank exposed to the fire. They should not be for the gas which is burning unless both are the same. See model description for further details.

PROPERTY DATA REQUIRED FOR TANK HEATING MODEL

Chemical Name	Code	1010 VPE COEFF A	1011 VPE COEFF B	1012 VPE COEFF C
Acetaldehyde	AAD	7.798	1444.0	273.2
Ammonia, anhydrous	AMA	8.022	1233.0	273.2
Boron trichloride	BRT	7.573	1340.0	273.0
Butadiene, inhibited	BDI	6.859	935.5	239.6
Butane	BUT	6.830	945.9	240.0
Butylene	BTN	7.378	1200.0	273.2
Carbon monoxide	CMO	7.194	352.4	273.0
Chlorine	CLX	7.418	1086.0	273.2
Chlorine trifluoride	CTF	7.367	1097.0	232.8
Cyanogen	CYG	7.847	1251.0	273.0
Cyanogen chloride	CCL	7.875	1430.0	273.2
Cyclopropane	CPR	7.816	1186.0	273.0
Dichlorodifluoromethane	DCF	?	?	?
1, 1-Difluoroethane	DFE	7.509	1150.0	273.0
Dimethylamine	DMA	8.297	1517.0	273.2
Dimethyl ether	DIM	7.818	1227.0	273.0
Ethane	ETH	7.211	800.0	273.2
Ethylamine	EAM	15.010	3514.0	273.0
Ethyl chloride	ECL	7.691	1375.0	273.2
Ethylene	ETL	6.748	585.0	255.0
Ethylene oxide	EOX	7.672	1359.0	273.2
Ethyl nitrite	ETN	10.050	2080.0	273.0
Hydrogen bromide	HBR	7.414	935.6	273.2
Hydrogen chloride	HDC	7.429	856.0	273.2
Hydrogen cyanide	HCN	7.791	1467.0	273.2
Hydrogen fluoride	HFX	7.394	1317.0	273.2
Hydrogen, liquefied	HXX	5.355	50.1	273.0
Hydrogen sulfide	HDS	7.434	970.0	273.2
Isobutane	IBT	6.748	882.8	240.0
Isobutylene	IBL	7.376	1197.0	273.2
Liquefied natural gas	LNG	6.612	389.9	266.0
Liquefied petroleum gas	LPG	6.830	813.2	248.0
Methane	MTH	6.612	389.9	266.0
Methylacetylene-propadiene mixture	MAP	7.021	962.0	273.0
Methylamine	MTA	8.348	1458.0	273.0

PROPERTY DATA REQUIRED FOR TANK HEATING MODEL
(Concluded)

Chemical Name	Code	1010 VPE COEFF A	1011 VPE COEFF B	1012 VPE COEFF C
Methyl bromide	MTB	6.960	986.6	238.3
Methly chloride	MTC	7.481	1148.0	273.2
Methly mercaptan	MMC	8.006	1432.0	273.0
Monochlorodifluromethane	MCF	7.625	1104.0	273.2
Nitrogen, liquefied	NXX	7.069	325.0	273.0
Nitrogen tetroxide	NOX	8.917	1799.0	276.8
Nitrous oxide	NTO	7.426	835.0	273.0
Oxygen, liquefied	OXY	7.056	377.0	273.0
Phosgene	PHG	7.511	1303.0	273.2
Propane	PRP	6.830	813.2	248.0
Propylene	PPL	6.820	785.0	247.0
Sulfur dioxide	SFD	7.282	999.9	237.2
Trichlorofluoromethane	TCF	7.524	1380.0	273.2
Trifluorochloroethylene	TFC	6.681	931.0	273.0
Trimethylamine	TMA	7.600	1303.0	273.2
Vinyl chloride	VCM	7.441	1183.0	273.2
Vinyl fluoride, inhibited	VFI	7.208	869.8	273.0
Vinyl methyl ether, inhibited	VME	7.420	1265.0	273.0

TABLE B2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM	Molecular weight of chemical	
1010	VPE COEFF A*	LOG FCN	Coefficients of a vapor pressure equation in the form of the one in Section 2.4.3 but which gives an answer in mm Hg.	Required only for execution of tank heating model B3
1011	VPE COEFF B*	C		
1012	VPE COEFF C*	C		
1016	AD FLAME TEMP	C K F	Theoretical adiabatic flame temperature of chemical	
1017	MOLEC RATIO	ND	Molar ratio of combustion reactants to products	
1018	STO AIR/FUEL	ND	Stoichiometric air to fuel ratio	
1019	FLAME TEMP	C K F	Flame temperature of burning chemical	Data not presently in HACS. default value will be used unless user provides data.

* These coefficients must be for the compressed, liquefied gas in the tank exposed to the fire. All other items on this page are for the gas which is burning. See model description for further details.

TABLE B3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4006	FLAME LENGTH	CM M FT MI	Length of flame jet	Computed by Model B1 Used by Models B2 and B3.
4007	DIAM FLAME	CM M FT MI	Diameter of a cylinder of flame which has the same volume as the cone of flame which occurs.	Computed by Model B1. Used by Models B2 and B3.
4009	SAF SEP WOOD	CM M FT MI	Maximum distance from flame at which wood will ignite if exposed for a prolonged period of time.	Measured from edge of flame.
4015	SAF SEP SKIN	CM M FT MI	Maximum distance from flame at which people will immediately be burned.	Measured from edge of flame.
4017	SAF SEP PBRN	CM M FT MI	Maximum distance from flame at which people will be burned if exposed for a prolonged period of time.	Measured from edge of flame.
4034	SAF SEP USER	CM M FT MI	Distance from the edge of the flame at which the user specified thermal radiation flux will occur.	Output will not appear if user does not input value for 2010 RAD FLUX.
		OUTPUT DATA FROM TANK HEATING MODEL B3:		
4051	OUT FAIL STR	D/CM2 N/M2 PSI MM HG	Failure stress at outside of wall.	Output if failure occurs at outside of wall.
4052	OUT WALL TMP	C K F	Temperature at outside of wall.	Output if failure occurs at outside of wall.
4053	IN FAIL STRS	D/CM2 N/M2 PSI MM HG	Failure stress at inside of wall.	Output if failure occurs at inside of wall.

TABLE B3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS (CONT'D)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4054	IN WALL TEMP	C K F	Temperature at inside of wall.	Output if failure occurs at inside of wall.
4055	FAILURE TIME	S MIN HR	Time in which tank will rupture.	Output only if it is determined that tank will rupture.

TABLE B4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3003	PLOT FLG B/E	ND (Integer)	Flag indicating whether a plot of thermal radiation flux versus distance from the flame center is desired.	0 = plot not desired 1 = plot is desired

MODEL C

Purpose

Model C is the primary vapor dispersion hazard assessment model in HACS. As such, it is called by, and functionally replaces, Models G, J, N, S and W.

The model works for either instantaneous or continuous releases of gases or vapors evolved from holes in tanks, evaporating pools of spilled liquid, or both.

Modules Which Constitute Model C

The model is comprised of two modules (i.e., parts) which are designated Model C1 and Model C2 respectively. Model C1 computes the downwind distance over which a flammable or toxic cloud or plume of gas or vapor is hazardous. Model C2 computes the time of arrival, duration, and width of the cloud or plume (for given hazardous concentrations of the gas or vapor) at a user specified downwind location and time.

Restrictions and Cautions or Model Use

Many of the assumptions upon which the model is based directly affect the degree to which the model is realistic in its assessment of hazards. It is advised that the user read and understand these assumptions. A brief discussion of them is given in the next section.

Model C, per se, is the vapor dispersion model for gas being released directly from a ruptured pipe or tank. When used to functionally replace Models G, J, N, S, or W, it acts as the dispersion model for vapors being evolved from the surface of a body of water.

In some situations, significant quantities of gas or vapor will only be discharged from a ruptured tank or pipe. In others, significant quantities may only be evolved from the surface of a water body after a volatile liquid is spilled. In yet other cases, significant quantities of gas or vapor may be evolved both from the initial venting process and from a spilled liquid. Since many hazard assessment codes contain both the letters C and either G, J, or N, it is important that the user realize that execution of Model C, when used as Model C, is not appropriate if volatile liquid has also been released. In these situations, Models G, J, or N are considerably better in that, for instantaneous releases at least, they can account for all gas or vapor sources.

This vapor dispersion model is only intended for use for chemicals which are released in gaseous form. It may provide inaccurate answers for chemical fumes, mists, or dusts which become airborne.

The accuracy of the model is completely unknown when so small an amount of gas is released that the downwind hazard extent is less than 100 meters.

Important Assumptions of the Model

The model assumes that the gas or vapor which is released is always the same density as air (i.e., it is neutrally buoyant in air). If the gas or vapor is actually lighter-than-air, it will tend to rise quickly into the sky. If the gas or vapor is actually heavier-than-air, it will tend to hug the ground as it moves downwind. In the former case, the model can give extremely conservative answers, since it assumes the cloud or plume stays near the ground whereas it actually starts to climb into the sky. In the latter case, the model is somewhat less conservative than the neutrally buoyant case, but not very much so if the cloud or plume gets lighter as it warms up to ambient temperature (if it was colder than ambient on release) or becomes so quickly diluted that its density, when mixed with large volumes of air, approaches that of air. To help the user properly take the effects of this assumption into account, the model outputs the relative density of the vapor or gas at its release temperature to air at ambient temperature.

The wind velocity is assumed to be the same at all distances above the ground through which the cloud or plume will pass.

The model assumes that the surface over which the cloud or plume is travelling is perfectly flat. Since any obstructions in the path of the cloud or plume will tend to accelerate mixing and dilution, this assumption can in many situations make the answers conservative.

The model uses the Threshold Limit Value (TLV) of the gas or vapor as the toxic concentration in air unless the user overrides the value. The TLV value for the gas or vapor is harmless to people for the short-term exposures under consideration by HACS. For more realistic answers, it is suggested that the user provide a value which is more representative of a concentration which can be harmful to health in the time spans of concern. Some such data are given in CG-446-2 and the Chemical Properties File for concentrations which can cause headaches, coughing, eye irritation, and other usually minor and temporary effects. Concentrations which can cause more significant effects are usually higher, and can be found in texts concerned with industrial hygiene and/or toxicology.

The model also assumes that the wind stays constant in intensity and direction. When it actually doesn't, the accuracy of the answers can be affected.

Most of the above assumptions tend to make HACS produce a conservative answer under most circumstances. Without going into details, let the user note that some gases and vapors have been known to be ignitable, even though their time averaged concentration at the center of the cloud or plume is substantially less than their lower flammable limit concentration. Thus, the user should not consider the answers given by this model for the maximum extent of flammable cloud or plume hazard to be conservative, unless the gas or vapor is lighter-than-air at the point of release.

Input Data Considerations

If at all possible, the user should determine and input a more realistic value for field number 2032, the lower toxic limit concentration for the gas or vapor in air. See the preceding section for reasons why.

Note that the size and shape of the source from which the vapor or gas is being generated must be more fully specified for this model than was necessary for Models A or B. This was necessitated by the fact that Model C will work not only for gases venting from a hole in a tank but also for those vapors evolving from a circular or rectangular pool of evaporating liquid. In actuality, it is not important to the model what the size or shape of the hole is when the release is from a hole in a tank. Thus, if Model C is being used for such a situation, and the hole size and shape were not determined, the user should simply allow field number 2018 to obtain a default value and input a value of zero for field number 2019.

Model C will handle either instantaneous releases of gas or vapor, or continuous releases. To make HACS as self-sufficient as is practical, there is at least one model in each hazard assessment (estimation route) path containing a vapor dispersion model that estimates whether the release should be considered as instantaneous or continuous. All of these models use an arbitrarily chosen time period of 10 minutes as the dividing line. The user may input his own choice by providing data for field number 2061.

Besides the wind speed, the model requires that the user define the type of weather condition which prevails in the spill area. This is done by inputting a number from 1 to 6 inclusive for data field number 2017. These six numbers correspond to the letters A to F in the following table (i.e., 1 = A, 2 = B, etc.) The phrase "Daytime insolation" refers to the degree of sunshine which reaches the earth. A bright, hot, sunny day would have "strong" insolation while a cloudy, dull day would have "slight" insolation.

RELATION OF TURBULENCE TYPES TO WEATHER CONDITIONS

A — Extremely unstable conditions
B — Moderately unstable conditions
C — Slightly unstable conditions
D — Neutral conditions*
E — Slightly stable conditions
F — Moderately stable conditions

Surface wind speed, m/sec	Daytime insolation			Nighttime conditions	
	Strong	Moderate	Slight	Thin overcast or ≥ 4/8 cloudiness†	≤ 3/8 cloudiness
<2	A	A–B	B		
2	A–B	B	C	E	F
4	B	B–C	C	D	E
6	C	C–D	D	D	D
>6	C	D	D	D	D

*Applicable to heavy overcast, day or night.
†The degree of cloudiness is defined as that fraction of the sky above the local apparent horizon which is covered by clouds.

Output of the Model

Model C1, using the lower flammable limit concentration and a lower toxic limit concentration for the gas or vapor released, determines the maximum downwind distances over which the center of the cloud or plume exceeds these concentrations. Additionally, it gives an estimate of the relative density of the chemical gas or vapor at its release temperature to air at ambient temperature. Model C2, again for each of two concentrations, gives the time of arrival of the hazardous concentrations at some user specified downwind location, the durations for which the concentration will exceed the hazardous concentrations, and the widths of the hazard zones (measured from the downwind centerline direction) defined by these concentrations.

Numerous optional plots and tables are available to the user. These are described in Table C4.

Data Specification

Table C1 defines the on-scene and operational data which the model requires.

Table C2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table C3 defines the output of the model.

Table C4 defines the data necessary for production of the optional tables and plots.

TABLE C1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2061	SPILL TYPE C	ND (Integer)	Flag indicating whether discharge is instantaneous or continuous.	0 = instantaneous 1 = continuous Will generally be estimated by preceding models.
2012	COORD X	CM M FT MI	Distance in downwind centerline direction	These 3 coordinates define the downwind location for which the user desires data.
2013	COORD Y		Distance in cross-wind direction (measured from centerline)	
2014	COORD Z		Height above groundlevel or water surface.	
2015	HOLE HEIGHT	CM M FT MI	Height of the centerline of the hole from which gas is escaping (measured up from groundlevel or water surface).	To be set to zero if Model C used to replace Models G,J,N, S, or W.
2016	WIND VELOC	CM/S M/S MPH KNOTS	Average wind velocity in vicinity of discharge.	
2017	ATMOS COND	ND (Integer)	Atmospheric condition flag (1 to 6 correspond to conditions A to F as defined in table in model description). Condition 6(F) is the worst case and is used as a default value.	1 = extremely unstable (A) 2 = moderately unstable (B) 3 = slightly unstable (C) 4 = neutral (D) 5 = slightly stable (E) 6 = moderately stable (F)
2018	DIM FLAG	ND (Integer)	Flag indicating whether source of gas or vapor discharge is circular or rectangular in shape.	1 = rectangular 2 = circular Will be estimated for user by any preceding pool spreading model.

TABLE C1: ON-SCENE AND OPERATIONAL DATA (CONT'D)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2019	DIM SPILL	CM M FT MI	Size of gas or vapor source. If source is circular in shape, it is the radius of the circle. If source is rectangular, it is the length of the source.	Will be estimated by any preceding pool spreading model.
2020	CHAN L WIDTH	CM M FT MI	The width of the gas or vapor source.	Required only if 2018 DIM FLAG = 1.
2032	LOW TOX LIM	PPM	The concentration of the gas or vapor in air which is considered to be toxic. See model description for details.	Utilizes Threshold Limit Value (TLV) for 8-hr exposure unless overridden.
2054	AIR TEMP	C K F	Temperature of ambient air in discharge area.	
4001	TOT MASS GAS	G KG LB TN	Total weight of gas or vapor which enters the atmosphere.	Required only for instantaneous discharges. Computed by Model A, and by Model K for underwater releases > 10' deep. May be modified by other preceding models.
4044	AVG VAP RATE	G/S KG/S LB/S TN/HR	Average flowrate at which gas or vapor enters atmosphere. Required only for continuous discharges.	Will be estimated by Models A, D, I, R, or V if any of them precede this model.
4045	EVOLVE TIME	S MIN HR	Time span over which discharge takes place. Required only for continuous discharges.	Same as above.
4068	AVG GAS TEMP	C K F	Temperature of gas or vapor being released.	Will be estimated by Models A, D, I, K, R, or V if any of them precede this model.

TABLE C2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	
2033	LOW FLAM LIM	PERCENT	The lowest concentration of the gas or vapor in air which can support combustion	Utilizes lower limit of flammability range (LFL or LEL)

TABLE C3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4010	MAX DIST FIR	CM M FT MI	The maximum distance downwind in the centerline direction over which the cloud or plume is flammable	
4043	MAX DIST TOX	CM M FT MI	The maximum distance downwind in the centerline direction over which the cloud or plume is toxic	
4069	VP DEN RATIO	ND	Ratio of gas or vapor density at release temperature to density of air at ambient temperature	
4011	1/2 HAZ ZONE	CN M FT MI	One-half the width in the cloud or plume which is at or above the toxic concentration	Measured from the centerline downwind direction at groundlevel. Given for user specified distance 2012 COORD X
4012	DUR HAZ CLD	S MIN HR	Duration for which hazardous toxic concentration exists at user specified point	
4013	ARRL TIME HAZ	S MIN HR	Time of arrival of hazardous toxic concentration at user specified point	
4065	1/2 HAZ ZONE	CM M FT MI	One-half the width in the cloud or plume which is at or above the lower flammable limit concentration	Measured from the centerline downwind direction at groundlevel. Given for user specific distance 2012 COORD X
4066	DUR HAZ CLD	S MIN HR	Duration over which flammable cloud or plume exists at user specified point.	
4067	ARRL TME HAZ	S MIN HR	Time of arrival of flammable concentration at user specified point	

TABLE C4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3004	PLOT FLAG C	ND (Integer)	Flag indicating which plots, if any, are desired.	0 = plots not desired 1 = plot concentration vs time at user specified point 2 = plot maximum ground level concentration vs time and distance * 3 = give both above plots *
3005	TABLE FLAG C	ND (Integer)	Flag indicating which tables, if any, are desired.	0 = tables not desired 1 = give tables of arrival times, durations, and 1/2 widths of toxic and flammable clouds or plumes as a function of downwind distance 2 = give table of concentration vs time at user specified point 3 = give all tables described above
2035	MAX HAZ ZONE	CM M FT MI	Maximum downwind X distance for table and plot.	Required only if 3004 PLOT FLAG C is 2 or 3, or 3005 TABLE FLAG C is 1 or 3.

*For continuous vapor discharges, the user must realize that vapor concentrations are constant at any given location over the duration of discharge. The time axis for the max ground level concentration vs time and distance plot, therefore, indicates the time at which the plume will arrive at the corresponding downwind distance. For instantaneous spills, it shows the single instant peak concentration will occur.

