**Final Report of the Accident
Phenomenology and Consequence
(APAC) Methodology Evaluation**

Spills Working Group

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Glossary

Accident	An unplanned event or sequence of events that results in safety consequences or impacts.
Aerosol	A solid or liquid particle existing as a dispersed phase in the atmospheric medium.
Accident Analysis	A process to systematically identify the hazards at a facility, to describe and analyze the adequacy of measures taken to eliminate, control, and mitigate identified hazards, and to analyze and evaluate potential accidents and their associated impacts to people, equipment, structures, and the environment.
Airborne Release Fraction	The fraction of material affected by an accident stress that can be suspended into the air and become available for airborne transport.
Adiabatic	No heat exchange occurs across the system boundaries; all energy comes from within the system.
Ambient	Surrounding. Ambient temperature is the temperature of the surrounding air.
Boiling Point	The temperature at which the equilibrium vapor pressure of a material equals the surrounding ambient pressure. The normal boiling point is the temperature at which the equilibrium vapor pressure is equal to 1 atm.
Choked Flow	Flow at the sonic velocity; the maximum flow, which is pressure independent.
Dense Gas	Gas or vapor emission that exhibits a density significantly greater than that of the surrounding ambient air at existing temperature conditions (also called heavy gas).
Dike	A barrier such as a low wall or embankment designed to prevent a spill from spreading or flooding.
Entrainment	The mixing of a gas/vapor cloud, plume or jet, liquid aerosol, or solid particulate with the surrounding air, due to such physical phenomena as advection (spatial variation in temperature of a medium through which a

	parcel of vapor is moving), momentum exchange induced by shear flow, molecular transport across a flow boundary, or turbulent mixing.
Free-fall Spill	An elevated release of powder or liquid as a slug of material that falls without obstruction and impacts a hard, essentially unyielding surface.
Flashing	A process whereby a portion (in some cases all) of a liquid suddenly vaporizes. A liquid that experiences a sudden change in pressure such that it's temperature is above the boiling point at the new pressure conditions will undergo a phase change to gas.
Hazardous Material	Any substance or material in a quantity or form that might be harmful to humans or the environment. Hazardous materials include: explosives, gases (compressed, liquefied, or dissolved), flammable and combustible liquids, flammable substances, oxidizing substances, toxic and infectious substances, radioactive materials, and corrosives.
Hazards Analysis	The procedure for identifying potential sources of hazardous material release and determining the vulnerability of an area to a hazardous material release.
Insolation	Energy transfer into a system as a result of exposure to solar energy.
Neutrally Buoyant Gas	Gas or vapor releases that exhibit essentially the same material density as air and therefore behave as a passive tracer that follows the same bulk movements and behavior as the surrounding ambient air.
Positively Buoyant Gas	Gas or vapor releases that exhibit a density significantly less than that of the surrounding air at existing temperature conditions.
Resuspension	Re-entrainment of solid particulate into the wind field, making the material available for downwind dispersion.
Sonic Flow	Flow at the sonic velocity. Below the sonic velocity, the velocity of flow is a function of the pressure differential. At the sonic velocity, further pressure reductions cannot be transmitted upstream. Hence, flow velocity cannot exceed the sonic velocity.

Sonic Velocity	The speed at which pressure waves are transmitted in a given medium
Source Term	The amount and characteristics of hazardous material emitted to the air at the location of an unplanned occurrence.
Sublimation	The process by which a solid changes to a vapor without passing through the liquid phase.
Vapor Pressure	The equilibrium pressure of the pure component vapor over the pure component liquid.

Acronyms

ADAM	Air Force Dispersion Assessment Model
ALOHA	Areal Locations of Hazardous Atmospheres
APAC	Accident Phenomenology and Consequence
ARF	Airborne Release Fraction
BIO	Basis for Interim Operation
CASRAM-SC	Chemical Accident Stochastic Risk Assessment Model - Single Case
CCPS	Center for Chemical Process Safety
DOE	Department of Energy
EFCOG	Energy Facilities Contractors Group
EMGRES	Emergency Response
EPA	Environmental Protection Agency
HGSystem	Heavy Gas System
HOTSPOT	Hot Simulations Portable Model
ID	Inside Diameter
JCO	Justification for Continued Operation
KBERT	Knowledge-Based System for Estimating Hazards of Radioactive Material Release Transients
MISM	Modified Ille Springer Model
NOAA	National Oceanic and Atmospheric Administration
RF	Respirable Fraction
RH	Relative Humidity
SAR	Safety Analysis Report
SCAPA	Subcommittee on Consequence Assessment and Protective Actions
TScreen	Toxic Screen
TSR	Technical Safety Requirement
VOC	Volatile organic compound