MODEL D

Purpose

Model D is utilized for liquids which are lighter-than-water, insoluble or slightly soluble in water, and which have a boiling point less than the ambient temperature. It computes the size of the pool which forms when such a substance is discharged either instantaneously or continuously onto water. For the instantaneous discharge case, it also estimates the time it will take for all the liquid to evaporate.

Restrictions and Cautions on Model Use

Model D only works for spills onto the surface of the water body. It will not work for underwater discharges or spills onto land.

Important Assumptions of the Model

For continuous discharges, the model assumes that all spreading takes place radially. For instantaneous releases, it can determine and indicate whether or not the pool becomes confined by channel banks.

The model assumes that the chemical which is spilled will not be depleted by dissolution into water, i.e., it assumes that the chemical is completely insoluble in water.

It is assumed that the chemical spills onto calm water.

Input Data Considerations

The model allows the user to specify whether or not the model is to assume that ice formation occurs. It is recommended that it be specified that ice formation does not occur unless the user has specific information that it does. If the results of the model are to be for some critical use, the model may be run twice (once for each option), the results compared, and the more conservative values utilized.

Output of the Model

Output of Model D for continuous releases includes the radius and diameter of the pool at a user specified time. It also indicates that the spreading has occurred radially, but this "computed" answer is necessitated by the fact that the model only works for radial spreading.

For instantaneous releases, the model gives the maximum size the pool will reach before completely evaporating and indicates whether or not the pool is confined by channel banks. If the pool is confined, the size given is the maximum length of channel which is covered by the chemical. If the pool is not confined, the size is the maximum radius of the pool. In either of the cases, the model also returns the time it takes for the pool to completely vaporize and the diameter of a circular pool of equivalent surface area to the pool which forms. This latter

output is provided in case Model E follows.

Optional output from the model consists of a table and plot of pool size versus time.

Data Specification

Table D1 defines the on-scene and operational data which the model requires.

Table D2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table D3 defines the output of the model. The user may override any computed output data with his own values.

Table D4 defines the data necessary for production of the optional table and plot.

TABLE D1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2060	SPILL TYPE D	ND (Integer)	Flag indicating whether discharge is instantaneous or continuous	0 = instantaneous 1 = continuous
2008	HOLE DIAM	CM M FT MI	Diameter of the hole from which discharge takes place. Required only if discharge is continuous.	Hole is assumed to be circular. If it is not, provide diameter for a hole of equivalent area to actual hole.
2020	CHAN L WIDTH	CM M FT MI	The average width of the water body into which the discharge occurs.	Required only if spill is instantaneous
2022	FLUX VAR	ND (Integer)	Flag indicating whether heat transfer from water to pool of chemical is limited by ice formation or is a constant.	1 = constant (no ice) 2 = ice forms See model description for discussion.
2023	WATER TEMP	C K F	Temperature of water body onto which discharge occurs.	
2024	HEAT FLUX	CL/CM2S W/M2 BT/FT2H KC/M2H	Heat flux between water and pool of chemical. Required only if 2202 FLUX VAR is 1	HACS will estimate a value and use it if the user does not provide one.
2026	POOL SIZE TM	S MIN HR	Elapsed time from the start of discharge at which the pool size is desired to be known.	Required only for continuous discharged.
2059	HOLE HGT UP	CM M FT MI	The height from the center of the discharge hole to the surface of the water.	Required only for continuous discharges.
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid which is discharged required only for instantaneous releases.	Will be computed by Model A. Not required if 4003 TOT VOL LIQ is given instead.
4003	TOT VOL LIQ	CM3 M3 FT3 GALS	The total volume of liquid which spills. Required only for instantaneous releases.	Will be computed by Model A. Not required if 4002 TOT MASS LIQ is given instead.

TABLE D1: ON-SCENE AND OPERATIONAL DATA (CONT'D)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4049	LIQ FLWRATE	G/S KG/S LB/S TN/HR	The average flowrate of the chemical being discharged. Required only for continuous discharges.	Will be computed by Model A.
4050	LIQ FLW TIME	S MIN HR	The time span over which liquid chemical is discharged. Required only for continuous discharges.	Will be computed by Model A.

TABLE D2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1003	BOIL TEM LIQ	C K F	Boiling point temperature of the chemical.	
1005	VISCOSITY-BP	DS/CM2 NS/M2 CP	Viscosity of the chemical at its boiling point.	Required only if the discharge is instantaneous
1014	HEAT OF VPR	CL/G J/KG BT/LB	Heat of vaporization of the chemical.	
1021	LIQ DENS BP	G/CM3 KG/M3 LB/FT3	Density of the liquid chemical at its boiling point.	

TABLE D3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2018	DIM FLAG	ND (Integer)	Flag indicating whether spill pool is circular or is confined by channel banks and rectangular	1 = pool is rectangular 2 = pool is circular
2019	DIM SPILL	CM M FT MI	Size of the spill pool. For continuous releases, it is the radius of the pool at the user specified input time. For instantaneous releases, it is the maximum length of the channel covered by the chemical or the maximum radius of the pool, depending upon the answer for 2018 DIM FLAG.	
4007	DIAM FLAME	CM M FT MI	For pools which are rectangular, it is the diameter of a circle of equivalent area to the spill pool. For circular pools, it is the diameter of the pool itself.	Used by Model E.
4016	TIME LQ EVAP	S MIN HR	The time it will take for all the chemical to vaporize.	Output only for instantaneous discharges.
Data Estimated in Case Model G Follows:				
2019	DIM SPILL	CM M FT MI	Takes value shown as computed for this field number, computes its mean with zero, and stores value as a SYSTEM value.	Done to provide more realistic value to subsequent models. User may override value before its mean is taken by providing this as input.
2061	SPILL TYPE C	ND (Integer)	An estimate of whether the spill should be considered to be an instantaneous one or a continuous one by the vapor dispersion models.	0 = instantaneous spill 1 = continuous discharge

TABLE D3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS (CONT'D)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4044	AVG VAP RATE	G/S KG/S LB/S TN/HR	Average vapor evolution rate from spill pool.	Output only if vapor evolution is estimated to be continuous.
4045	EVOLVE TIME	S MIN HR	Estimated time span over which vapor is evolved.	Output only if vapor evolution is estimated to be continuous.
4068	AVG GAS TEMP	C K F	Temperature of vapors being released.	Same as the boiling point of the chemical.

TABLE D4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3006	PLOT FLAG D	ND (Integer)	Flag indicating whether a plot of pool size vs. elaspsed time for spill is desired.	0 = plot not desired 1 = plot is desired
3013	TABLE FLAG D	ND (Integer)	Flag indicating whether a table of pool size vs. elapsed time from spill is desired.	0 = table not desired 1 = table is desired

MODEL E

Purpose

Model E is to be used in situations where a pool of flammable liquid (either on land or water) has been ignited or has the potential to be ignited. It computes the height of the flame, the angle it will bend because of wind forces, and the distances from the flame which are "safe" for people and combustible materials. It can also determine whether or not an intact tank containing a compressed liquefied gas will rupture if exposed to the flame, and how long the tank must be exposed before it does rupture.

Model E is the primary pool fire hazard assessment model in HACS. As such, it is called by, and functionally replaces, Models H, L, Q, and U.

Modules Which Constitute Model E

The model is comprised of four modules (i.e., parts) which are designated Models E1, E2, B2, and B3. Model E1 computes the height of the flame and Model E2 computes the tilt of the flame from plumb vertical due to wind forces. Models B2 and B3 are the same ones used as parts of Model B. As for that model, Model B2 calculates the safe separation distances from the flame, and Model B3 determines whether or not an intact tank containing compressed liquefied gas will rupture if exposed to the flame, how long it will take to do so, etc.

Restrictions and Cautions on Model Use

Heavy hydrocarbon liquids (such as fuel oil or other petroleum products) and many other liquid chemicals burn with a sooty flame. This model can be conservative from a safety point of view when such liquids are addressed.

The user should give consideration to the nature of the chemical spilled, the location in which it has spilled, the time the spill pool has been spreading, and the burning rate of the chemical for a realistic assessment of hazards. If the spill has been on water, the chemical will burn for only a short period of time if the pool is very thin or has become diluted with water.

Important Assumptions of the Model

The model assumes that the flame is "clean" and radiates the maximum possible amount of energy. Many liquids, such as fuel oil, however, burn with an extremely sooty flame. Since substantially less heat is generated from sooty flames, the answers of the model represent conservative estimates of the hazard in such cases.

Thermal radiation flux is a measure of the heat energy from the flame which reaches an object near the flame. As noted, the model

outputs safe separation distances from the flame for people exposed for a very short period of time, people exposed for a long period of time, and wooden structures. These distances are computed using three corresponding radiation flux levels. These levels are:

0.0339 cal/cm^2-sec: Causes burns to people exposed to the flame for a long period of time. It is about 1.5 times the energy flux that the sun can generate on earth on a very hot, bright, sunny day.

0.113 cal/cm^2-sec: Causes light burns to people almost instantaneously.

0.753 cal/cm^2-sec: Eventually causes wooden structures to ignite.

Input Data Considerations for Flame Size and Safe Separation Distance Computations

An optional input to the model is a thermal radiation flux for which a safe separation distance will be calculated. The model will not accept as input any value which is less than 0.0226 cal/cm^2-sec. This flux corresponds to that generated by the sun on a hot, bright, sunny day. If the user does not provide a value for this data item, he should ignore the default data warning message which appears for it.

HACS contains little data for field number 1019 FLAME TEMP. For precise answers from the model, he must provide this value himself. The default file contains a value which will give a reasonable estimate of the hazard.

Input Data Considerations for Tank Heating Model

Models E1, E2, and B2, as noted above, compute flame parameters and safe separation distances from the flame. Chemical property data these models require, therefore, are those for the liquid which is burning. Model B3 determines what will happen to an intact tank which contains a compressed, liquefied gas and which is exposed to thermal radiation from the flame. Model B3 utilizes certain data, therefore, for the substance within the tank. When Model B3 is requested for execution, the user must input chemical property data required by the model. These data, represented by fields 1010, 1011, and 1012, are listed for each pertinent chemical in a table following Table E2.

A considerable amount of tank construction data is also required if Model B3 is desired to be executed. These data will be extremely difficult for a user to provide unless he has access to the blueprints and specifications of the tank which is exposed to the fire. To enable the user to execute this model in emergency situations, the HACS default

file has been provided actual data from a pressurized propylene barge used by the Union Carbide Corporation and built by the Bethlehem Steel Corporation. If the user utilizes these data, he must be aware that the reliability of the answers given is only as good as the degree to which these "typical" data apply to the tank in question. He is urged, therefore, to provide as much actual data as he possible can. The relief valve setting and the wall thickness are of particular importance.

Input 2066 HEAT FLUX is an optional input value by which the user may specify the thermal radiation flux to which a tank is exposed. HACS computes a value for this flux and uses it if the user does not provide a value.

Output of the Model

Output of Model E consists of the height of the flame, its angle of tilt from plumb vertical due to wind effects, and safe separation distances from the flame for people exposed for a very short period of time, people exposed for a long period of time, and wooden structures. If the user desires, the model will also compute a safe separation distance for a thermal radiation flux level which he specifies. The minimum safe separation distance which can be computed in any case is 5 feet, with an accuracy of $\pm$ 5 feet. For longer distances, the accuracy of the model is $\pm$ 10 feet.

If execution of Model B3 is requested, the model will also determine if and how rupture of the tank may occur, how long it will take for rupture to occur, what the temperature of the tank wall is, and what stress is placed on the wall at failure.

Optional output from the model consists of a plot of radiation flux versus distance from the flame.

Data Specification

Table E1a defines the on-scene and operational data which the model requires for execution of Models E1, E2, and B2.

Table E1b defines the tank construction specification data required for execution of Model B3. These data have been placed in a separate table because it is not expected that the tank heating model will be used as often as the other parts of Model E.

Table E2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table E3 defines the output of the model.

Table E4 defines the data necessary for production of the optional plot.

TABLE E1a: ON-SCENE AND OPERATIONAL DATA
(EXCEPT THOSE SPECIFICALLY REQUIRED FOR TANK HEATING MODEL)

FIELD NUMBERS	FIELD NAME*	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2082	TNK HEAT FLG	ND (Integer)	Flag telling HACS which parts of the model to use. The input data required for execution of the tank heating model (B3) are described in Table E1b. The data in this table are required for execution of either of both models.	0 = compute flame size, safe separation distances 1 = execute tank heating Model B3 2 = do both of the above
2010	RAD FLUX	CL/CM2S W/M2 BT/FT2H KC/M2H	A thermal radiation flux for which a safe saparation distance from the flame will be calculated.	This is an optional user input. Ignore the default data warning message if it is not provided.
2016	WIND VELOC	CM/S M/S MPH KNOTS	Wind velocity in area of fire	
4007	DIAM FLAME	CM M FT MI	Diameter of the burning pool	Will be computed by Models D or T or estimated by Models H, L, or Q if any of these precede or call this model.

*Note: All data items on this page must be provided, with the exception of optional data item 2010, under all circumstances. The chemical recognition code specified for field 1001 should be for the substance which is burning.

TABLE E1b: ON-SCENE AND OPERATIONAL DATA
(FOR TANK HEATING MODEL)

FIELD NUMBERS	FIELD NAME*	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2062	TANK DIAM	CM M FT MI	Internal diameter of the tank exposed to fire	
2063	WALL THICKNS	CM M FT MI	Wall thickness of the tank exposed to fire	1 inch = 2.54 centimeters
2064	ULLAGE FRACTN	ND	Fraction of the tank volume which does not contain liquid	
2065	RLF VALV SET	D/CM2 N/M2 PSI MM HG	Pressure setting for the relief valve on the tank (gauge pressure)	1,013,250 dynes/cm^2 = 1 atm 14.7 lb/in^2 = 1 atm
2066	HEAT FLUX	CL/CM2S W/M2 BT/FT2H KC/M2H	Radiation flux to which the tank is exposed (optional input)	Will be computed by HACS if user does not provide a value
2067 2068 2069 2070 2071	THR CND 0 DG THR CND 400 THR CND 800 THR CND 1200 THR CND 1600	CL/CMSC W/MK BT/FTHF KC/MHK	Thermal conductivity of the tank wall at 0, 400, 800, 1200, and 1600 degrees F respectively	Default data is for a typical propylene barge. See model description.
2072 2073 2074 2075 2076	SPEC HT 0 DG SPEC HT 400 SPEC HT 800 SPEC HT 1200 SPEC HT 1600	CL/GC J/KGK BT/LBF	Specific heat of the tank wall at 0, 400, 800, 1200, and 1600 degrees F respectively	Default data is for a typical propylene barge. See model description.
2077 2078 2079 2080 2081	TNS STR 0 DG TNS STR 400 TNS STR 800 TNS STR 1200 TNS STR 1600	D/CM2 N/M2 PSI MM HG	Ultimate tensile strength of the tank wall at 0, 400, 800, 1200, and 1600 degrees F respectively	Default data is for a typical propylene barge. See model description.
2083	TANK-FIRE DIS	CM M FT MI	Distance from the flame to the tank exposed to the fire.	

*Note: Data also required for fields 1010, 1011, and 1012. See next page and model description for details.

TABLE E2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	
1003	BOIL TEM LIQ	C K F	Boiling point temperature of chemical	
1009	DENS FUEL VPR	GM/CM3 KG/M3 LB/FT3	Density of chemical vapor at its boiling point	Estimated automatically by HACS from ideal gas law equation
1010	VPE COEFF A^*	LOG FCN	Coefficients of a vapor pressure equation in the form of the one in Section 2.4.3 but which gives an answer in mm Hg.	Required only for execution of tank heating model B3
1011	VPE COEFF B^*	C		
1012	VPE COEFF C^*	C		
1015	BURNING RATE	CM/S M/S IN/MIN MM/MIN	Burning rate of liquid (decrease in pool depth with time)	
1019	*FLAME TEMP*	*C K F*	*Flame temperature of chemical.*	*Data not presently in HACS. Default value will be used unless user provides data.*
1021	LIQ DENS BP	GM/CM3 KG/M3 LB/FT3	Density of liquid chemical at its boiling point	
			* These coefficients must be for the compressed, liquefied gas in the tank exposed to the fire. All other items on this page are for the gas which is burning. See model description for further details. A list of coefficients for pertinent chemicals is given on the next page for the user's convenience.	

PROPERTY DATA REQUIRED FOR TANK HEATING MODEL

Chemical Name	Code	1010 VPE COEFF A	1011 VPE COEFF B	1012 VPE COEFF C
Acetaldehyde	AAD	7.798	1444.0	273.2
Ammonia, anhydrous	AMA	8.022	1233.0	273.2
Boron trichloride	BRT	7.573	1340.0	273.0
Butadiene, inhibited	BDI	6.859	935.5	239.6
Butane	BUT	6.830	945.9	240.0
Butylene	BTN	7.378	1200.0	273.2
Carbon monoxide	CMO	7.194	352.4	273.0
Chlorine	CLX	7.418	1086.0	273.2
Chlorine trifluoride	CTF	7.367	1097.0	232.8
Cyanogen	CYG	7.847	1251.0	273.0
Cyanogen chloride	CCL	7.875	1430.0	273.2
Cyclopropane	CPR	7.816	1186.0	273.0
Dichlorodifluoromethane	DCF	?	?	?
1, 1-Difluoroethane	DFE	7.509	1150.0	273.0
Dimethylamine	DMA	8.297	1517.0	273.2
Dimethyl ether	DIM	7.818	1227.0	273.0
Ethane	ETH	7.211	800.0	273.2
Ethylamine	EAM	15.010	3514.0	273.0
Ethyl chloride	ECL	7.691	1375.0	273.2
Ethylene	ETL	6.748	585.0	255.0
Ethylene oxide	EOX	7.672	1359.0	273.2
Ethyl nitrite	ETN	10.050	2080.0	273.0
Hydrogen bromide	HBR	7.414	935.6	273.2
Hydrogen chloride	HDC	7.429	856.0	273.2
Hydrogen cyanide	HCN	7.791	167.0	273.2
Hydrogen fluoride	HFX	7.394	1317.0	273.2
Hydrogen, liquefied	HXX	5.355	50.1	273.0
Hydrogen sulfide	HDS	7.434	970.0	273.2
Isobutane	IBT	6.748	882.8	240.0
Isobutylene	IBL	7.376	1197.0	273.2
Liquefied natural gas	LNG	6.612	389.9	266.0
Liquefied petroleum gas	LPG	6.830	813.2	248.0
Methane	MTH	6.612	389.9	266.0
Methylacetylene-propadiene mixture	MAP	7.021	962.0	273.0
Methylamine	MTA	8.348	1458.0	273.0

PROPERTY DATA REQUIRED FOR TANK HEATING MODEL
(Concluded)

Chemical Name	Code	1010 VPE COEFF A	1011 VPE COEFF B	1012 VPE COEFF C
Methyl bromide	MTB	6.960	986.6	238.3
Methly chloride	MTC	7.481	1148.0	273.2
Methly mercaptan	MMC	8.006	1432.0	273.0
Monochlorodifluromethane	MCF	7.625	1104.0	273.2
Nitrogen, liquefied	NXX	7.069	325.0	273.0
Nitrogen tetroxide	NOX	8.917	1799.0	276.8
Nitrous oxide	NTO	7.426	835.0	273.0
Oxygen, liquefied	OXY	7.056	377.0	273.0
Phosgene	PHG	7.511	1303.0	273.2
Propane	PRP	6.830	813.2	248.0
Propylene	PPL	6.820	785.0	247.0
Sulfur dioxide	SFD	7.282	999.9	237.2
Trichlorofluoromethane	TCF	7.524	1380.0	273.2
Trifluorochloroethylene	TFC	6.681	931.0	273.0
Trimethylamine	TMA	7.600	1303.0	273.2
Vinyl chloride	VCM	7.441	1183.0	273.2
Vinyl fluoride, inhibited	VFI	7.208	869.8	273.0
Vinyl methyl ether, inhibited	VME	7.420	1265.0	273.0

TABLE E3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4008	FLAME ANGLE	RAD DEG	Angle of the flame from plumb vertical (straight up = 0)	Output of Model E2; used by Models B2 and B3
4009	SAF SEP WOOD	CM M FT MI	Maximum distance from flame at which wood will ignite if exposed for a prolonged period of time.	Measured from edge of burning pool
4015	SAF SEP SKIN	CM M FT MI	Maximum distance from flame at which people will immediately be burned	Measured from edge of burning pool
4017	SAF SEP PBRM	CM M FT MI	Maximum distance from flame at which people will be burned if exposed for a prolonged period of time	Measured from edge of burning pool
4018	POOL FLM HGT	CM M FT MI	Flame height. Field number and name are changed to 4006 FLAME LENGTH before use in Model B2.	Output of Model E1
4034	SAF SEP USER	CM M FT MI	Distance from the edge of the flame at which the user specified thermal radiation flux will occur	Output will not appear if user does not give input value for 2010 RAD FLUX
Output Data From Tank Heating Model B3:				
4051	OUT FAIL STR	D/CM2 N/M2 PSI MM HG	Failure stress at outside of wall	Output if failure occurs at outside of wall.
4052	OUT WALL TMP	C K F	Temperature at outside of wall.	Output if failure occurs at outside of wall.
4053	IN FAIL STRS	D/CM2 N/M2 PSI MM HG	Failure stress at inside of wall.	Output if failure occurs at inside of wall.

TABLE E3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS (CONT'D)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4054	IN WALL TEMP	C K F	Temperature at inside of wall.	Output if failure occurs at inside of wall.
4055	FAILURE TIME	S MIN HR	Time in which tank will rupture.	Output only if it is determined that tank will rupture.

TABLE E4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3003	PLOT FLG B/E	ND (Integer)	Flag indicating whether a plot of thermal radiation flux versus distance from the flame center is desired.	0 = plot not desired 1 = plot is desired

MODEL F

Model F does not really do anything in this version of HACS. Its function was incorporated into Model D for the sake of simplification of use. If called, it simply states, "Model F Has Been Functionally Incorporated into Model D."

MODEL G

Model G is the vapor dispersion model for insoluble or slightly soluble liquids which are lighter-than-water and have boiling points lower than the ambient temperature. If the gas or vapor release is estimated as best being represented as an instantaneous one, it takes the amount of gas which is released from the tank and the amount of liquid which has been discharged, adds them together, and stores the sum for use by the vapor dispersion model. It then calls Model C, the primary vapor dispersion model in HACS, for assessment of hazards.

If the release is estimated to be best represented as being a continuous release, Model G directly calls Model C without performing any intermediate calculations. The user should be cautioned that no attempt is made in this case to take into account any gas or vapor which discharges from the leaking tank or pipe after the liquid stops venting. If such gas or vapor discharge is significant (as can be determined from inspection of Model A output), he may wish to adjust the flow rate and time for vapor evolution as appropriate.

The input data required for execution of Model G, and the definitions of the data it may compute, are presented in Table G1. The user must refer to Model C for further information required to execute this model.

MODEL H

Model H is the pool fire hazard assessment model for insoluble or slightly soluble flammable liquids which have a boiling point less than the ambient temperature and which are heavier-than-water. It estimates the diameter of the base of the flame as being twice the volume of liquid discharged raised to the 1/3 power, and then calls Model E, the primary pool fire hazard assessment model in HACS.

The only input data item which Model H itself requires is that for field number 4003, the total volume of liquid released (see Table A3 for a full description of this item). The user must refer to Model E for further information required to execute this model.

TABLE G1: INPUT/OUTPUT DATA SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
INPUT:				
2061	SPILL TYPE C	ND (Integer)	Flag indicating whether discharge is instantaneous or continuous. Will be estimated by Model D.	0 = instantaneous 1 = continuous
4001	TOT MASS GAS	G KG LB TN	Total weight of gas which discharged from tank.	Required only if discharge is instantaneous.
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid which discharges from tank	Required only if discharge is instantaneous.
OUTPUT:				
4001	TOT MASS GAS	G KG LB TN	Total weight of chemical which escapes into the environment in gaseous form. This is a SYSTEM value.	Computed only if discharge is instantaneous. It is the sum of 4001 and 4002 above.

*** THE USER MUST ALSO PROVIDE DATA FOR EXECUTION OF MODEL C ***

MODEL I

Purpose

Model I is utilized for liquids which are insoluble or slightly soluble in water, are heavier-than-water, and have a boiling point which is less than the ambient temperature. It computes the time it will take for all the chemical to evaporate, and the depth in water at which the chemical will not boil. Other parameters of the release phenomena are given in optional tables and plots.

Restrictions and Cautions on Model Use

Model I can only be used for instantaneous releases of chemical into or onto water.

If a liquid to which this model applies is released below a certain depth in water, called its "critical depth" here, it will not boil, and thus, will not result in the evolution of a large amount of vapor from the surface of the water. This phenomenon occurs because the pressure of the water on the chemical raises its boiling point above the ambient water temperature. Since Model I would generally be followed by execution of Model J, and Model I does not prevent Model J from assuming that all the liquid released will vaporize, the user must take this phenomenon into consideration when the release is underwater. To aid him in his assessment of hazards, Model I estimates and prints out the critical depth for the particular chemical of concern.

If the release occurs underwater, Model A should not be used to precede execution of Model I. Model A is only valid when the hole from which the chemical is being released is at or above the surface of the water.

Important Assumptions of the Model

Model I assumes that all the liquid released is discharged instantaneously.

The model assumes that, as soon as the liquid is released, it breaks up into small drops due to surface tension effects and these drops evaporate (boil) as they sink down through the water.

The model assumes that the liquid is released at a depth in water which is considerably less than its critical depth. See above for a definition of "critical depth".

Output of the Model

Model I computes the time it will take for all the liquid discharged to vaporize, and the critical depth in water below which the liquid will not boil.

Optional output consists of a table and two plots. The table gives the evaporation rate of the liquid and the volume of liquid remaining as a function of elapsed time from spill. The plots give the same data arrays separately.

Data Specification

Table I1 defines the on-scene and operational data which the model requires.

Table I2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table I3 defines the output of the model. The user may override any output data with his own values.

Table I4 defines the data necessary for production of the optional table and plots.

TABLE I1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2023	WATER TEMP	C K F	Temperature of water into which chemical spills	
2036	TEMP LIQ	C K F	Temperature of chemical which spills	
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid which spills	Will be computed by Model A
4050	LIQ FLW TIME	S MIN HR	Time span over which liquid discharges	Will be computed by Model A

TABLE I2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1003	BOIL TEM LIQ	C K F	Boiling point temperature of the chemical	
1008	SURF TENSION	D/CM N/M LB/FT	Surface tension of liquid chemical	
1010	VPE COEFF A	LOG FCN	Coefficients of a vapor pressure equation in the form of the one in Section 2.4.3 but which gives an answer in mm Hg.	
	VPE COEFF B	C		
	VPE COEFF C	C		
1014	HEAT OF VPR	CL/G J/KG BT/LB	Heat of vaporization of chemical	
1021	LIQ DENS BP	G/CM3 K/M3 LB/FT3	Density of liquid chemical at its boiling point.	

TABLE I3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4021	EVAP TIME LQ	S MIN HR	Time required for all discharged liquid to evaporate.	Answer is valid only if chemical has not been released beneath its critical depth and if part of it does not sink beneath its critical depth before vaporizing.
4046	CRIT DEPTH	CM M FT MI	Depth in water below which chemical will not boil (due to hydrostatic pressure effects)	This is the "critical depth" for the chemical.
Data Estimated in Case Model J Follows:				
2018	DIM FLAG	ND (Integer)	Flag indicating whether vapor source is rectangular or circular in shape.	Since chemical sinks, Model I estimates source to be circular (DIM FLAG = 2)
2019	DIM SPILL	CM M FT MI	The size of the vapor source; in this case, its radius.	Model I arbitrarily gives a value of 150 cm as the source radius.
2061	SPILL TYPE C	ND (Integer)	Flag indicating whether vapor evolution is instantaneous or continuous	0 = instantaneous 1 = continuous
4044	AVG VAP RATE	G/S KG/S LB/S TN/HR	Average rate at which liquid vaporizes	Computed only if discharge is estimated to be continuous
4045	EVOLVE TIME	S MIN HR	Time span over which vapor evolves.	Computed only if discharge is estimated to be continuous.
4068	AVG GAS TEMP	C K F	Temperature of vapors being generated.	Same as boiling point of chemical.

TABLE I4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3007	PLOT FLAG I	ND (Integer)	Flag indicating whether plots of volume of liquid remaining and evaporation rate versus time are desired.	0 = plots not desired 1 = plots are desired
3016	TABLE FLAG I	ND (Integer)	Flag indicating whether a table of mass of liquid remaining and evaporation rate versus time is desired.	0 = table not desired 1 = table is desired

MODEL J

Model J is the vapor dispersion model for insoluble or slightly soluble liquids which are heavier-than-water and have boiling points lower than the ambient temperature. If the vapor release is estimated as best being represented as an instantaneous one, it takes the amount of gas which is released from the tank and the amount of liquid which has been discharged, adds them together, and stores the sum. It then calls Model C, the primary vapor dispersion model in HACS, for assessment of hazards.

If the release is estimated to be best represented as being a continuous release, Model J directly calls Model C without performing any intermediate calculations. The user should be cautioned that no attempt is made in this case to take into account any gas or vapor which discharges from the leaking tank or pipe after the liquid stops venting. If such gas or vapor discharge is significant (as can be determined from inspection of Model A output), he may wish to adjust the flow rate and time for vapor evolution as appropriate.

The input data required for execution of Model J, and the definitions of the data it may compute, are presented in Table J1. The user must refer to Model C for further information required to execute this model.

TABLE J1: INPUT/OUTPUT DATA SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
INPUT:				
2061	SPILL TYPE C	ND (Integer)	Flag indicating whether discharge is instantaneous or continuous.	0 = instantaneous 1 = continuous Will be estimated by Model I
4001	TOT MASS GAS	G KG LB TN	Total weight of gas which discharges from tank	Required only if discharge is instantaneous
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid which discharges from tank	Required only if discharge is instantaneous
OUTPUT:				
4001	TOT MASS GAS	G KG LB TN	Total weight of chemical which escapes into the environment in gaseous form. This is a SYSTEM value.	Computed only if discharge is instantaneous. It is the sum of 4001 and 4002 above.

*** THE USER MUST ALSO PROVIDE DATA FOR EXECUTION OF MODEL C ***

MODEL K

Purpose

Model K is utilized for liquids which are soluble in water and which have boiling points less than the ambient temperature. When the release takes place at a sufficient depth underwater, it determines the amount of chemical which dissolves in the water and the amount which evolves from the surface as vapor or gas. It then calls Model P for assessment of the water pollution hazard presented by the dissolved chemical. If the release takes place on or near the surface of the water, it simply calls Model P with no intermediate computations.

Internal Decisions

The internal decision processes of Model K are complex because of the large variety of phenomena which may occur when chemicals addressed by Model K are discharged at various locations in a water body. For the benefit of interested users, a simplified logic chart for the important decisions is presented in Figure K1.

The "critical depth" for a chemical is here defined as that depth in water below which the chemical will not boil because of the effects of water pressure acting upon it.

Restrictions and Cautions on Model Use

Model A should not precede execution of Model K if the release takes place underwater. Model A only works when the hole from which the chemical is being discharged is at or above the surface level of the water. Its improper execution will cause Models L, M, and N to produce wrong answers.

Model K only works for releases which are into or onto water.

Model K does not address the possibility that a release of a reactive chemical (such as liquid anhydrous ammonia) underwater may result in a vapor heat explosion.

The phenomena which may occur when a chemical addressed by Model K is released on or underwater are influenced by a large number of factors. Although the model has been prepared in a manner which minimizes the risk that it will be used or its results interpreted improperly, it is advised that the user take all answers with a "grain of salt" unless he is thoroughly familiar with the actions of such chemicals.

Important Assumptions of the Model

Figure K1 points out three situations in which Model K assumes that all of the liquid discharged dissolves into the water. This forces Model P, the water pollution hazard assessment model, to provide worst

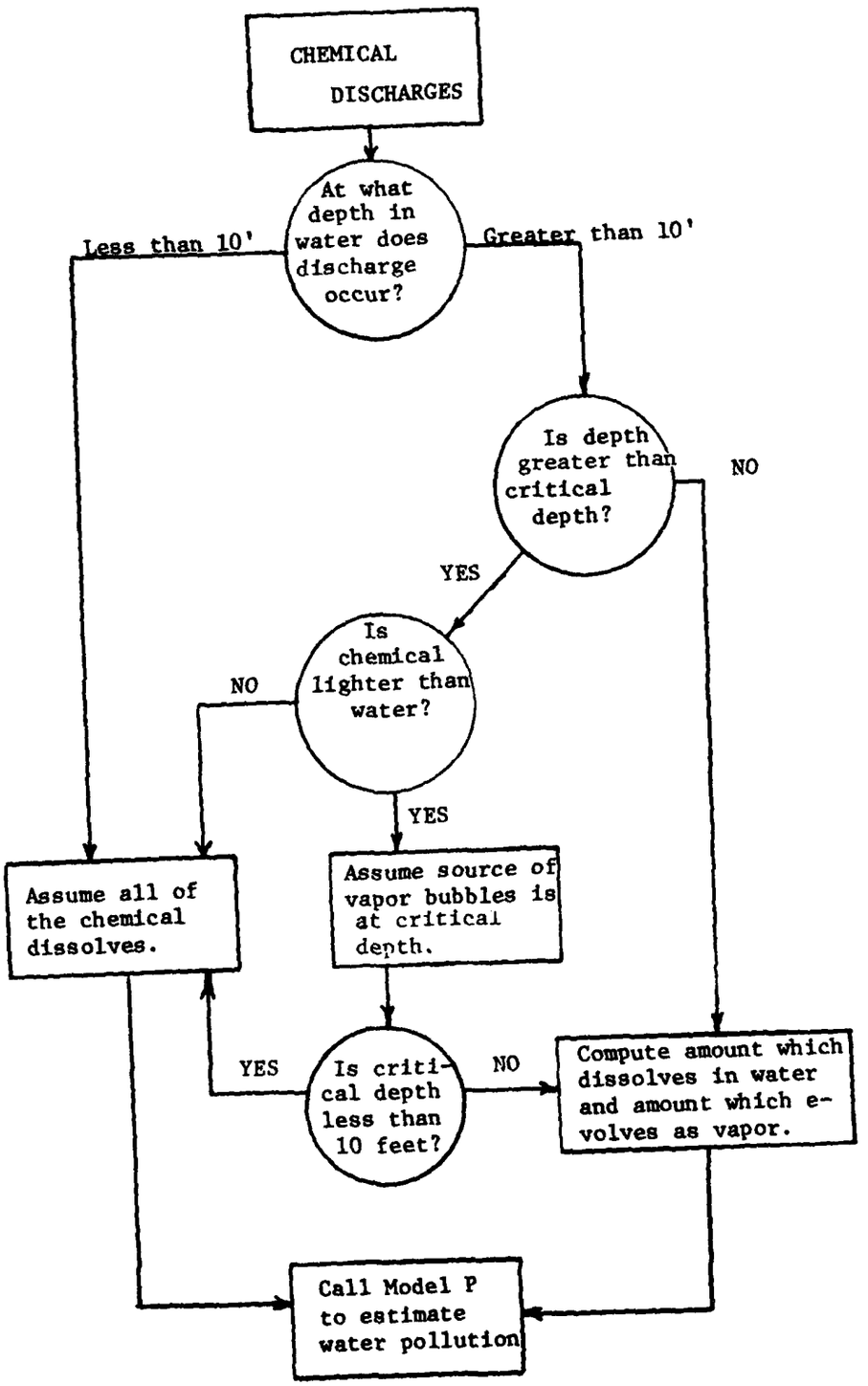


FIGURE K1. LOGIC CHART FOR MODEL K

case answers. To reiterate, these situations are (1) when the release takes place on the surface of the water; (2) when the release takes place less than 10 feet underwater; (3) when the release takes place at a depth which is greater than the "critical depth" of the chemical and the density of the chemical is greater than that of water; and (4) when the release takes place at a depth greater than the critical depth, the chemical is lighter-than-water and its critical depth is less than 10 feet.

The answers provided by Model P for situations (1), (2) and (4) may be overly conservative by anywhere from an estimated 10 to 90% or so depending upon the degree of solubility of the chemical and its boiling point. If the chemical is very soluble in water, it can be expected that a large portion of it actually will dissolve in water before the rest of it boils off. Alternatively, if the chemical is not exceedingly soluble in water, a large portion of it may vaporize before it has chance to contact a sufficient amount of water to dissolve in. The boiling point is a factor because the lower the boiling point of a substance is, in general, the faster that it can be expected to vaporize. In situation (3) described above, the assumption of complete dissolution is considerably more realistic.

If a chemical was completely soluble in water (miscible in all proportions), a value of zero was placed in the Chemical Properties File. This was done because the true value is infinity and cannot be properly represented. The unfortunate consequence of this act is that it is now impossible for the computer to determine whether the chemical is indeed completely miscible in water or is of some finite but unknown solubility. Since any chemical which has been assigned the hazard assessment code letter K is at least 5% soluble in water, Model K assumes that a solubility value of zero indicates that the chemical is completely soluble in water and in this case also assumes that all of it will dissolve.

Input Data Considerations

If the release takes place on the surface of the water body, or less than 10 feet underwater, Model K itself only requires input of the depth of release by use of field number 2021. This is pointed out in Table K1.

In all cases, the user must provide the input data necessary for execution of Model P.