1. Executive Summary

The Spills Working Group was one of six working groups established under the Accident Phenomenology and Consequence (APAC) methodology evaluation program. The objectives of APAC were to assess methodologies available in the accident phenomenology and consequence analysis area and to evaluate their adequacy for use in preparing DOE facility safety basis documentation, such as Basis for Interim Operation (BIO), Justification for Continued Operation (JCO), Hazard Analysis Documents, and Safety Analysis Reports (SARs). Additional objectives of APAC were to identify development needs and to define standard practices to be followed in the analyses supporting facility safety basis documentation. The Spills Working Group focused on methodologies for estimating four types of spill source terms: liquid chemical spills and evaporation, pressurized liquid/gas releases, solid spills and resuspension/sublimation, and resuspension of particulate matter from liquid spills.

The APAC activity began in late 1994. By December 1994, the membership of the Spills Working Group had been established. The working group consisted of six members with broad experience in safety analysis, chemical accident emergency planning and response, risk assessment, source term model development, air pollution meteorology, chemical engineering, and mathematics. The bulk of the work was carried out during 1995. Working group members performed the work at their home sites, and communicated regularly through email and telephone. The group met three times: in January, in May, and in August of 1995. An initial draft report was issued in December 1995. After an initial review and comment period, a second draft of the Spills Working Group report was issued in September of 1996. A second review and comment period was held from the fall of 1996 through the early summer of 1997. Revisions were made, resulting in this final report documenting the work and findings of the Spills Working Group.

The Spills Working Group first reviewed regulatory documents, standards, and guidance documents to identify requirements that the methodologies must meet. These requirements, supplemented by the knowledge of the materials and types of events that might occur at DOE facilities, led to a set of review criteria for model evaluation. A set of publicly available computer models with capabilities for quantifying release rates or released amounts from spills of chemical or radiological materials was identified. Additionally, a set of sample test problems was established to evaluate the general applicability and suitability of a specific model to some common or probable accident release scenarios.

The working group initially compiled a list of 24 computer codes. Initial screening reduced the set to 11 codes, which were then evaluated.

Code reviews allowed the working group to identify those models with appropriate and/or unique capabilities important for DOE safety analysis applications. After reviewing the code evaluations and the results of the test problem exercise, the working group agreed on a set of recommended computer codes. These models included:

- (1) ADAM, ALOHA, TScreen, CASRAM-SC, and HGSystem for liquid chemical spills and evaporation;
- (2) ALOHA, TScreen, CASRAM-SC, and HGSystem for pressurized liquid/gas releases;
- (3) KBERT (an expert user interface accessing the data in HDBK-3010-94 (DOE, 1994a)) and HOTSPOT for solid spills and resuspension; and
- (4) HOTSPOT for resuspension of dissolved/suspended material from liquid spills.

CASRAM-SC and HGSystem are more sophisticated codes, and may be more useful for evaluating source terms for higher hazard facilities. KBERT was conditionally recommended as it is still under development and was not fully evaluated as part of this activity. It was included here because of its unique capabilities and the widespread use of DOE-HDBK-3010-94 (DOE, 1994a), on which it is based.

The test problem exercise was performed with the purpose of testing the capabilities of the codes. Some previously established problems applying to liquid chemical spills and evaporation and pressurized liquid/gas releases were adopted for the exercise. The code results for a given problem varied by up to an order of magnitude. This was primarily attributed to the differences in how the models treated the physics and thermodynamics of the problems.

In general, the working group felt that hand calculations are acceptable, but they typically may only be practical for simple problems. When analysis requires the use of formulations that can readily be done by hand, this approach is recommended. Hand calculations may be particularly useful for problems like resuspension, where only a limited number of codes are available. Additionally, DOE (1994a) was identified as an excellent source of information for estimating source terms by hand.

Several areas for follow on work and source term model development needs were also identified. These would be helpful in implementing the objectives of APAC, and are summarized below. More details are provided in Section 7.2.

Suggestions for Follow-on Work:

- (1) It would be valuable to expand and conduct a more thorough search of models available, first in the U.S., and then internationally. This wider search for state-of-the-science models could include private sector codes if

certain conditions are met pertaining to documentation and ultimately to licensing fees.