Use of Model X Instead of Model P

When a chemical is released at a depth greater than its critical depth it will not boil. If, additionally, the chemical is heavier-than-water, it will sink to the bottom of the water body and dissolve at a rate dependent upon its solubility in water.

In most cases, execution of Model P is appropriate for obtaining an acceptable evaluation of water pollution hazards, since most chemicals which have been assigned the hazard assessment code letter K are appreciably soluble in water. However, when a chemical has been released in

a situation analagous to that described above, and the chemical is not considerably soluble in water (say 5-10% soluble), there may be advantage to executing Model X instead of Model P. A part of Model X provides water pollution information in the manner as Model P. It has the advantage, however, of assuming that the chemical is dissolving on the bottom of the water body and of being able to estimate and use the specific rate of dissolution.

Output of the Model

If the release takes place on the surface of the water or less than 10 feet underwater, Model K simply calls for execution of Model P. The output of Model P is described elsewhere in this manual.

If the release takes place in a situation which allows HACS to estimate the specific amount of chemical which dissolves in water and the amount which is evolved from the surface, Model K will output these values.

Data Specification

Table K1 defines the on-scene and operational data which Model K requires.

Table K2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table K3 defines the output of the model. The user may override any computed output data with his own values.

Model K itself does not have any optional output. Thus, there is no Table K4 for this model.

TABLE K1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2021	SPILL DEPTH	CM M FT MI	Depth in water at which chemical is released; measured from the surface, down is the positive direction.	Model A must not precede this model if the chemical is released underwater.
2004	TEMP START	C K F	Temperature of the liquid before discharge starts	Required only if release is at a depth > 10 feet (3.05m)
2007	INITIAL MASS	G KG LB TN	Initial weight of the chemical in the tank	Required only if release is at a depth > 10 feet (3.05 m)
2023	WATER TEMP	C K F	Temperature of water body into which discharge occurs	Required only if release is at a depth >10 feet (3.05 m)
2043	DIF COEF H20	CM2/S M2/S FT2/S	Diffusion coefficient of the chemical in water. Required only if release is at a depth >10 feet (3.05 m)	HACS will automatically estimate a value and use it if the user does not provide one.

*** THE USER MUST ALSO PROVIDE DATA FOR EXECUTION OF MODEL P ***

TABLE K?: CHEMICAL PROPERTY DATA UTILIZED*

FIELD NUMBERS *	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	
1003	BOIL TEM LIQ	C K F	Boiling point temperature of the chemical	
1010	VPE COEFF A	LOG FCN	Coefficients of a vapor pressure equation in the form of the one in Section 2.4.3 but which gives an answer in mm Hg.	
1011	VPE COEFF B	C		
1012	VPE COEFF C	C		
1021	LIQ DENS BP	G/CM3 KG/M3 LB/FT3	Density of the liquid chemical at its boiling point	
1025	CRIT TEMP	C K F	Critical temperature of the chemical	
1026	SOLUBILITY	G/HG	Solubility of the chemical in water at a fixed temperature	Value used only if coefficients of solubility as a function of temperature equation are not in data base.
1028	SOL EQ COEF1	G/HG	First coefficient of a solubility equation in the form of the one in Section 2.4.3	
1029	SOL EQ COEF2	G/HGC	Second coefficient of a solubility equation in the form of the one in Section 2.4.3. Temperature used for computation is 2023 WATER TEMP.	Answer from solubility equation should be in units of grams per 100 grams.

*These data are not utilized if the spill depth is less than 10 feet.

TABLE K3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS*

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2029	SPILL TYPE P	ND (Integer)	Flag indicating whether discharge is instantaneous or continuous for Model P (0 = instantaneous, 1 = continuous)	HACS always estimates the discharge is instantaneous. The user may override this value at will.
2084	MODK FLAG	ND (Integer)	Flag indicating whether or not Model K has been able to estimate the specific portion of the spilled chemical which vaporizes	0 = has estimated portion which vaporizes; this portion to be used by Models M and N 1 = has not estimated portion which vaporizes; Models M and N will assume a certain portion has vaporized.
4001	TOT MASS GAS	G KG LB TN	Weight of vapor which Model K estimates will be evolved from surface of water	
4002	TOT MASS LIQ	G KG LB TN	Weight of chemical which Model K estimates will be dissolved in water	
4003	TOT VOL LIQ	CM3 M3 FT3 GALS	Total volume of liquid which dissolves in water	
4046	CRIT DEPTH	CM M FT MI	Depth in water below which the chemical will not boil (due to hydrostatic pressure effects)	This is the "critical depth" for the chemical.
4068	AVG GAS TEMP	C K F	Temperature of vapors evolved, if any.	Same as boiling point of chemical.

*Only 2084 MODK FLAG is given if spill depth is less than 10 feet. If spill depth is greater than 10 feet but solubility is unknown, only 2084, 4001, 4002 and 4003 are given.

MODEL L

Model L is the pool fire hazard assessment model for soluble liquids which have a boiling point less than the ambient temperature. It very roughly estimates the diameter of the base of the flame and then calls Model E, the primary pool fire hazard assessment model in HACS.

The only input data item which Model L itself requires is that for field number 4003, the total volume of liquid released (see Table A3 for a full description of this item). The user must refer to Model E for further information required to execute this model.

MODELS M and N

Models M and N are the sequence of models called for assessment of the vapor dispersion hazards caused when a chemical which is soluble in water and has a boiling point less than ambient is spilled on or in water.

Model M was originally intended to be capable of estimating the rate at which vapor is being generated from the spill site. Unfortunately, such a model could not be developed. Thus, Model M Simply informs the user that HACS assumes that all vapor is evolved instantaneously, and then goes on to store the appropriate spill duration flag for Model C (for data field number 2061).

Model N is the vapor dispersion hazard assessment model for these chemicals. If Model K has been able to estimate the specific amount of chemical which has evolved from the surface of the water body, Model N provides rough estimates of the size and shape of the vapor source, and then calls Model C, the primary vapor dispersion model in HACS. If Model K has not been able to estimate the specific amount of chemical which has evolved from the surface of the water body, Model N does the following: (1) it asks for the amount of gas or vapor which was released while the chemical was venting from its ruptured container; (2) it asks for the amount of low-boiling point liquid which was discharged from the tank; (3) it asks that the user provide an estimate of the fraction of the discharged liquid which vaporizes; and (4) it sums the amount of gas plus the fraction of liquid vaporized times the amount of liquid discharged to arrive at a total amount of gas released which can be used by Model C.

The default file value for the fraction of liquid which vaporizes is 0.10. In actuality, this fraction might range from less than 0.10 to over 0.90 depending on the nature of the chemical and the conditions under which it has spilled. The user is therefore required to make an educated guess based on his knowledge of spill phenomena. As guidance, it can only be stated that a fraction of 0.50 was found to be accurate in an experimental program specifically concerned with liquid anhydrous ammonia spills on the surface of water.

The input data required for execution of Model N, and the definitions of the data items it estimates, are presented in Table N1. The user must refer to Model C for the information required to execute the primary vapor dispersion model.

TABLE N1: INPUT/OUTPUT DATA SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
INPUT:	Besides the inputs listed below, Model N also calls field numbers 1021 and 2021. See tables K1 and K2 for the definitions of these.			
2084	MODK FLAG	ND (Integer)	Flag indicating whether Model K has estimated specific portion of liquid which vaporizes	0 = it has 1 = it has not
2085	GAS FRACTION	ND	Fraction of the amount of liquid which spills which Model N is to assume has vaporized.	Required only if 2084 MODK FLAG is 1. Default value = 0.10.
4001	TOT MASS GAS	G KG LB TN	Weight of gas which escapes from tank while it is discharging.	Will be computed by Model A. Required only if 2084 MODK FLAG is 1.
4002	TOT MASS LIQ	G KG LB TN	Weight of liquid which escapes from tank while it is discharging	Will be computed by Model A. Required only if 2084 MODK FLAG is 1. Not required if 4003 is given.
4003	TOT VOL LIQ	CM3 M3 FT3 GALS	Volume of liquid which escapes-not required if 4002 is given.	
OUTPUT:				
4001	TOT MASS GAS	G KG LB TN	Total weight of vapor and gas which enters the atmosphere due to this incident. Will be computed only if 2084 MODK FLAG is 1.	Stored as a SYSTEM value. See model description for discussion of how computed.
2018	DIM FLAG	ND (Integer)	Flag indicating whether vapor source is rectangular or circular. Always estimated to be circular for use by Model C.	1 = rectangular 2 = circular
2019	DIM SPILL	CM M FT MI	The size of the vapor source. Since the source is assumed to be circular, it is the radius of the source in this case.	This radius is very roughly estimated and should be replaced with better data, if available.

THE USER MUST ALSO PROVIDE DATA REQUIRED FOR EXECUTION OF MODEL C

MODEL 0

Model 0 does not exist as a separate model. The appearance of this path code in a hazard assessment code is only meant to indicate that the chemical somehow reacts with water.

To accomplish hazard assessments for such water-reactive chemicals it is necessary for the user to determine what the products of reaction are and to conduct assessments for these products. To aid the user in this task, Table 0.1 is presented. This table lists the water reactive chemicals found in the first 900 CHRIS chemicals, and for each, gives their products of reaction with water and the amounts of these products which form per ton of the chemical spilled on water (e.g. one ton of anhydrous ammonia spilling on water results in ∿1.37 tons of concentrated ammonium hydroxide and ∿.50 tons of ammonia vapor).

For chlorosulfonic acid (CSA), nitrogen tetroxide (NOX) and phosgene (PHG), specialized procedures have been developed for hazard assessments. These procedures are discussed in the following.

CHLOROSULFONIC ACID (CSA)

Chlorosulfonic acid is a colorless to pale yellow liquid at all temperatures from -112°F to 311°F. It is classified as a corrosive liquid.

When in contact with moist air, CSA fumes strongly. The fumes released presumably consist of fine droplets of sulfuric acid in air. As such, they are persistent and very damaging to nasal passages and lungs.

In contact with water, CSA reacts quite violently and rapidly, to form sulfuric acid (SFA) and hydrogen chloride (HDC). The hydrogen chloride formed is volatile, but also quite soluble in water. Dissolved in water, it is known as hydrochloric acid (HCL).

In contact with most metals, CSA generates hydrogen (HXX), a lighter-than-air highly flammable and explosive gas. Contact with combustible materials may cause ignition of them, although chlorosulfonic acid itself is not flammable.

The heat of solution of CSA in water is 623 Btu/lb of acid (40.3 kcal/g mol). Thus, a very large amount of water must be available to dissolve the reaction products without large temperature rises or steam evolution. As an approximate rule, at least 10 lbs of water per lb of acid are necessary to keep the increase in water temperature below 65-80°F.

For hazard assessment purposes, we are concerned with what will happen if CSA is discharged underwater and what will happen if it is

TABLE 0.1[†]

LIQUID CHEMICALS WHICH REACT WITH WATER

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Acetyl bromide	Acetic acid	APQ	.49	Reacts violently.
	Hydrogen bromide	AC	some	
	Hydrobromic acid	(no code)	⩽.66	
Acetyl chloride	Acetic acid	APQ	.76	Reacts vigorously.
	Hydrochloric acid	AP	⩽.46	
	Hydrogen chloride	AC	some	
Allyl chloroformate	Allyl alcohol	APQ	.48	Reaction is *slow*.
	Hydrochloric acid	AP	.30	
	Carbon dioxide	AC	.37	
Allyltrichlorosilane	Silicone type polymer	(no code)	.67	Reacts vigorously.
	Hydrochloric acid	AP	.62	
	Hydrogen chloride	AC		
Ammonia, anhydrous	Ammonia, anhydrous (vapor)	ABC	≈ .50	Quite vigorous dissolution with heat evolution.
	Ammonium hydroxide	APRS	~1.37	

TABLE O.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
n-Amyltrichlorosilane	Silicone type polymer	(no code)	.72	Reacts vigorously.
	Hydrochloric acid	AP	.53	
	Hydrogen chloride	AC		
Anisoyl chloride	Hydrochloric acid	AP	.21	Reacts slowly.
	Hydrogen chloride	AC		
	p-anisic acid	(no code)	.89	
Antimony pentachloride	Hydrochloric acid	AP	≤.61	
	Hydrogen chloride	AC	some	
	Antimonic acid	(no code)	.62	
Antimony pentafluoride	Hydrofluoric acid	AP	.46	Reacts vigorously.
	Hydrogen fluoride	AC		
	Antimonic acid	(no code)	.85	
Arsenic trichloride	Hydrochloric acid	AP	≤.60	Not vigorous.
	Hydrogen chloride	AC	very little	
	Antimonous acid	(no code)	.69	
Benzene phosphorus dichloride	Hydrochloric acid	AP	.60	Reacts vigorously.
	Hydrogen chloride	AC		
	Benzene phosphonous acid	(no code)	.79	

TABLE O.1[†] (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Benzene phosphorus thiodichloride	Hydrochloric acid	AP	≤.35	Reaction slow unless water is hot. HCl fume unlikely unless water hot.
	Hydrogen chloride	AC	see remark	
	Benzenethiophosphonic acid	(no code)	.82	
Benzoyl chloride	Benzoic acid	II	.87	Reacts *slowly*.
	Hydrochloric acid	AP	≤.26	
	Hydrogen chloride	AC	some	
Benzyl bromide	Benzyl alcohol	APTX	.63	Reacts *slowly*.
	Hydrogen bromide	AC	little, if any	
	Hydrobromic acid	(no code)	≤.47	
Benzyl chloride	Benzyl alcohol	APTX	.85	Reacts *slowly*.
	Hydrochloric acid	AP	~.29	
	Hydrogen chloride	AC	little, if any	
Benzyl chloroformate	Benzyl alcohol	APTX	.63	Not vigorous in cold water.
	Hydrochloric acid	AP	.21	
	Carbon dioxide	AC	.26	
Boron tribromide	Boric acid	SS-II	.25	Reacts violently.
	Hydrogen bromide	AC	.97	
	Hydrobromic acid	(no code)		

TABLE O.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Boron trichloride	Boric acid	SS-II	.55	Reacts vigorously.
	Hydrochloric acid	AP	.93	
	Hydrogen chloride	AC		
Bromine pentafluoride	Bromine	APX	.46	Reacts violently. Reactions not stoichiometric. Products and weight fractions are best guesses.
	Hydrofluoric acid	AP	.57	
	Hydrogen fluoride	AC		
	Oxygen	no hazard	.23	
Bromine trifluoride	Bromine	APX	.58	Reacts vigorously. Reactions not stoichiometric. Products and weight fractions are best guesses.
	Hydrofluoric acid	AP	.44	
	Hydrogen fluoride	AC		
	Oxygen	no hazard	.18	
Butyltrichlorosilane	Silicone type polymer	(no code)	.70	Reacts vigorously.
	Hydrochloric acid	AP	.57	
	Hydrogen chloride	AC		
Chlorine trifluoride	Chlorine	AC	.38	Reacts explosively.
	Hydrofluoric acid	AP	.65	
	Hydrogen fluoride	AC		
	Oxygen	no hazard	.26	

TABLE O.1[†] (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Chloroacetyl chloride	Monochloroacetic acid	AP	.84	Reacts vigorously.
	Hydrochloric acid	AP	.32	
	Hydrogen chloride	AC		
Chloromethyl methyl ether	Formaldehyde	APQ	.37	Not violent.
	Methyl alcohol	APQRS	.40	
	Hydrochloric acid	AP	<.45	
	Hydrogen chloride	AC	little, if any	
Chlorosulfonic acid	Sulfuric acid	AP	.84	Reacts violently.
	Hydrochloric acid	AP	.31	
	Hydrogen chloride	AC		
Chromyl chloride	Chromic acid	(no code)	<.76	Reacts violently.
	Chromium dioxide	(no code)	little, if any	
	Hydrochloric acid	AP	<.47	
	Hydrogen chloride	AC		
	Chlorine	AC	some	
	Hydrogen	ABC	maybe some	

TABLE 0.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Cyclohexenyltrichloro-silane	Silicone type polymer	(no code)	.73	
	Hydrochloric acid	AP	.51	
	Hydrogen chloride	AC		
Diethylzinc	Ethane	ABC	.49	Reacts violently with water and may ignite spontaneously.
	Zinc oxide	(no code)	.66	
Difluorophosphoric acid, anhydrous	Phosphoric acid	AP	.95	Reacts vigorously.
	Hydrofluoric acid	AP	.39	
	Hydrogen fluoride	AC		
Dimethyldichlorosilane	Silicone type polymer	(no code)	.70	Reacts vigorously.
	Hydrochloric acid	AP	.57	
	Hydrogen chloride	AC		
Dimethylzinc	Methane	ABC	.34	Reacts vigorously with water and may ignite spontaneously.
	Zinc oxide	(no code)	.85	
Diphenyldichlorosilane	Silicone type polymer	(no code)	.95	
	Hydrochloric acid	AP	.29	
	Hydrogen chloride	AC		

TABLE O.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Dodecyltrichlorosilane	Silicone type polymer	(no code)	.77	
	Hydrochloric acid	AP	.36	
	Hydrogen chloride	AC		
Ethylaluminum dichloride	Ethane	ABC	.23	Reacts violently with water and may ignite spontaneously. Smoke may be irritating and cause metal fume fever.
	Hydrochloric acid	AP	.56	
	Hydrogen chloride	AC		
	Aluminum oxide	(no code)	.39	
Ethylaluminum sesquichloride	Ethane	ABC	.36	Reacts violently with water and may ignite spontaneously. Smoke may be irritating and cause metal fume fever.
	Hydrochloric acid	AP	.44	
	Hydrogen chloride	AC		
	Aluminum oxide	(no code)	.41	
Ethyl chloroformate	Carbon dioxide	AC	.41	Reaction is *slow*.
	Ethyl alcohol	APQRS	.42	
	Hydrochloric acid	AP	.34	
Ethyldichlorosilane	Silicone type polymer	(no code)	.70	Reacts vigorously.
	Hydrochloric acid	AP	.57	
	Hydrogen chloride	AC		

TABLE O.1[†] (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Ethylphenyldichlorosilane	Silicone type polymer	(no code)	.81	
	Hydrochloric acid	AP	.36	
	Hydrogen chloride	AC		
Ethyl phosphonothioic dichloride, anhydrous	Ethanephosphonothioic acid	(no code)	.77	
	Hydrochloric acid	AP	.45	
	Hydrogen chloride	AC		
Ethyl phosphorodichloridate	Ethyl dihydrogen phosphate	(no code)	.77	Ethyl dihydrogen phosphate may or may not react with water to form ethyl alcohol and phosphoric acid.
	Hydrochloric acid	AP	.45	
	Hydrogen chloride	AC		
Ethyl silicate	Ethyl alcohol	APQRS	.88	Products may include silica gel *or* o-silicic acid. Reaction is *slow*.
	Silica gel	(no code)	.46	
	o-silicic acid	(no code)		
Ethyltrichlorosilane	Silicone type polymer	(no code)	.64	Reacts vigorously.
	Hydrochloric acid	AP	.67	
	Hydrogen chloride	AC		

TABLE O.1[†] (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Fluosulfonic acid	Hydrofluoric acid	AP	.20	Reacts violently.
	Hydrogen fluoride	AC		
	Sulfuric acid	AP	.98	
Hydrogen bromide	Hydrobromic acid	(no code)	1.00	Moderate reaction with evolution of heat.
Hydrogen chloride	Hydrochloric acid	AP	1.00	Moderate reaction with evolution of heat.
Hydrogen fluoride	Hydrofluoric acid	AP	1.00	Dissolves with liberation of heat.
Methyl chloroformate	Carbon dioxide	AC	.47	Reacts slowly. Reaction can be hazardous and hydrogen chloride formed if water is hot.
	Hydrochloric acid	AP	.39	
	Hydrogen chloride	AC		
	Methyl alcohol	APQRS	.34	
Methyldichlorosilane	Silicone type polymer	(no code)	.66	Reacts violently.
	Hydrochloric acid	AP	.63	
	Hydrogen chloride	AC		

TABLE O.1[†] (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Methyl phosphonothioic dichloride, anhydrous	Hydrochloric acid	AP	.49	May be violent reaction.
	Hydrogen chloride	AC		
	Methanephosphonothioc acid	(no code)	.75	
Methyltrichlorosilane	Silicone type polymer	(no code)	.63	Reacts violently.
	Hydrochloric acid	AP	.73	
	Hydrogen chloride	AC		
Nitrogen tetroxide	Nitric acid	AP	.91	
	Nitric oxide	AC	.22	
Nitrosyl chloride	Hydrochloric acid	AP	.56	
	Hydrogen chloride	AC		
	Nitrogen dioxide	(no code)	.70	
	Nitrogen tetroxide	ACO		
Oleum	Sulfuric acid	AP	?	Vigorous reaction; spatters. Weight fraction depends on SO_3 content of oleum. Use 1.15 if better value not available.

TABLE O.1[†] (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Parathion, liquid	Ethyl alcohol	APQRS	.32	*Slow* reaction.
	4-Nitrophenol	II-SS	.48	
	Thionophosphonic acid	(no code)	.39	
Pentaborane	Hydrogen	ABC	.38	Reacts *slowly*. Not hazardous unless water is hot or unless confined.
	Boric acid	SS-II	4.89	
Perchloromethyl mercaptan	Carbon dioxide	AC	.24	Reacts only when hot.
	Hydrochloric acid	AP	.79	
	Sulfur (solid)	(no code)	.17	
Phenyldichloroarsine, liquid	Benzenearsenic acid	(no code)	.83	*Very slow* reaction.
	Hydrochloric acid	AP	.33	
Phosgene	Carbon dioxide	AC	.44	Decomposes, but not vigorously.
	Hydrochloric acid	AP	.74	
Phosphorus oxychloride	Hydrochloric acid	AP	.71	Vigorous reaction.
	Hydrogen chloride	AC		
	Phosphoric acid	AP	.64	

TABLE O.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Phosphorus tribromide	Hydrobromic acid	(no code)	.90	Reacts violently.
	Hydrogen bromide	AC		
	Phosphorous acid	(no code)	.30	
Phosphorus trichloride	Hydrochloric acid	AP	.80	Reacts violently and may cause flashes of fire.
	Hydrogen chloride	AC		
	Phosphorous acid	(no code)	.60	
Polymethylene polyphenyl isocyanate	Carbon dioxide	AC	?	Reacts *slowly*, forming heavy scum and carbon dioxide. Reaction is not stoichiometric.
	Some sort of polymer	(no code)	?	
Polyphosphoric acid	Phosphoric acid	AP	?	Reaction not *violent*. Weight fraction depends upon acid content of initial reactant.
Propionic anhydride	Propionic acid	APQ	1.14	Reacts *slowly* to form weak acid.
Propyleneimine, inhibited	Monoisopropanolamine	APQ	1.31	Reaction is *slow*.

TABLE O.1[†] (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Silicon tetrachloride	Hydrochloric acid	AP	.86	Reacts vigorously.
	Hydrogen chloride	AC		
	Silica gel	(no code)	.57	
	o-Silicic acid	(no code)		
Sulfur monochloride	Hydrochloric acid	AP	.54	Reacts violently.
	Hydrogen chloride	AC		
	Hydrogen sulfide	ABC	< .24	
	Sulfur dioxide	AC	< .47	
	Sulfur (solid)	(no code)	?	
	Polythionic acids	(no code)	?	
Sulfuric acid	Sulfuric acid (in solution)	AP	1.00	Reacts violently with evolution of heat. Spattering occurs when water added to compound.
Sulfuryl chloride	Hydrochloric acid	AP	.54	Reacts vigorously.
	Hydrogen chloride	AC		
	Sulfuric acid	AP	.73	

TABLE O.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Tetrabutyl titanate	n-Butyl alcohol	APQ	.87	
	Titanium dioxide	(no code)	.24	
Thiophosgene	Carbon dioxide	AC	.38	Reaction is slow unless water is hot.
	Hydrochloric acid	AP	.63	
	Hydrogen sulfide	ABC	.30	
Titanium tetrachloride	Hydrochloric acid	AP	.77	Heat generated.
	Hydrogen chloride	AC		
	Titanium dioxide	(no code)	.42	
Trichlorosilane	Hydrochloric acid	AP	.81	Reacts violently.
	Hydrogen chloride	AC		
	Silanetriol polymer	(no code)	.57	
Triethylaluminum	Aluminum oxide	(no code)	.45	Reacts violently, ignites spontaneously at all temperatures. Smoke may cause metal fume fever.
	Ethane	ABC	.79	
Triisobutylaluminum	Aluminum oxide	(no code)	.26	Reacts violently and may ignite spontaneously. Smoke may cause metal fume fever.
	Isobutane	ABC	.88	

TABLE O.1[†] (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Trimethylchlorosilane	Hydrochloric acid	AP	.34	Reacts vigorously.
	Hydrogen chloride	AC		
	Trimethylsilanol	(no code)	.83	
Vanadium oxytrichloride	Hydrochloric acid	AP	.63	
	Hydrogen chloride	AC		
	Vanadic acid	(no code)	.68	
Vinyltrichlorosilane	Silicone type polymer	(no code)	.64	Reacts vigorously.
	Hydrochloric acid	AP	.68	
	Hydrogen chloride	AC		

†Notes for Table O.1

1) The *pertinent* hazard assessment codes of this table were especially chosen to best reflect the hazards from the products of reaction. They may or may not be the same as those found for these chemicals in CG-446-2.

2) Many lists of products of reaction include hydrogen chloride and hydrochloric acid, *or* hydrogen fluoride and hydrofluoric acid, *or* hydrogen bromide and hydrobromic acid. In most cases where this occurs, it is not possible to estimate how much hydrogen chloride, fluoride, or bromide will enter the atmosphere as a vapor or acid mist, or how much will mix with the water. Consequently, one "weight fraction of spill" has been given which shows the total of the two possible products. The user must decide how to apportion the weight fraction between the two products. As a general guideline it can only be said that the slower the reaction is, the more that will mix with water, and vice versa.

3) The products of reaction and their weight fractions were estimated, with one exception, by assuming that all of the reactant compound reacts with the water. When the reactant compound boils at less than ambient temperatures or reacts slowly, however, this assumption may not be completely true. In such cases, a large portion of the chemical may vaporize or otherwise disperse before reacting. For example, about 50% of any liquid anhydrous ammonia spilled on water is known to vaporize before reacting. For such chemicals, therefore, the user may wish to assume that some portion of the originally spilled chemical does not react and to utilize the hazard assessment code for the unreacted chemical to determine additional hazards.

4) The hazard assessment code "B" should not be utilized for a product of reaction, unless the reaction takes place *within* a punctured tank or other container.

5) "No code" indicates that the chemical is not contained in CHRIS. It should not be interpreted as signifying that the substance is non-hazardous.

spilled onto or near the surface of a water body. Hazards associated with the generation of hydrogen gas and the ignition of combustible materials are beyond the predictive capabilities of HACS at the present time.

Underwater Discharges

Discharges under a large head of water would probably result in little evolution of gas or steam from the surface since any sulfuric acid or hydrogen chloride formed would dissolve in the water and any steam formed would recondense before reaching the surface. If any harmful gas or fume were to reach the surface, it would most likely entirely consist of hydrogen chloride or steam. Water pollution hazards from such a discharge would stem from the sulfuric and hydrochloric acid which would dissolve in the water.

Model K in HACS estimates the amount of a soluble gas which will evolve from the surface of a water body when it is discharged at a water depth greater than 10 feet. It, and subsequent models M and N, can therefore be used to estimate the amount of hydrogen chloride which escapes to the atmosphere and the air pollution hazards of this amount. Execution of Model K also runs Model P, the water dispersion model, to estimate downstream concentrations of hydrochloric acid in water.

The only unusual step in setting up a HACS run for this situation is the necessity for the user to calculate the amount of hydrogen chloride which is evolved (data item with field number 2007). This is simply done by multiplying the amount of CSA discharged by 0.31.

A separate HACS run must be made to determine the water pollution hazards of the sulfuric acid (SFA) which forms. Since we would not be concerned with any vapor dispersion hazards, the only model to be run would be Model P. As before, a special calculation is necessary to determine the amount of SFA formed. In this instance, the amount of CSA spilled is multiplied by a factor of 0.84 and used as the input value for the data item with field number 4002.

Table 0.2 summarizes the run set-ups which may be utilized.

Near or On-Surface Spills

Spills on or near the surface would quite definitely result in a significant cloud (of steam, sulfuric acid, and hydrogen chloride gas or hydrochloric acid fume) which would move downwind and only slowly be dissipated. Large spills in a local area could, in fact, generate so much steam and hydrogen chloride that the reaction could resemble a flameless explosion. As would also be true for underwater discharges, any sulfuric or hydrochloric acid dissolving into the water could be harmful to aquatic life and to industrial or public facilities which intake water from the polluted water body.

TABLE 0.2

POSSIBLE RUN SET-UPS FOR

CHLOROSULFONIC ACID SPILLS

UNDERWATER DISCHARGE (>10' underwater)

1. For determining the amount of HDC which escapes the surface and that which dissolves, and for assessing HDC air and water pollution hazards:

   Col #1
   *TITLE CARD
   K␣␣␣M␣␣␣N
   1001HDC
   2007 (0.31 x amount of CSA discharged) (wt units)
   Rest of deck would be exactly the same as normally used for the K-M-N execution sequence.

2. For determining the SFA water pollution hazard:

   TITLE CARD
   P
   1001SFA
   4002 (0.84 x amount of CSA discharged) (wt units)
   Rest of deck would be exactly the same as normally used for Model P execution.

NEAR OR ON SURFACE DISCHARGES*

3. For air pollution hazards of HDC evolved:

   TITLE CARD
   C
   1001HDC
   4001 (0.31 x amount of CSA discharged) (wt units)
   Rest of deck would be exactly the same as normally used for the Model C execution.

*Note: These set-ups assume that the release of CSA is instantaneous. They may, however, be used for continuous discharges if Model A is first (and separately) run to find the liquid discharge rate of CSA, and if the factors 0.31 and 0.84 were applied, as appropriate, to this rate.

TABLE 0.2 (continued)

4. For water pollution hazards of HCL:

   TITLE CARD

   P

   1001HCL

   4002 (0.31 x amount of CSA discharged) (wt units)

   Rest of deck would be exactly the same as normally used for Model P execution.

5. For the water pollution hazard of SFA:

   Set-up is same as for #2 above.

To assess the vapor dispersion hazards for this type of spill, the user can assume as the worst case situation that all of the hydrogen chloride generated escapes as a gas or vapor. Thus, he would execute Model C for a hydrogen chloride evolution amount which is 0.31 times that of the amount of CSA which is released.

To assess the water pollution hazards of the spill, Model P can be run the same way as described for underwater releases of SFA. For the HCL hazard, as a worst case, the user could run Model P in a similar fashion with a factor of 0.31 being used instead of 0.84.

Table 0.2 also summarizes the run set-ups for these cases.

NITROGEN TETROXIDE (NOX)

Nitrogen tetroxide (NOX) has a boiling point of 70° F and a specific gravity of 1.45. It is a powerful oxidizing agent, and either liquid or vapor is toxic to life. Contact of the liquid with combustible material may lead to ignition and, if spilled on the skin, severe burns result. The symptoms of NOX inhalation include pulmonary edema, cyanosis, and other serious effects.

In contact with water, NOX eventually reacts to form nitric acid (HNO_3) and nitric oxide (NO). The nitric acid formed will remain predominantly in the water phase and disperse downstream in a manner similar to other soluble chemicals; the nitric oxide will, to a certain extent, dissolve, but most will leave the aqueous phase and disperse downwind as a vapor. The time span over which the NOX contacts water determines how much NOX or its reaction products with water will enter the aquatic or atmospheric environments, and hence, determines the hazard extents in these media.

The determining factors for the contact time between NOX and water are the temperature and pressure to which the liquid is subjected. If the liquid may boil in its environment, it can be expected that it will vaporize before much of it can react with water. If the liquid may not boil, due to low ambient temperature and/or hydrostatic pressure, all of it can be assumed to react with water.

In the following, we describe how HACS may be used to assess hazards in both of these situations. To be noted is that these cases are somewhat idealized extremes and that the realistic case may lie somewhere between them.

Boiling Liquid Case

If the water temperature is greater than 70°F, and a surface spill occurs, liquid NOX will immediately begin to boil upon contact with the water and will continue to boil as it sinks until all of it has vaporized. In this case, it can be assumed that little NOX will have time to react with water and that a significant portion of it will cause an air pollution hazard.

This scenario of events is represented by the hazard assessment path A-I-J and can be simply executed by reference to the instructions for these models.

Non-Boiling Liquid Case

If the water temperature is less than 70°F, or if the NOX is released at a depth at which it may not boil due to hydrostatic pressure effects, it can be expected that the NOX will form a pool on the bottom of the water body. This pool will relatively slowly dissolve into and react with water.

Assessment of the air and water pollution hazards in this case requires the procedure outlined below.

Step 1. Execute Model X for the amount of NOX spilled in order to determine the time it takes the chemical to reach the bottom of the waterbody, the distance downstream that it travels, the area of the pool on the bottom, and the length of the pool. Ignore other outputs as they will not be applicable.

Step 2. Find R from the equation:

$$R = (5.75)\ (10^{-4})\ \frac{(uL)^{0.8}}{L}$$

where u = stream velocity, m/sec

L = pool length, m

Step 3. Find the rate at which nitric acid is evolved from the pool from the equation:

$$\frac{1}{\text{Rate } HNO_3} = 757.6 + \frac{1}{R}$$

Step 4. Find the rate at which nitric oxide is formed from the equation:

$$\text{Rate NO} = 0.5 \times \text{Rate } HNO_3$$

Step 5. Find how long it will take for the spill pool to completely dissolve and react from the equation:

$$T = \frac{(1.45)\ (10^{-2})\ (W)}{(A)\ (\text{Rate } HNO_3)} \quad \text{seconds}$$

where W = weight of NOX spilled, Kg

A = area of pool on bottom, m^2

T = time for all of pool to dissolve, s

Step 6. Execute Model P to determine water pollution hazards of nitric acid (NAC). For continuous evolution of nitric acid, the spill rate is given by the equation (for 4049 LIQ FLWRATE):

$$\text{Rate} = (\text{Rate } HNO_3)\ (A)\ (92)\ \frac{kg}{s}$$

The total amount of NAC generated (for 4002 TOT MASS LIQ) is given by this rate multiplied by the "T" computed in Step 5.

Step 7. Execute Model C to determine air pollution hazards of nitric oxide. For continuous evolution of nitric oxide from the surface of the water, the evolution rate (for 4044 AVG VAP RATE) is given by the equation:

$$\text{Rate} = (\text{Rate NO})\ (A)\ (30)\ \frac{kg}{s}$$

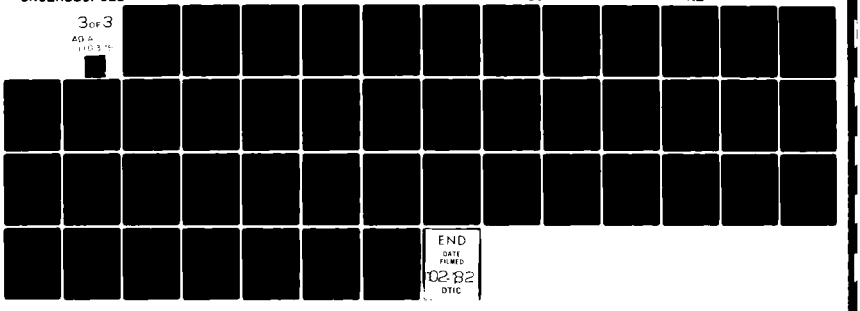
The time span over which vapor will be generated is given by the "T" calculated above (for 4045 EVOLVE TIME). For an instantaneous release calculations, the total gas amount (for 4001 TOT MASS GAS), in units of kg, is given by multiplication of the "rate" computed directly above by the T computed in step 5 above.

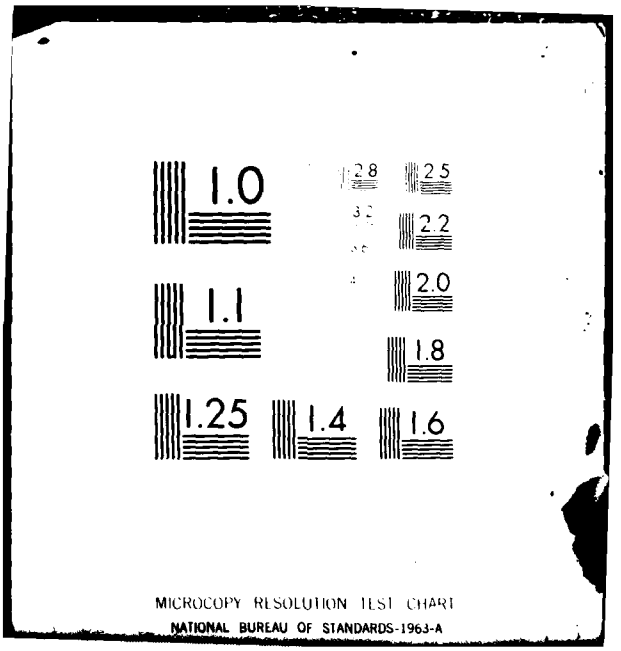
At the time that this procedure was written, HACS did not contain chemical property data for nitric oxide. To run Model C, it is necessary, therefore, that the user provide certain data. These, and other suggested data for use, are given below.

Field number	Data value
1001	leave blank
1002	30.0
2015	0.0
2018	2 (Integer)
2019	300.0
2032	25.0 (TLV*)
2033	0.0

*Value given is Threshold Limit Value (in ppm) for 8-hr exposures. Concentrations of 60 to 150 ppm can result in serious delayed injury some 6 to 24 hours after 30 to 60 minute exposure. Concentrations of 200 to 700 ppm may be fatal after even very short exposures.