- (2) A performance evaluation of evaporating pool models against as complete a data set as possible should be conducted. A search for spill and evaporation experimental data for comparison with predictions would be valuable. A comparison against measured data would provide insight on model performance.
- (3) A more thorough review of the codes, including understanding why the sample problem results were different, would be beneficial. The review could include a sensitivity/uncertainty analysis.
- (4) Some effort should be directed towards providing better guidance on selection of spill pool depth. The 1 cm depth commonly used appears to be arbitrary.

Recommended Areas for Model Improvement:

- (1) Improved modeling is needed to handle flash fraction formation properly.
- (2) Improvements in aerosol generation and entrainment modeling would be beneficial.
- (3) A good model does not currently exist for liquid pool evaporation inside a facility (still air or near still air model).
- (4) The capability to model water reactives would be valuable.
- (5) Spills involving multi-components or chemical mixtures cannot currently be properly modeled. Consideration should also be given to potential chemical reactions that may occur subsequent to a spill.
- (6) A code should be developed to specifically model solid sublimation.
- (7) A better understanding of the resuspension process during the evaporation phase of a spilled liquid containing dissolved/suspended solid material would be beneficial.
- (8) Any final validation of KBERT should be completed so that the code can further reviewed.

The Spills Working Group identified a set of good engineering or good safety analysis practices for use in preparation of safety analysis documentation. A summary of these recommendations follows.

- (1) Chemical Lists: The group recommends consulting the following lists for assistance in identifying chemicals of greatest concern for analysis:
 - EPA list (40CFR68)
 - OSHA list (29CFR1910.119)
 - DOE-EH list of unique chemicals in the DOE complex (provided in Appendix E)
 - Sample list of hazardous chemicals within the DOE complex (from DOE (1994b), see Appendix E).
- (2) Chemical Selection Criteria: If the analyst chooses to evaluate chemicals not on the lists noted above, EPA criteria noted below can be used as an additional basis for selection:
 - include chemicals with vapor pressure above 10 mm Hg (interpreted to be at 20 °C)
 - include chemicals in concentrations above 1 %wt.
- (3) Consult EPA Documents, where appropriate: An earlier methodology study that was performed for the EPA was identified (EPA, 1993). This reference was found to provide useful guidance for selecting parameter values.
- (4) Release Diameter/Area: Some specific guidance on estimating source release diameters or areas is provided. The details are given in Section 7.3.2.
- (5) Ground Surface Temperature. If ground surface temperature data are not available from routine on-site measurements, it is recommended that the ground surface temperature be set to the ambient temperature.
- (6) Dense Gas Effects. If a release can be considered denser than air, standard passive dispersion modeling does not apply. To determine if a release is denser than air, the Richardson number should be calculated. A formulation for the friction Richardson number is provided. If greater than ~1 - 10, dense gas effects are important (Spencer and Havens (1989), NOAA (1992)).
- (7) Consistency in Parameter Selection: The analyst should be consistent in making realistic selection of parameters for a given problem. Some specific guidance is provided in Section 7.3.2.
- (8) Caution for Cryogenic Releases: An instantaneous spill is not always the worst case. For example, when the boiling point of the material is significantly below ambient, an instantaneous release may result in freezing of the ground. This may change the ground thermal conductivity in such a fashion that the source term is not maximized.

2. Acknowledgments

The Spills Working Group would like to acknowledge and thank the sponsors, contributors, and reviewers of this work. The support and technical guidance of Dr. Dae Chung, U.S. Department of Energy (DOE/DP-45), the sponsor of this work, is very much appreciated. In addition, we would like to recognize Dr. Kevin O’Kula of Westinghouse Savannah River Company, and Dr. Louis Restrepo of Omicron Safety and Risk Technologies for their leadership as co-chairs of the overall APAC effort. We would also like to acknowledge the other members of the APAC Executive Committee for their valuable guidance and input, as well as their assistance in managing interface issues between working groups under the APAC activity.

3. Introduction

The Accident Phenomenology and Consequence (APAC) Methodology Evaluation Program was a Defense Programs activity aimed at providing guidance for improving the quality and consistency of the analysis approaches used for Safety Analysis Reports, Basis for Interim Operation, and Hazard Analysis documents. The objectives of this effort were to:

- establish current analysis needs and requirements reflected in the DOE Orders, Standards, and Guidance for safety analysis,
- evaluate the status, adequacy (detailing both strengths and limitations) of models and computer codes available in the accident phenomenology and consequence analysis area,
- identify any model development needs,
- provide recommendations and guidance to DOE on the selection and applicability of state-of-the-art models, and
- define key standard practices to be followed in the analyses supporting facility safety basis documentation.

The APAC activity was overseen by an Executive Committee, and the work was carried out by six working groups. The working groups reviewed methodologies in the following areas:

- source term development, from accidents involving fires, spills, and energetic events (e.g., explosions),
- in-facility transport, and
- ex-facility transport/consequences, for both chemical and radiological releases.

The APAC activity began in late 1994. By December 1994, the membership of the Spills Working Group had been established. The bulk of the Spills Working Group effort was carried out during 1995. Working group members performed the work at their home sites, and communicated regularly through email and telephone. The group met three times: in January, in May, and in August of 1995. An initial draft report was issued in December 1995. An initial review and comment period occurred during the first half of 1996. Comments were incorporated and a second draft of the Spills Working Group report was issued in September of 1996. A second review and comment period was held from the fall of 1996 through the early summer of 1997. Revisions were made, resulting in this final report documenting the work and findings of the Spills Working Group.

The Spills Working Group was comprised of six individuals representing various DOE sites. The membership was as follows:

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The overall process followed by the Spills Working Group effort is summarized in Figure 1. First, DOE regulatory documents, guidance documents, and standards were reviewed to identify requirements for spills methodologies. Although the requirements for spill event source terms were not specifically given, an attempt was made to interpret them as a specific basis for judging the capabilities of each code.

The identified requirements were developed into a set of criteria for code evaluation and comparison. This included a set of general criteria as well as a set of specific criteria, focusing on technical capabilities and limitations of each code. The criteria reflected the requirements as well as the nature of the materials and types of events that might be encountered across the DOE complex. The adequacy of each code was also evaluated in terms of DOE's graded approach philosophy.

Coincident with this, an initial set of codes to review was established. This was based on existing compilations (O'Kula, 1994; SCAPA, 1995; EFCOG, 1993), and knowledge about codes used for safety analysis at the various DOE sites. The survey was limited to codes in the public domain. This groundrule was established primarily because of the difficulty in obtaining the source code for proprietary models. In most cases, source code for proprietary models is not available for independent inspection, nor are the full details of the models utilized published and available for review by the public. The working group did recognize that some proprietary codes may offer modeling capabilities not available from the codes in the public domain. A future activity of the Spills Working Group may include a review of proprietary models.

The codes were evaluated by assessing them with respect to the various criteria. This included an evaluation of the availability, current status, and technical adequacy of the computer models. A set of sample problems were identified to test the code capabilities. Results of the sample problems were folded into the evaluations.

As the evaluations were performed, a set of recommended practices was collected. This included guidance on input parameter selection, computational assumptions and procedures, and cautionary notes. Final conclusions were drawn by comparing the evaluations and the results of the sample problem exercise. Key model development areas were also identified.

Figure 1: Overall Process followed by the Spills Working Group

3.1 Background

The missions within the DOE complex have required the use of a variety of hazardous chemicals, ranging from common acids, bases, oxidizing agents, solvents, and heavy metals, to specialty organics, explosives, hydrocarbon fuels, toxics, corrosives, and flammables. Although chemical hazards are a more recent concern, hazards associated with the use of radioactive solids, liquids, and gases continue to exist. The quantity of these substances used varies widely, ranging from small laboratory amounts to large volumes of hazardous chemicals needed for defense-related manufacturing or large-scale processing operations. In addition, most, if not all, of the DOE sites store and conduct some limited treatment and disposal of a variety of hazardous wastes.

Under a recent broad-based internal review to identify and characterize adverse conditions or circumstances involving potentially hazardous chemicals, the DOE uncovered a number of safety vulnerabilities within the DOE complex (DOE, 1994b). These vulnerabilities represent circumstances or conditions that could lead to chemical accidents. Such accidents could involve chemical releases and exposures to workers, the public, and the environment, and health and safety hazards to workers and the public from fires and explosions (e.g., from uncontrolled chemical reactions). The more significant hazards appear to be spills of chlorine, refrigerated ammonia, sulfuric acid, nitric acid, hydrochloric acid, sodium hydroxide, and many VOCs. Simple asphyxiants, which are not chemically toxic, but which, if present in sufficient quantity, can lead to an oxygen deficient atmosphere, are also of interest. These chemicals include nitrogen, carbon dioxide, argon, and sulfur hexafluoride. Solid materials of potential concern include beryllium and lithium hydride. Appendix E provides a sample list of hazardous chemicals within the DOE complex. In addition to chemical hazards, radioactive source terms resulting from spills of radioactive powders or solutions containing radioactive materials were of interest to the Spills Working Group.