AD-A110 375 LITTLE (ARTHUR D) INC CAMBRIDGE MA F/G 7/1
HAZARD ASSESSMENT COMPUTER SYSTEM HACS/UIM USERS' OPERATION MAN--ETC(U)
SEP 81 R G POTTS DOT-CG-941999-A
UNCLASSIFIED USCG-D-75-81 NL

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1.1
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2.0
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MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

PHOSGENE (PHG)

Phosgene (PHG) has a boiling point of 46.8%, and a specific gravity of about 1.38 at 20°C. It is a highly toxic substance which was once used as a war gas. A vapor exposure to only 1 ppm for 5 minutes is sufficient to cause toxic effects.

In contact with water, PHG eventually reacts to form aqueous hydrochloric acid and carbon dioxide gas. The acid formed will remain predominantly in the water phase and disperse downstream in a manner similar to other soluble chemicals. The fate of any carbon dioxide formed is irrelevent in that this substance is completely non-toxic and non-flammable. The time span ever which PHG contacts water determines how much PHG or its reaction products with water will enter the aquatic or atmospheric environments, and hence, determines the hazard extents in these media.

The determining factors for the contact time between PHG and water are the temperature and pressure to which the liquid subjected. If the liquid will boil in its environment, it can be expected that it will vaporize before much of it can react with water. If the liquid may not boil, due to low ambient temperature and/or hydrostatic pressure, most of it can be assumed to react with water.

In the following, we describe how HACS may be used to assess hazards in these cases. To be noted is that these situations are somewhat idealized extremes and that the realistic case may be somewhere between them.

Boiling Liquid Case

If the water temperature is greater than 46.8°F, and a surface spill occurs, liquid PHG will immediately begin to boil upon contact with water and will continue to boil as it sinks until all of it has vaporized. In this case, it can be assumed that little PHG will have time to react with water and that a significant portion of it will cause an air pollution hazard.

This scenario of events is represented by the hazard assessment path A-I-J and can be simply executed by reference to the instructions for these models.

Non-Boiling Liquid Case

If the water temperature is less than 46.8°F, or if the PHG is released at a depth at which it may not boil due to hydrostatic pressure effects, it can be expected that the PHG will form a pool on the bottom of the water body. This pool will relatively slowly dissolve into and react with water. Since PHG generates only one product of reaction which is hazardous, hydrogen chloride, only water pollution hazards need be addressed.

The procedure to be used is outlined below.

Step 1. Execute Model X for the amount of PHG spilled in order to determine the time it takes the chemical to reach the bottom of the water body, the distance downstream that it travels, the area of the pool on the bottom, and the length of the pool. Ignore other outputs as they will not be applicable.

Step 2. Find R from the equation:

$$R = (3.49)\ (10^{-6})\ \frac{(uL)^{0.8}}{L}$$

where u = stream velocity, m/s

L = pool length, m

Step 3. Find X from the equation:

$$\frac{1}{X} = 102{,}041 + \frac{1}{R}$$

Step 4. Find the rate at which hydrochloric acid (HCL) is formed from the equation:

$$\text{Rate HCL} = (26.53)\ (X)\ (A)\ \frac{kg}{s}$$

where A = pool area, m^2

Step 5. Find how long it will take for the spill pool to completely dissolve and react from the equation:

$$T = \frac{(0.0101)\ (W)}{(X)\ (A)} \quad \text{seconds}$$

where W = weight of PHG spilled, kg

A = area of pool on bottom, m^2

T = Time for all of pool to dissolve, s

Step 6. Execute Model P to determine water pollution hazards of hydrochloric acid (HCL). For continuous evolution of HCL, the spill rate (for 4049 LIQ FLWRATE) is given by the "Rate HCL" computed in Step 4 above. The total amount of HCL generated (for 4002 TOT MASS LIQ) is simply the "Rate HCL" multiplied by the "T" computed in Step 5.

MODEL P

Purpose

Model P computes the concentration of a water-miscible liquid or solid at any specified point and given time for a discharge in a lake, river, or estuary. All the chemical discharged is assumed to go into solution with water. This same program can also be used for the dispersion of insoluble solids which are neutrally buoyant or whose settling times are large compared to mixing times. It can be used approximately for concentration predictions for those fluids which react with water or whose boiling point is less than that of ambient temperature.

Restrictions and Cautions on Model Use

Model P only works for chemical spills into or onto water.

The model is only approximately correct when used for chemicals which are significantly heavier- or lighter-than-water or which are not very soluble in water.

If the release occurs deep underwater, the answers which Model P gives for locations very near the spill site may be only approximately correct.

Model P cannot be used for spills which occur offshore in the ocean in a region which is not part of an estuary. (An estuary is defined as a water passage where the tide meets a river current; esp: an arm of the sea at the lower end of a river).

Important Assumptions of the Model

The actual dispersion equations in Model P were developed with the assumptions that the chemical which spills is not very much heavier- or lighter-than-water and is fully soluble in water (miscible in all proportions).

Model P assumes that the spill occurs near or on the surface of the water body.

Input Data Considerations

An important input to the model is the Manning Roughness Factor, a number which describes to the model the type of water body into which the chemical has spilled. To aid the user in choosing a proper value, the following table is presented. (The default value for this data item is 0.030).

Natural-stream Channels	Manning Factor
Clean, straight bank, full stage	0.030
Winding, some pools, and shoals	0.040
Same, but with stony sections	0.055
Sluggish reaches, very deep pools, very weedy	0.070-0.125

If the spill is in an estuary, a water body affected by tidal action, the model requires that the user input the maximum amplitude of the tidal current velocity for data field number 2048. This data item can be found by the user by accessing the Tidal Current Tables for the region of concern and by computing the average of the maximum ebb and flood current velocities. The default value for this data item is 0.97 knots (50 cm/sec). To convert knots to units of cm/sec, the user must multiply the number in units of knots by 51.5.

The stream velocity in a river affected by tidal action is the sum of a constant outflow stream velocity and a velocity caused by the tides. The data item described in the preceding paragraph gives HACS the second part of this sum, the velocity caused by the tides. The outflow stream velocity (for data field number 2047) can be provided by determining the stream velocity of the river at an upstream point in the river which is not affected by tidal action. Alternatively, it can be estimated from the Tidal Current Tables by subtracting the maximum flood current velocity from the maximum ebb current velocity.

The tidal period is another data item required if the spill is in an estuary (for data field number 2049). This time period is the time from one high tide to the next, or from one low tide to the next. Since there are two high tides or low tides in any given day, the default file value for this data item is 12 hours (43,300 seconds).

The last data item which is specifically required when the spill is into an estuary is the phase lag (for data field number 2050). This value is simply the time to the next highwater slack tide (high tide) from the time of spill. The default file value is zero, but the actual value might range from zero to 12 hours.

Output of the Model

Model P computes the concentration of the chemical in water at a user specified time and location.

Optional output consists of two tables and two plots. One table and one plot give the concentration as a function of time at the user specified point. The other table and plot give the peak concentration versus distance downstream.

Data Specification

Table P1 defines the on-scene and operational data which the model requires.

Table P2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table P3 defines the output of the model.

Table P4 defines the data necessary for production of optional tables and plots.

TABLE P1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2028	WAT TYPE P/R	ND (Integer)	Flag indicating type of water body into which spill occurs.	1 = still water 2 = non-tidal river 3 = estuary or tidal region
2029	SPILL TYPE P	ND (Integer)	Flag indicating whether discharge is instantaneous or continuous.	0 = instantaneous 1 = continuous
2039 2040 2041	CONC PT X CONC PT Y CONC PT Z	CM M FT MI	Downstream distance from spill site. Cross-stream position (measured from center of river) Depth (measured from surface; down is positive direction)	These 3 coordinates define the point at which the concentration of the chemical in water is desired.
2042	TIME CONC PT	S MIN HR	Time at which concentration is desired to be known at point specified above.	
2044	RIVER DEPTH	CM M FT MI	Mean depth of water body	
2045	RIVER WIDTH	CM M FT MI	Mean width of water body	
2046	OFF DIST	CM M FT MI	Distance from center of water body at which discharge occurs.	Center is 0.0 Bank is width/2.
2047	STREAM VEL	CM/S M/S MPH KNOTS	Mean current velocity of water body. See model description if spill is in estuary.	Required only if spill is in flowing water 1 knot = 51.48 cm/sec
2048	TIDAL VEL	CM/S M/S MPH KNOTS	Maximum amplitude of tidal current velocity. See model description for details.	Required only if spill is in estuary or tidal region.
2049	TIDAL PERIOD	S MIN HR	Tidal period. See Model description for details.	Same as above.

TABLE P1: ON-SCENE AND OPERATIONAL DATA (CONT'D)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2050	PHASE LAG	S MIN HR	Time to next highwater slack tide from time of discharge. See model description for details.	Same as above.
2051	DECAY COEFF	/S /MIN /HR	Decay coefficient, to be given only if pollutant decays as per first order decay equation.	Data not in HACS for individual chemicals. Default value of 0.0 reflects fact that vast majority of pollutants do not decay.
2052	MANNING FACT	ND	Manning Roughness Factor for river. See model description for table.	Required only if spill is into flowing water.
2043	DIF COEF H20	CM2/S M2/S FT2/S	Diffusion coefficient of the chemical in water. Required only if spill is into still water.	HACS will estimate and use a value if user does not provide one.*
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid chemical which enters the water.	Computed by Model A.
4049	LIQ FLWRATE	G/S KG/S LB/S TN/HR	Average rate at which chemical enters water.	Required only for continuous discharges. Computed by Model A.
2004	TEMP START	C K F	Temperature of liquid chemical before discharge starts.	

* Estimated as being 1000 times the molecular diffusion coefficient for the liquid.

TABLE P2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	Required only if spill is in still water
1003	BOIL TEM LIQ	C K F	Boiling point temperature of chemical	Required only if spill is in still water.
1004	DENS LIQ AMB*	G/CM3 KG/M3 LB/FT3	Density of liquid chemical at ambient temperature	
1021	LIQ DENS BP	G/CM3 KG/M3 LB/FT3	Density of liquid chemical at its boiling point	Required only if spill is in still water.
1025	CRIT TEMP	C K F	Critical temperature of chemical	Required only if spill is in still water.

* Computed automatically at temperature 2004 TEMP START.

TABLE P3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4022	LIQ-H2O CONC	G/CM3 KG/M3 LB/FT3	Concentration of the chemical in water. For chemicals which are diluted with water before they spill, it is necessary for the user to multiply this answer by the fraction of the spilled solution which consisted of the chemical. For example, if 28% hydrochloric acid is spilled instead of 100% hydrochloric acid, the answer given should be multiplied by 0.28 to obtain the true answer.	Answer is also printed in units of ppm and mg/liter

TABLE P4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3008	PLOT FLAG P	ND (Integer)	Flag indicating which plots, if any, are desired.	0 = plots are not desired 1 = plot concentration vs time at user specified point 2 = plot maximum concentration vs distance downstream* 3 = give both plots above*
3015	TABLE FLAG P	ND (Integer)	Flag indicating which tables, if any, are desired.	0 = tables are not desired 1 = print table of concentration vs time at user specific point 2 = print table of maximum concentration vs distance downstream* 3 = print both tables above*
2037	MAX TIME CONC	S MIN HR	Maximum elasped time from start of spill for various tables and plots. HACS is capable of automatically decreasing this value under some circumstances if the user given value is too large.	Not required if tables or plots are not desired.
			*Not appropriate for spills into still water or estuaries.	

MODEL Q

Model Q is the pool fire hazard assessment model for soluble liquids which have a boiling point greater than the ambient temperature. It estimates the diameter of the base of the flame as being twice the volume of liquid discharged to the 1/3 power, and then calls Model E, the primary pool fire hazard assessment model in HACS.

The only input data item which Model Q itself requires is that for field number 4003, the total volume of liquid released (see Table A3 for a full description of this item). The user must refer to Model E for further information required to execute this model.

MODEL R

Purpose

Model R is used for volatile liquids which are soluble in water and have a boiling point greater than the ambient temperature, but less than 100 degrees centigrade (i.e., the chemical has a considerable vapor pressure at ambient temperatures - and is miscible in water). The model computes the amount of vapor which is evolved from the surface of the water and the downstream distances over which the water body can liberate vapors which are toxic or flammable. It also estimates other data required to execute vapor dispersion Model S.

Restrictions and Cautions on Model Use

It must be cautioned that the rate of vapor liberation is not uniform as the chemical/water solution moves downstream. It is likely that more will be liberated near the spill origin than further on. The model, as presently developed, outputs the average vapor evolution rate as the solution moves downstream.

The model can only be used for chemical spills into still water or into river stretches which are not affected by tidal action. It cannot be used for spills into estuaries.

The model may not produce realistic answers if the chemical spilled is significantly heavier - or lighter-than-water or is not very soluble in water.

The model may not produce realistic answers if the discharge of the chemical occurs over a long period of time.

The user must realize that the "slug" of chemical/water solution which moves downstream at the current velocity is representative of a moving vapor source. Any answers resulting from the execution of Model S will apply not to the spill site but to the actual location of the "slug".

Important Assumptions of the Model

The actual water dispersion equations in Model R were developed with the assumptions that the chemical which spills is not very much heavier - or lighter-than-water and is fully soluble in water (miscible in all proportions).

Model R assumes that the spill occurs near or on the surface of the water body.

The model assumes that the liquid discharge occurs instantaneously.

Input Data Considerations

An important input to the model is the Manning Roughness Factor, a number which describes to the model the nature of water body into which the chemical has spilled. To aid the user in choosing a proper value, a table was presented in the description of Model P.

The model uses the Threshold Limit Value (TLV) of the volatile liquid in order to determine the chemical concentration in water below which the chemical/water solution cannot generate toxic vapors - unless the user overrides the value. The TLV concentration for the vapor is harmless to people for the short-term exposures under consideration by HACS. *For more realistic answers, it is suggested that the user provide* a value which is more representative of a concentration which can be harmful to health in the time spans of concern. Some such data are given in CG-446-2 and the Chemical Properties File for concentrations which can cause headaches, coughing, eye irritation, and other usually minor and temporary effects. Concentrations which can cause more significant effects are usually higher and can be found in texts concerned with industrial hygiene and/or toxicology. The data field number of concern here is 2032.

Output of the Model

For either or both of the lower flammable limit concentration in air or a lower toxic limit concentration in air for the chemical, Model R computes the total mass of vapor liberated, the distance downstream over which the chemical/water solution is "strong" enough to liberate flammable or toxic vapors, the average vapor evolution rate, and the time span over which hazardous concentrations of vapor will be liberated from the surface of the water. It also estimates that the vapor source is a circular one (DIM FLAG = 2) to facilitate data input in case Model S immediately follows.

If both the lower toxic concentration and the lower flammable limit concentration are given for the chemical (i.e., the data for field numbers 2032 and 2033 are both greater than zero), the model stores the output for the lower toxic concentration for use by Model S. This also occurs if the lower flammable limit concentration is zero. If only the flammable limit is given, the model stores the output for this concentration for subsequent use by Model S.

Data Specification

Table R1 defines the on-scene and operational data which the model requires.

Table R2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table R3 defines the output of the model. The user may override any computed data with his own values.

Model R does not have any optional tables or plots. Thus, there is no Table R4 for this model.

TABLE R1; ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2028	WAT TYPE P/R	ND (Integer)	Flag indicating type of water body into which discharge occurs. A value of 3 will be replaced with a 2 by HACS.	1 = still water 2 = non-tidal river
2004 2023	TEMP START WATER TEMP	C K F C K F	Temperature of liquid discharged Temperature of the water body	
2032	LOW TOX LIM	PPM	The concentration of the vapor in air which is considered to be toxic. See model description for discussion.	Utilizes Threshold Limit Value (TLV) for 8-hr exposure unless overridden
2044	RIVER DEPTH	CM M FT MI	Mean depth of water body	Required only if spill is in flowing water
2045	RIVER WIDTH	CM M FT MI	Mean width of water body	Required only if spill is in flowing water
2047	STREAM VEL	CM/S M/S MPH KNOTS	Mean current velocity of river.	Required only is spill is in flowing water.
2052	MANNING FACT	ND	Manning Roughness Factor for rivers. see description of Model P for table.	Required only if spill is in flowing water.
2054	AIR TEMP	C K F	Ambient air temperature in area of discharge.	
2053	DIF COEF V-A	CM2/S M2/S FT2/S	Diffusion coefficient of the chemical vapor in air	HACS will estimate and use a value if the user does not provide one
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid chemical which enters the water.	
2043	DIF COEFF H20	CM2/S M2/S FT2/S	Diffusion coefficient of the chemical liquid in water. Required only for spills into still water	HACS will estimate a value and use it if the user does not provide one. (Estimated as being 1000 times molecular diffusion coefficient.)

TABLE R2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	
1003	BOIL TEM LIQ	C K F	Boiling point temperature of chemical	Required only if spill is in still water
1004	DENS LIQ AMB	G/CM3 KG/M3 LB/FT3	Density of liquid chemical at ambient temperature	Computed automatically at temperature 2004 TEMP START
1010	VPE COEFF A	LOG FCN	Coefficients of a vapor pressure equation in the form of the one in Section 2.4.3 but which gives an answer in mm Hg.	
1011	VPE COEFF B	C		
1012	VPE COEFF C	C		
1021	LIQ DENS BP	B/CM3 KG/M3 LB/FT3	Density of liquid chemical at its boiling point	
1025	CRIT TEMP	C K F	Critical temperature of chemical	Required only if spill is in still water
2033	LOW FLAM LIM	PERCENT	Lower flammability limit of chemical vapor in air (LFL or LEL)	

TABLE R3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4023	MASS VAP LIB	G KG LB TN	Total weight of vapor which evolves while the concentration of the chemical in water is sufficient to produce toxic vapors.	If the lower toxic limit concentration is zero, this field # will be used for flammable vapors.
4024	SAFE DIST	CM M FT MI	Distance downstream over which toxic vapors will be generated	Same as above.
2019	DIM SPILL	CM M FT MI	Maximum radius of vapor source which evolves toxic vapors (source is assumed to be circular).	Same as above.
4044	AVG VAP RATE	G/S KG/S LB/S TN/HR	Average rate at which toxic vapors will be evolved.	Same as above.
4045	EVOLVE TIME	S MIN HR	Time span from spill over which toxic vapors will be evolved.	Same as above.
4056	MASS VAP LIB	G KG LB TN	Total weight of vapor which evolves while the concentration of the chemical in water is sufficient to produce flammable vapors.	Used only if model is executed for both toxic and flammable concentrations.
4057	SAFE DIST	CM M FT MI	Distance downstream over which flammable vapors will be generated.	Same as above.
4058	DIM SPILL	CM M FT MI	Maximum radius of vapor source which evolves flammable vapors (source is assumed to be circular).	Same as above.
4059	AVG VAP RATE	G/S KG/S LB/S TN/HR	Average rate at which flammable vapors will be evolved.	Same as above.
4060	EVOLVE TIME	S MIN HR	Elapsed time from spill over which flammable vapors will be evolved.	Same as above.