A spectrum of possible spill-type releases can be envisioned. These may range from spills of fairly small quantities of materials in a laboratory environment, to leakage from drums in a waste storage facility, to failures associated with larger storage containers or failures of multiple containers/components. Thus, safety analysis methodologies for spill-type events must be capable of addressing this range of possible events. In particular, reasonable bounding estimates of accidental source terms from the different types of spills must be provided.

3.2 Objectives of this Study and Scope

- The objectives of the Spills Working Group activity included:
- assessment of existing public domain models for estimating spill source terms;
 - identification of the models with the best physics and thermodynamics, applicable for estimating spill source terms for DOE safety analysis documentation;
 - identification of a set of good engineering and good safety analysis practices, i.e. assumptions, parameter values, etc., for use when estimating spill source terms for hypothetical or credible worst-case scenarios;
 - identification of future development needs.

The scope of this work is limited to the evaluation of methodologies for estimating an initial source term. That is, this assessment does not include an evaluation of barrier integrity (i.e. it is assumed that any barrier has been breached), nor does it include an assessment of methodologies describing phenomena occurring after the material leaves the immediate location of the spill event. The concern addressed by this working group is the initial source as the material is emitted into the air during and/or after the spill, from the location of the spill. The behavior of the material during in-facility and/or ex-facility transport is beyond the group's scope of work.

Originally, the Spills Working Group's focus was on liquid spills and evaporation. However, it was recognized that limiting the scope to just liquid spills would ignore several other important classes of spill-type accidents. Thus, the Spills Working Group expanded its scope to look at four distinct areas:

- (1) liquid chemical spills and evaporation;
- (2) pressurized liquid/gas releases;
- (3) solid spills and resuspension/sublimation;
- (4) resuspension of dissolved/suspended solid material from spilled liquids.

Many safety analysis codes span more than one working group. For example, several codes estimate an initial source term and also estimate dispersion in the environment. In instances like this, the Spills Working Group only evaluated the source term component of the code. As an example, the initial characterization of liquid aerosol formation (e.g., droplet diameter, initial trajectory of flow) falls within the scope of the source term. Other facets of the vapor source term (e.g., aerosol evaporation rate, fraction of aerosol component that falls to the ground prior to complete evaporation) may more reasonably fall within the scope of dispersion. Communication between working groups provided assurance that other parts of the code would also be evaluated in the appropriate working group. In many cases, recommending a code would necessitate that all its parts are acceptable,

because intermediate information (e.g. source term) is not provided. For example, many codes that have a source term model linked to a dispersion model do not directly provide source term information. Rather, the source term information is directly fed into the dispersion model, with the final consequences being the only output.

It is recognized for spills occurring in the outdoor environment, the development of the source term, e.g. a release rate, depends on the same atmospheric/ambient conditions (e.g. wind speed and stability class), which also influence the transport and dispersion of the released material. Thus, in addition to code evaluations traversing the working group interface, ultimate recommendations on parameter values may result from the convolution of input from multiple working groups. The reader is referred in particular to the APAC Chemical Dispersion and Consequence Analysis Working Group Report (Lazaro et al., 1997) and the APAC Radiological Dispersion and Analysis Working Group Report (O'Kula et al., 1997) for a more thorough discussion of the dispersion aspect of consequence assessment.

3.3 Phenomenology

The process by which a spilled material becomes an airborne source term is dependent upon the initial form of the material spilled. Four types of spill events, based on material form, are the subject of this report. The purpose of this section is to provide some background on the phenomena involved in generating a spill source term and on the effects of the physical characteristics of the release and the chemical properties of materials involved.