TABLE R3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS (CONT'D)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
Data Estimated in Case Model S Follows:				
2019	DIM SPILL	CM M FT MI	Mean size of vapor source which generates hazardous vapors.	Stored as a SYSTEM value to provide Model S more realistic answer. May be overridden before its mean is taken.
2061	SPILL TYPE C	ND (Integer)	Flag indicating whether vapor evolution is estimated to be instantaneous or continuous	0 = instantaneous 1 = continuous
2018	DIM FLAG	ND (Integer)	Flag indicating whether vapor source is circular or rectangular	Model R always estimates that the source is circular.
4001	TOT MASS GAS	G KG LB TN	Total weight of vapor which enters the atmosphere. Stored as a SYSTEM value. User may override value only by providing data for 4023 MASS VAP LIB	Given only if the vapor evolution is estimated to be instantaneous. This simply transfers answer from 4023 to 4001 for use by Model S.
4068	AVG GAS TEMP	C K F	Temperature of vapors being evolved	Same as water temperature.

MODEL S

Model S is the vapor dispersion model for chemicals of the type addressed by Model R. Since all computed data necessary for a vapor dispersion hazard assessment are computed or estimated by Model R, Model S simply calls Model C, the primary vapor dispersion model in HACS. The user must therefore refer to Model C for the information required to execute this model.

CAUTION: The vapor dispersion model assumes that all of the vapor liberated is generated at the spill origin. This is not entirely true in this case because of the fact that some vapor will be generated throughout the travel zone of the chemical from the origin to what is referred to as the SAFE DIST in Model R. Though it is true that most of the vapor will be evolved near the spill origin, it is important to realize that populated areas immediately adjacent to the travel path of the chemical/water solution could be subjected to toxic and/or flammable vapor concentrations.

MODEL T

Purpose

Model T contains spreading and dispersion models for chemicals which are insoluble or slightly soluble in water, have a boiling point greater than the ambient temperature, and which are lighter-than-water. It may be used to determine the size of the spill pool at a given time for both instantaneous or continuous releases, or may be used to find the concentration of the chemical in water which results from the dissolution of a floating pool of a slightly soluble chemical.

Restrictions and Cautions on Model Use

The user should refer to the description of Model V for further explanation of the function of Model T when the hazard assessment (estimation route) code for the chemical also contains the letter V.

Model T only works for spills of chemicals into water. It does not work for spills on land.

The continuous pool spreading model in the Model T only works for spills onto the surface of water. It does not work when the chemical is continuously released from an underwater source.

Model A should not precede the execution of Model T if the release takes place underwater. Model A only works when the hole from which the chemical is being discharged is at or above the surface level of the water.

Although the instantaneous spill pool spreading part of Model T can determine whether or not the spill pool has been confined by channel banks at a user specified elapsed time, the continuous discharge

spreading model cannot. It can only give the user the radius of the spill pool at a given time regardless of whether or not the diameter of the pool is greater than the channel width.

The part of Model T which computes the concentration of the chemical in water resulting from dissolution of a slightly soluble pool of chemical only works for instantaneous spills of chemical. It cannot be used for continuous releases. Neither can it be used for spills into estuaries.

The density of a liquid chemical changes with temperature; the higher the temperature, the lighter it becomes, and vice versa. If HACS should determine that the density of the liquid at its temperature of release is greater than that of water, it will print out a message that the chemical may or may not float and then assume that the density of the chemical is slightly less than that of water. In such situations, the user must realize that the chemical may not actually float on the surface of the water, but may be suspended at some point beneath the surface. The answers obtained from Model T in such a situation will be invalid.

Important Assumptions of the Model

The pool spreading models in Model T assume mass conservation; i.e., they assume that the amount of chemical on the surface of the water does not become depleted due to evaporation of volatile constituents or other such factors.

The pool spreading model for continuous discharges assumes that the pool will not become confined by channel banks.

The part of Model T which can be used to compute the concentration of a chemical in water resulting from dissolution of a slightly soluble pool of chemical assumes that the discharge has been instantaneous. Additionally, it assumes that the user will ask for the concentration of the chemical in water at some point outside of the spill pool.

The instantaneous spill spreading model assumes that the pool will stop spreading when it reaches a thickness of 0.01 centimeters.

The chemical is assumed to have spilled onto calm water.

Input Data Considerations

An important input to the model when it is to be used for a dispersion problem is the Manning Roughness Factor. This number describes to the model the nature of the water body onto which the chemical has spilled. To aid the user in choosing a proper value, a table was presented in the description of Model P.

Output of the Model

The instantaneous and continuous discharge pool spreading models compute the size of the spill pool at a user specified time. For the instantaneous spill case, the model indicates whether or not the pool has been confined by channel banks. If it has, it gives the length of the channel which is covered by the chemical and the diameter of a circular spill pool of equivalent area. This latter value is required in case Model U follows. For the continuous discharge case, the model always indicates that the spill pool is circular and gives the radius and diameter of the pool.

The dispersion model outputs the dissolution rate of the spill pool (the rate at which it dissolves), the time it will take for all the chemical to dissolve into water, the distance the center of the spill pool will move downstream in a user specified time, and the concentration of the chemical in water at a user specified time and location.

Optional output consists of three tables and two plots. These are:

1. Table of pool size versus time
2. Table of peak concentration at middepth and bottom of river versus time and distance
3. Table of concentration versus time at a user specified point
4. Plot of pool size versus time
5. Plot of concentration versus time at a user specified point

Data Specification

Table T1 defines the on-scene and operational data which the various parts of the model require.

Table T2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table T3 defines the output of the model. The user may override any computed output data with his own values.

Table T4 defines the data necessary for production of optional tables and plots.

TABLE T1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2086	MODEL TYPE-T	ND (Integer)	Flag indicating which parts of Model T are to be executed	0 = execute pool spreading part 1 = execute pool dissolution and dispersion part 2 = do both of the above
2004	TEMP START	C K F	Temperature of liquid discharged	
DATA REQUIRED FOR POOL SPREADING PART OF MODEL T.				
2058	SPILL TYPE T	ND (Integer)	Flag indicating whether spill is instantaneous or continuous	0 = instantaneous 1 = continuous
2008	HOLE DIAM	CM M FT MI	Diameter of hole through which discharge takes place	Required only for continuous spill. If hole not circular, provide diameter of hole of equivalent area
2020	CHAN L WIDTH	CM M FT MI	Width of the channel or river into which the spill occurs	
4049	LIQ FLWRATE	G/S KG/S LB/S TN/HR	Average flow rate of chemical which enters water	Required only for continous spill. Will be computed by Model A
4050	LIQ FLW TIME	S MIN HR	Elapsed time from start of spill over which spill occurs	Same as above
2056	LIQ SPR TIME	S MIN HR	Elapsed time from start of spill at which the user desires the pool size	
2059	HOLE HGT UP	CM M FT MI	Distance from center of discharge hole to water surface	Required only for continuous spill
4002	TOT MASS LIQ	G KG LB TN	Total weight of chemical which enters water	

TABLE T1: ON-SCENE AND OPERATIONAL DATA (cont.)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
DATA REQUIRED FOR POOL DISSOLUTION AND DISPERSION PART OF MODEL T:				
2020	CHAN L WIDTH	CM M FT MI	Width of the channel or river into which the spill occurs	Required for other part of model also. Need not be specified twice.
2023	WATER TEMP	C K F	Temperature of water body into which spill occurs.	
2039	CONC PT X	CM M FT MI	Downstream distance from spill site	These 3 coordinates define the location at which the concentration of chemical in water is desired to be known.
2040	CONC PT Y		Cross-stream position (measured from center of channel)	
2041	CONC PT Z		Depth (measured from surface, down is positive direction	
2042	TIME CONC PT	S MIN HR	Time at which concentration is desired at above point	
2043	DIF COEF H2O	CM2/S M2/S FT2/S	Diffusion coefficient of the chemical in water	HACS will estimate a value and use it if the user does not provide one.
2044	RIVER DEPTH	CM M FT MI	Mean depth of the water body into which the spill occurs	
2047	STREAM VEL	CM/S M/S MPH KNOTS	Mean current velocity of water body into which spill occurs	
2052	MANNING FACT	ND	Manning Roughness Factor for water body. See Model P description for a table.	
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid chemical which enters water	Will be computed by Model A.

TABLE T2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	
1003	BOIL TEM LIQ	C K F	Boiling point temperature of liquid chemical	
1004	DENS LIQ AMB	G/CM3 KG/M3 LB/FT3	Density of liquid chemical at ambient temperature	Computed automatically at temperature 2004 TEMP start.
1006	VISCOSITY-AM	DS/CM2 NS/M2 CP	Viscosity of liquid chemical at ambient temperature	Same as above.
1008	SURF TENSION	D/CM N/M LB/FT	Surface tension of liquid chemical	
1021	LIQ DENS BP	G/CM3 KG/M3 LB/FT3	Density of liquid chemical at its boiling point	
1025	CRIT TEMP	C K F	Critical temperature of chemical	
1026	SOLUBILITY	G/HG	Solubility of chemical in water at a fixed temperature	Will be used only if data for 1028 and 1029 are unavailable.
1028	SOL EQ COEF1	G/HG	First coefficient of a solubility equation in the form of the one in Section 2.4.3	Answer from solubility equation should be in units of grams per 100 grams. Equation used at 2023 WATER TEMP.
1029	SOL EQ COEF2	G/HGC	Second coefficient of a solubility equation in the form of the one in Section 2.4.3	
1031	INTRFACE TEN	D/CM N/M LB/FT	Interfacial tension between the liquid chemical and water	

*The pool spreading model requires data for field numbers 1004, 1006 and 1031. Rest of data is used by pool dissolution and dispersion model.

TABLE T3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
OUTPUT FOR POOL SPREADING PART OF MODEL T:				
4025	POOL SZ HBTL	CM M FT MI	Size of the pool at the user specified time. If the pool is confined by channel banks, it is the length of the channel covered. If the pool is not confined, it is the radius of the pool.	HACS always assumes that the spill pool is circular in the continuous spill case.
4007	DIAM FLAME	CM M FT MI	Size of spill pool to be used by Model U. If pool is circular, it is the diameter of the pool. If the pool is confined by channel banks, it is the diameter of a circular pool of equivalent area.	
OUTPUT FOR POOL DISSOLUTION AND DISPERSION PART OF MODEL T:				
4061	DISOLVE RATE	G/CM2S KG/M2S LB/FT2S	Rate at which pool dissolves into water	
4062	DISOLVE TIME	S MIN HR	Elapsed time it takes for all of the pool to dissolve	
4063	POOL CENT X	CM M FT MI	Distance downstream the center of the pool has travelled at user specified time	
4064	CONC AT XYZ	G/CM3 KG/M3 LB/FT3	Concentration of the chemical in water at the user specified time and location.	

TABLE T4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3009	PLOT FLAG T	ND (Integer)	Flag indicating which plots, if any, are desired*	0 = plots are not desired 1 = plot pool size vs. time 2 = plot concentration vs time at user specified point 3 = plot both above plots
3017	TABLE FLAG T	ND (Integer)	Flag indicating which tables, if any, are desired* * The user should not ask for a plot or table from a part of the model he has not specified to be executed. See 2086 MODEL TYPE-T ** Concentrations are given at center of river at mid-depth and bottom	0 = tables are not desired 1 = table of pool size vs time 2 = table of peak concentrations at middle and bottom of river** 3 = table of concentration vs time at user specified point 4 = tables described for 2 and 3 above 5 = all tables described above
2055	TIM LIQ SPR	S MIN HR	Maximum time range for various tables and plots	Required only if plots or tables are desired

MODEL U

Model U is the pool fire hazard assessment model for the types of substances addressed by Model T. It simply calls Model E the primary pool fire hazard assessment model in HACS. The user must refer to Model E for further information required to execute this model. (The size of the pool, for data field number 4007, is calculated by Model T.)

MODEL V

Purpose

Model V is used for volatile chemicals which are insoluble in water, have a boiling point greater than the ambient temperature (but less than 100 degrees Centigrade), and which are lighter-than-water (i.e., a chemical which forms a slowly evaporating, floating pool when spilled on water). The model computes a variety of data which characterize the size of the spill pool, the rate it is evaporating, the time it will take for all the chemical to vaporize, etc.

Relationship to Model T

A number of chemicals have hazard assessment (estimation route) codes which contain both the letter T and the letter V. It is to be noted that both these models have somewhat similar functions in that they both calculate the pool radius for the spill at a specified time. However, the answers which each give are slightly different. Model V, in virtually all cases, will calculate a pool size which is somewhat smaller than the pool size calculated by Model T. This occurs as a consequence of the fact that Model V can account for evaporation from the pool while Model T cannot. It is because of the uncertainties present in both models that it is not only Model V which is provided. To be somewhat conservative, it was decided that Model T should be utilized to calculate the pool size when the thermal radiation and flame size hazards are estimated and Model V utilized when the vapor dispersion hazards are evaluated. Larger pool sizes result in greater flammability hazards; smaller ones in greater vapor dispersion hazards. Thus, acceptable subsets of the code ATUVW consist of the codes ATU and AVW.

Restrictions and Cautions on Model Use

Model V works only for instantaneous releases of chemicals on water.

The model returns values of the temperature of the liquid remaining which often will appear to be unreasonably low. This is an unfortunate consequence of the manner in which the model is presently formulated and cannot be helped until a better model, if ever, becomes available.

Model V contains a numerical integration of coupled, non-linear differential equations. It has been noted that if the user should by some chance input an "elapsed time after discharge that conditions are to be calculated for", which is almost exactly the elapsed time within which all the chemical will evaporate, the model will calculate an answer which is somewhat higher than it should be for both the temperature of the liquid remaining and the total evaporation rate.

The density of a liquid chemical changes with temperature; the higher the temperature, the lighter it becomes, and vice versa. If HACS should determine that the density of the liquid at the temperature of release is greater than that of water, it will print out a message that the chemical may or may not float and then assume that the density of the chemical is slightly less than water. In such situations, the user must realize that the chemical may not actually float on the surface of the water, but may be suspended at some point beneath the surface. The answers obtained from Model V in such a situation will be invalid. To be also noted is that an evaporating pool of chemical cools down considerably as it evaporates. If it should cool down to a temperature where its density becomes greater than that of water, it may sink and then rise some time later when it has sufficiently warmed up.

Important Assumptions of the Model

Model V assumes that the spill takes place instantaneously onto calm water.

The model assumes that the chemical is completely insoluble in water, that none of the spill amount is depleted due to dissolution in water.

It is assumed that the density of the spilled chemical is less than that of water at all times after the spill takes place.

Input Data Considerations

There are no unusual input data required for execution of Model V.

Output of the Model

Input for Model V includes a time at which the user desires to know the condition of the chemical pool. If this time is less than the time in which it takes all the pool to evaporate, the model gives answers for the user specified time. If the user specified time is greater than the time it takes for all of the chemical to vaporize, the model returns answers for the spill pool at the time at which it disappears. The user can determine the time at which answers are given by inspecting the output 4030 EVP TIM HVPL. This value will be the lesser of his input time or the time it takes all of the pool to evaporate.

Output of the model for the time it computes conditions includes an indication of whether or not the pool has been confined by channel banks and the size of the pool. If the pool has been confined, the size given is the length of the channel which has been covered by the chemical. If the pool has not been confined, the size given is the radius of the pool.

Other answers which Model V computes are the volume of the spilled chemical remaining, the temperature of the chemical, the area the spill pool covers, and the evaporation rate of the chemical. In case Model W follows, it computes the overall average rate at which the pool has evaporated up to the specified time, and estimates whether the vapor release should be considered to have been instantaneous or continuous.

Another aspect which needs to be discussed concerns the capability of the model to decide whether conditions are such that flammable vapors might form over the spill area. As presently written, this model calculates the vapor pressure of the spilled chemical at the highest temperature which the chemical might attain, goes on to compute the highest possible concentration in air of the vapor which might occur, and then compares this value with the lower flammable limit of the material. If the concentration is less than this limit, the lower flammable limit is noted as being set to zero before HACS proceeds to a vapor dispersion model.

Optional output for Model V consists of a table and five plots. The table gives the size, temperature, evaporation rate, and area the pool covers as a function of time. Each of four plots gives these four data arrays in graphical form. The fifth plot is of volume of liquid remaining versus time.

Data Specification

Table V1 defines the on-scene and operational data which the model requires.

Table V2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table V3 defines the output of the model. The user may override any computed output data with his own values.

Table V4 defines the data necessary for production of the optional table and plots.

TABLE V1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2004	TEMP START	C K F	Temperature of chemical before it discharges	
2020	CHAN L WIDTH	CM M FT MI	Width of channel or river into which spill occurs	
2023	WATER TEMP	C K F	Temperature of water body into which spill occurs	
2054	AIR TEMP	C K F	Temperature of air in area in which spill occurs	
2057	TIM SPL COND	S MIN HR	Elapsed time from spill at which pool conditions are desired	
4002	TOT MASS LIQ	G KG LB TN	Total weight of liquid which spills. Will be computed by Model A	Not required if 4003 TOT VOL LIQ is given
4003	TOT VOL LIQ	CM3 M3 FT3 GALS	Total volume of liquid which spills. Will be computed by Model A	Not required if 4002 TOT MASS LIQ is given
2053	DIF COEF V-A	CM2/S M2/S FT2/S	Diffusion coefficient of the chemical vapor in air	HACS will estimate a value and use it if the user does not provide one

TABLE V2: CHEMICAL PROPERTY DATA UTILIZED

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	
1004	DENS LIQ AMB	G/CM3 KG/M3 LB/FT3	Density of liquid chemical at ambient temperature	Computed automatically at temperature 2004 TEMP START.
1006	VISCOSITY-AM	DS/CM2 NS/M2 CP	Viscosity of liquid chemical at ambient temperature	Same as above.
1007	HT CAP LQ-AM	CL/GC J/KGK BT/LBF	Heat capacity of the liquid chemical at ambient temperature	Same as above.
1010	VPE COEFF A	LOG FCN	Coefficients of a vapor pressure equation in the form of the one in Section 2.4.3 but which gives an answer in mm Hg.	
1011	VPE COEFF B	C		
1012	VPE COEFF C	C		
1014	HEAT OF VPR	CL/G J/KG BT/LB	Heat of vaporization of chemical	
1021	LIQ DENS BP	G/CM3 KG/M3 LB/FT3	Density of the liquid chemical at its boiling point	
1031	INTRFACE TEN	D/CM N/M LB/FT	Interfacial tension between the liquid chemical and water	
2033	LOW FLAM LIM	PERCENT	Lower flammability limit of chemical vapor in air (LFL or LEL)	

TABLE V3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2018	DIM FLAG	ND (Integer)	Flag indicating whether pool is confined by channel banks and is rectangular, or is not confined and is circular.	1 = rectangular (confined) 2 = circular (not confined)
4026	VOL REM HVPL	CM3 M3 FT3 GALS	Volume of liquid chemical not yet evaporated at time 4030 EVP TIM HVPL	
4027	SPL SZE HVPL	CM M FT MI	Size of pool at time 4030 EVP TIM HVPL. If the pool is confined by channel banks, it is the length of channel covered. If the pool is not confined, it is the radius of the pool.	
4028	TEMP HVPL	C K F	Temperature of liquid chemical at time 4030 EVP TIME HVPL	
4029	EVAP RT HVPL	G/CM2S KG/M2S LB/FT2S	Evaporation rate of chemical at time 4030 EVP TIME HVPL	
4030	EVP TIM HVPL	S MIN HR	Time for all liquid to evaporate or specified elapsed time, whichever is smaller.	
4031	AREA HVPL	CM2 M2 FT2	Area covered by pool at time 4030 EVP TIM HVPL	
4068	AVG GAS TEMP	C K F	Average temperature of vapors evolved.	

TABLE V3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS (cont.)

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
DATA ESTIMATED IN CASE MODEL W FOLLOWS:				
2033	LOW FLAM LIM	PERCENT	Lower flammability limit of chemical vapor in air.	Will be set to zero if HACS decides that pool cannot generate flammable vapors.
2061	SPILL TYPE C	ND (Integer)	Flag indicating whether vapor evolution is estimated to be instantaneous or continuous.	0 = instantaneous 1 = continuous
4044	AVG VAP RATE	G/S KG/S LB/S TN/HR	Average rate of vapor evolution up to time 4030 EVP TIM HVPL	
4045	EVOLVE TIME	S MIN HR	Same answer as 4030 EVP TIM HVPL. It is the time over which vapors are generated.	

TABLE V4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3010	PLOT FLAG V	ND (Integer)	Flag indicating whether plots are desired. See model description for what plots are available.	0 = plots not desired 1 = plots are desired
3014	TABLE FLAG V	ND (Integer)	Flag indicating whether table is desired. See model description for description of table.	0 = table not desired 1 = table is desired

MODEL W

Model W is the vapor dispersion model for chemicals of the type addressed by Model V.

If the vapor release is estimated as best being represented as an instantaneous one, it determines the amount of vapor which has evolved from the pool during the elapsed time span defined by 4030 EVP TIM HVPL (Model V output) and stores this value for use by Model C, the primary vapor dispersion model in HACS. It then transfers the pool size computed by Model V to the correct field number for use by Model C, and calls Model C.

If the vapor release is estimated as best being represented as a continuous one, Model W only transfers the pool size before calling Model C.

For the continous vapor release case, the user must take into consideration that the vapor source will be moving downstream. Answers derived from Model C will not necessarily pertain only to the spill site.

The input data specifications for execution of Model W itself are presented in Table W1. The user must refer to Model C for further information required to execute this model.

TABLE W1: INPUT/OUTPUT DATA SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
INPUT:				
2061	SPILL TYPE C	ND (Integer)	Flag indicating whether vapor evolution is estimated to be instantaneous or continuous	Estimated by Model V
2004	TEMP START	C K F	Temperature of liquid before discharge	
1004*	DENS LIQ AMB	G/CM3 KG/M3 LB/FT3	Density of liquid chemical at ambient temperature 2004 TEMP START	Computed automatically from data on property file tape
4026*	VOL REM HVPL	CM3 M3 FT3 GALS	Volume of liquid not yet evaporated at time 4030 EVP TIM HVPL	Computed by Model V
4003*	TOT VOL LIQ	CM3 M3 FT3 GALS	Total volume of liquid spilled	Computed by Model A
4027	SPL SZE HVPL	CM M FT MI	Size of spill pool	Computed by Model V
			* Required only if vapor evolution is estimated to be instantaneous	
OUTPUT:				
4001	TOT MASS GAS	G KG LB TN	Total weight of vapor which enters the atmosphere up to time 4030 EVP TIM HVPL	Stored as SYSTEM value
2019	DIM SPILL	CM M FT MI	Size of the spill pool. Same value as input for 4027 SPL SZE HVPL	Stored as SYSTEM value. Can be overridden by use of field number 4027.

*** THE USER MUST ALSO PROVIDE
INPUT DATA FOR EXECUTION OF MODEL C ***

MODEL X

Purpose

Model X is primarily intended for use for chemicals which are insoluble or slightly soluble in water, which have a boiling point greater than the ambient temperature, and which are heavier-than-water. Parts of it can also be used for otherwise similar chemicals which have a boiling point less than the ambient temperature when such chemicals are released at a depth in water which precludes their boiling because of hydrostatic pressure effects.

The model computes a variety of parameters which describe how the chemical sinks, how it spreads and then dissolves on the bottom on the water body, and how the chemical which dissolves disperses in water.

Restrictions and Cautions on Model Use

Model X only works for spills into or onto water.

The dispersion equations in the model were developed for releases into a river which is not effected by tidal action. They are not appropriate for use for spills into still waters or estuaries.

Model A should not precede the execution of Model X if the release takes place underwater. Model A only works when the hole from which the chemical is being discharged is at or above the surface level of the water.

The density of a liquid chemical changes with temperature; the higher the temperature, the lighter it becomes, and vice versa. If HACS should determine that the density of the liquid at the temperature of release is less than that of water, it will print out a message that the chemical may or may not sink and then assume that the density of the chemical is slightly greater than that of water. In such situations, the user must realize that the chemical may not actually sink to the bottom of the water body, but may be suspended at some point beneath the surface. The answers obtained from Model X in such a situation will be invalid.

Important Assumptions of the Model

Model X assumes that the spill occurs instantaneously.

The model assumes that the spill occurs in a non-tidal river.

It is assumed that the spill occurs in the center of the river.

Input Data Considerations

An important input to the model when it is used for a dispersion problem is the Manning Roughness Factor. This number describes to the model the nature of the water body into which the chemical has spilled. To aid the user in choosing a proper value, a table was presented in the description of Model P.

Output of the Model

For a spill from a given depth in water, Model X computes the time it takes the chemical to reach the bottom of the water body, the distance downstream the chemical travels before reaching the bottom, the area of the bottom which will be covered by the chemical, the length of the pool on the bottom, the time it will take for the pool to reach its maximum size, the average rate at which the chemical will dissolve into the water, and the time it will take for all the chemical to dissolve. At a user specified time and location, the model also gives the concentration of the chemical in water and the time it will take after the spill at which all of the pollutant will have passed the downstream point specified (called the CLEAR TIME).

Optional output for the model consists of two tables of the concentration of the chemical in water and the clear time as a function of downstream distance from the spill site. One table is for the maximum concentration at the surface of the water. The other is for the maximum concentration at the bottom of the water body.

Data Specification

Table X1 defines the on-scene and operational data which the model requires.

Table X2 contains a list of the chemical property data which HACS will automatically obtain from the Chemical Properties File.

Table X3 defines the output of the model.

Table X4 defines the data necessary for production of the optional table.

TABLE X1: ON-SCENE AND OPERATIONAL DATA

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
2021	SPILL DEPTH	CM M	Depth is water at which release occurs (measured from surface, down is positive direction)	
2023	WATER TEMP	C K F	Temperature of water body into which chemical spills	
2039	CONC PT X	CM M FT MI	Downstream distance from spill site	These 3 coordinates define point at which concentration of the chemical in water is desired.
2040	CONC PT Y		Cross-stream position(measured from center of river)	
2041	CONC PT Z		Depth (measured from surface, down is positive direction)	
2044	RIVER DEPTH	CM M FT MI	Mean depth of water body	
2045	RIVER WIDTH	CM M FT MI	Mean width of water body	
2047	STREAM VEL	CM/S M/S MPH KNOTS	Mean current velocity of water body	
2052	MANNING FACT	ND	Manning Roughness Factor for river. See description of Model P for table	
4002	TOT MASS LIQ	G KG LB TN	Total weight of chemical which enters water	
2043	DIF COEF H2O	CM2/S M2/S FT2/S	Diffusion coefficient of the chemical in water	HACS will estimate a value and use it if user does not provide one
2004	TEMP START	C K F	Temperature of liquid discharged.	

1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM	Molecular weight of chemical	
1003	BOIL TEM LIQ	C K F LB/FT3	Boiling point temperature of the chemical	
1004	DENS LIQ AMB	G/CM3 KG/M3	Density of liquid chemical at ambient temperature 200% TEMP START	Computed automatically.
1021	LIQ DENS BP	G/CM3 KG/M3 LB/FT3	Density of liquid chemical at its boiling point	
1025	CRIT TEMP	C K F	Critical temperature of chemical	
1026	SOLUBILITY	G/HG	Solubility of chemical in water at fixed temperature	Will be used only if data for *1028 and 1029 are unavailable*
1028	SOL EQ COEF1	G/HG	First coefficient of a solubility equation in the form of the one in Section 2.4.3	
1029	SOL EQ COEF2	G/HGC	Second coefficient of a solubility equation in the form of the one in Section 2.4.3	Answer of solubility equation should be in units of grams per 100 grams. Equation used at 2023 WATER TEMP.
1031	INTRFACE TEN	D/CM N/M LB/FT	Interfacial tension between the liquid chemical and water	

TABLE X3: OUTPUT DATA DEFINITIONS AND SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
4032	SINK TIME	S MIN HR	Time it takes chemical to sink to bottom of water body	
4033	DIST TRAV	CM M FT MI	Distance the chemical will travel downstream from the spill site before reaching the bottom of the water body	
4036	DISOLVE RATE	G/S KG/S LB/S TN/HR	Rate at which pool on bottom dissolves	
4037	DISOLVE TIME	S MIN HR	Time it takes for all of pool to dissolve	
4038	POOL AREA	CM2 M2 FT2	Maximum bottom area which chemical will cover	
4039	POOL LENGTH	CM M FT MI	Maximum length which pool on bottom will reach	
4040	SPRD TIME	S MIN HR	Time it takes pool to reach its maximum size	
4041	CLEAR TIME	S MIN HR	Time at which all pollutant will have passed by user specified point	
4042	CONC AT XYZ	G/CM3 KG/M3 LB/FT3	Concentration of the chemical in water at the user specified point	Answer will also print out in units of ppm and mg/liter

TABLE X4: OPTIONAL OUTPUT SPECIFICATIONS

FIELD NUMBERS	FIELD NAME	UNIT TYPES	DESCRIPTION	SPECIAL FEATURES
3012	TABLE FLAG X	ND (Integer)	Flag indicating whether tables are desired which give the peak concentration of the chemical in water at the water surface and at the bottom of the water body as a function of downstream distance and time from spill	0 = tables are not desired 1 = tables are desired
2031	MAX DISTANCE	CM M FT MI	Maximum distance range for tables	Required only if tables are desired

MODEL Y

Model Y does not exist. The flammability hazard of low vapor pressure substances which sink in water is limited under most circumstances if the substance is spilled into water.

MODEL Z

Model Z does not yet exist. The following message will be generated by HACS: "Model for self-reacting substances is not available."

MODEL II

Model II does not yet exist. The following message will be generated by HACS: "Model for insoluble solids is not available."

MODEL RR

Model RR does not exist as a separate model. The use of this path code in a hazard assessment code is meant only to indicate that the solid chemical somehow reacts with water. To accomplish a hazard assessment for such a chemical, it is necessary to determine what the products of the reaction are, especially for rapidly reacting materials, and to conduct hazard assessments for these products. To aid the user in this task, Table RR-1 is presented. The weight fraction of a product is to be interpreted as the amount of product which will form per unit amount of reacting solid spilled on water (e.g. one ton of aluminum chloride spilled on water results in 0.821 tons of hydrogen chloride and 0.584 tons of aluminum hydroxide after reaction is completed).

MODEL SS

Model SS does not exist as a separate model in HACS. If it is asked for, HACS will generate the message "Model for soluble solids is not available."

The user should realize that, once a soluble solid dissolves in water, the resulting solution behaves similarly to the solution resulting from a spill of soluble liquid into water. Hence, water pollution hazards for such spills can be determined by straightforward application of Model P.

MODEL ?

Unrecognizable model codes, i.e., any not specifically identified on the preceding pages will cause HACS to generate an error message, followed by immediate program termination.

TABLE RR.1†

SOLID CHEMICALS WHICH REACT WITH WATER

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Aluminum chloride	Aluminum hydroxide	(no code)	<.59	Reacts violently. Reaction is not stoichiometric
	Hydrochloric acid Hydrogen chloride	AP AC	<.82	
Antimony trichloride	Antimonous acid	(no code)	.76	Reacts vigorously
	Hydrochloric acid Hydrogen chloride	AP AC	.48	
Beryllium chloride	Beryllium oxide	II	.31	Reacts vigorously with heat evolution
	Hydrochloric acid Hydrogen chloride	AP AC	.91	
Calcium carbide	Acetylene	ABC	.40	Reacts vigorously. Acetylene may spontaneously ignite.
	Calcium hydroxide	II	1.16	
Calcium, metallic	Calcium hydroxide	II	1.85	Reaction not violent. Hydrogen may ignite
	Hydrogen	ABC	.05	
Calcium oxide	Calcium hydroxide	II	1.32	Heat may ignite combustibles. Swells during reaction

TABLE RR.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Calcium peroxide	Calcium hydroxide	II	1.03	Reacts *very slowly*
	Oxygen	AI	.22	
Calcium phosphide	Calcium hydroxide	II	1.22	Reacts vigorously. Phosphine is a poisonous, spontaneously flammable gas.
	Phosphine	(no code)	.37	
Chloroacetophenone	Hydrochloric acid	AP	.24	Reacts *slowly.*
	Hydroxyacetophenone	(no code)	.88	
Decaborane	Boric acid	SS-II	5.05	Reacts *slowly.*
	Hydrogen	ABC	.36	
Lead tetraacetate	Acetic acid	APQ	.54	Reaction not violent.
	Lead dioxide	(no code)	.54	
Lithium aluminum hydride	Aluminum hydroxide	(no code)	2.06	Reacts violently.
	Hydrogen	ABC	.21	
	Lithium hydroxide	(no code)	.63	
Lithium hydride	Hydrogen	ABC	.25	Reacts violently. Ignition may occur.
	Lithium hydroxide	(no code)	3.01	

TABLE RR.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Lithium, metallic	Hydrogen	ABC	.29	Reacts violently. Ignition usually occurs.
	Lithium hydroxide	(no code)	3.45	
Maleic anhydride	Maleic acid	SS	1.18	Reaction with cold water slow. Hot water may cause frothing.
Paraformaldehyde	Formaldehyde	APQ	1.00	
Phosphorus, white	Phosphoric acid (in water)	AP	1.58	Ignites spontaneously in air.
Phosphorus pentasulfide	Hydrogen sulfide	ABC	.76	
	Phosphoric acid	AP	.88	
Potassium, metallic	Hydrogen	ABC	.026	Reacts violently.
	Caustic potash solution	AP	1.44	
Potassium peroxide	Oxygen	AI	.073	Reacts violently with heat evolution.
	Caustic potash solution	AP	1.02	
Selenium trioxide	Selenic acid	(no code)	1.14	Reacts vigorously.
Sodium	Hydrogen	ABC	.043	Reacts violently. Fire often occurs.
	Caustic potash solution	AP	1.74	

TABLE RR.1† (Continued)

Reactant Compound	Products	Pertinent Code	Weight Fraction of Spill	Remarks
Sodium amide	Ammonia	ABC	.36	Reacts violently. Frequently bursts into flames.
	Caustic soda solution	AP	1.03	
Sodium borohydride	Boric acid	SS-II	<1.63	Boric acid and sodium hydroxide may form sodium borate solution.
	Hydrogen	ABC	.21	
	Caustic soda solution	AP	<1.06	
Sodium hydride	Hydrogen	ABC	.08	Vigorous reaction. Hydrogen ignition is infrequent.
	Caustic soda solution	AP	1.66	

†Notes for Table RR.1

1) The *pertinent* hazard assessment codes of this table were especially chosen to best reflect the hazards from the products of reaction. They may or may not be the same as those found for these chemicals in CG-446-2.

2) The products of reaction for aluminum chloride, antimony trichloride, and beryllium chloride include both hydrochloric acid and hydrogen chloride. Since it cannot be estimated how much hydrogen chloride vapor or acid mist will enter the atmosphere, or how much will mix with the water, a single "weight fraction of spill" has been given which shows the total of the two possible products. The user must decide how to apportion the weight fraction between the two products. As a general guideline, it can only be said that the slower the reaction is, the more that will mix with water, and vice versa.

3) The products of reaction and their weight fractions were estimated by assuming that all of the reactant compound reacts with water before it itself poses a hazard to the environment. When the reaction is slow, however, this assumption may not be true. Depending upon the circumstances, for slow-reacting substances, the user may wish to assume that some portion of the initially spilled chemical does not react and to utilize the hazard assessment code for the unreacted chemical also to determine hazards.

4) The hazard assessment code "B" should not be utilized for a product of reaction unless the reaction takes place *within* a punctured tank or other container.

5) "No code" indicates that the chemical is not contained in CHRIS. It should not be interpreted as signifying that the substance is non-hazardous.

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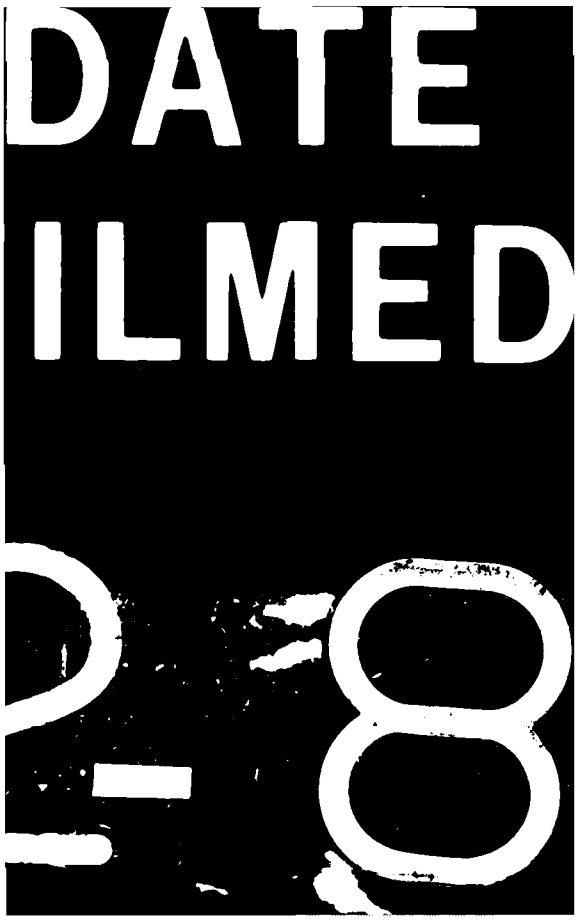
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