3.3.1 Liquid Chemical Spills and Evaporation

The simplest case of a liquid chemical spill and evaporation results if the material spilled has relatively low volatility and the material is normally a liquid at ambient conditions. The spilled liquid will form a pool, and release to the atmosphere will result from evaporation. The pool formation may take place essentially instantaneously, such as in the case of a catastrophic failure. Or, if the failure is better characterized as a leak, the rate at which the material enters the pool depends on the size of the hole in the container, and the height of the liquid level above the hole. The pool size will grow until the evaporation rate from the pool matches the release rate from the failed container. During the spill process, there may be some aerosolization caused by shear, as the liquid falls to the ground, and by impact forces (splashing) as the liquid impacts the ground. This is generally small relative to the vapor generation for volatile materials. For materials that are

less volatile, however, this initial phase of the spill event may represent a significant fraction of the material made airborne within a given time period.

The evaporation rate from a liquid pool is influenced by several parameters, in particular, pool area, pool and ambient temperature, ambient atmospheric conditions, and properties of the spilled material, such as vapor pressure, molecular weight, and latent heat of vaporization. Chemicals with lower vapor pressures will evaporate more slowly than chemicals with higher vapor pressures, when all other conditions are the same. A larger pool surface area will result in a higher evaporation rate. Physical barriers, such as a berm, a trench, or terrain features, can restrict the size of an expanding pool, and thus, limit the evaporation rate. Pool temperature is influenced by the initial conditions of the material and heat transfer mechanisms into the pool. Heat transfer into the pool is important, as the spilled liquid will take energy from the surroundings to provide the latent heat of vaporization. Heat transfer into the pool can occur as a result of conduction from the ground, convection from the ambient air, or solar radiation (insolation). Direct insolation on the pool surface can be a significant source of energy. Any cloud cover will tend to attenuate the sunlight and reduce this heat transfer mechanism. The surface substrate onto which the spill has occurred, and the roughness of that surface, influence the ground-to-pool heat transfer rate. Another critical parameter is wind speed. The evaporation rate from a liquid pool increases with increasing wind speed. Some models also include the influence of stability class, with less stable atmospheres leading to increased evaporation.

A liquid phase release of a volatile material may result if the material's vapor pressure is such that it would be in the gas phase at ambient conditions, but is stored as a liquid through refrigeration to a temperature below its boiling point (i.e., subcooled liquid). Some flashing may occur as the material is released. "Flashing" results from the abrupt growth of vapor bubbles that form in an attempt to attain a new equilibrium state. The released liquid will form a pool and will evaporate as it absorbs energy from the surroundings and from the spill surface. Conduction from the spill surface is the initial and primary source of energy input to the pool. Parameters that influence the conductive heat transfer and thus the evaporation rate include ambient temperature, pool surface area, and the thermal conductivity and diffusivity of the soil or other surface medium. If the liquid temperature is above the normal boiling point, but below ambient, some flashing will occur upon release, with the remaining material forming a liquid pool. This type of release is usually mildly flashing, since it is common to maintain the release temperature just above the material's normal boiling point. The flash fraction is usually much less than that of a two-phase pressurized liquid release. This is because the refrigerated liquid is typically stored near ambient pressure, and the evolution of pressure head upon loss of refrigeration does not usually occur rapidly enough to result in substantial pressurization.

within the vessel. Thus, the release rate of gas is usually lower than for a significantly pressurized material. The liquid pool will initially vaporize quickly as it absorbs energy from the surroundings and the spill surface. As evaporation continues, the pool will cool slightly (to its normal boiling point), and the rate of vapor generation will decrease.

3.3.2 Pressurized Liquid/Gas Releases

Under pressurized conditions, a more energetic release may occur. Pressurized liquids and vapors used or stored near their saturation temperatures may, upon release to ambient, "flash" to a liquid-vapor mixture. As the discharge stream experiences a sudden pressure decrease following release from storage, some of the liquid will flash immediately to vapor, whereas the remaining liquid will either be suspended as a finely distributed aerosol or fall to the ground forming a pool. Two-phase releases typically represent one of the most complex source emission phenomena. These sorts of releases may necessitate a treatment of the interphase heat, mass and momentum transfer rates accompanying changes in temperature or other conditions.

In the case of a compressed gas, a two-phase release occurs as a result of the reduction in pressure upon release and the cooling of the gas as it expands. The resulting adiabatic expansion subcools some or all of the material (cools the material to a temperature below its boiling point at ambient pressure). The liquid may "rain-out" from the vapor/liquid release and form a liquid pool, which will then evaporate. The condensed liquid may also form an aerosol in the jet emission from the source. The aerosol is a suspension of small liquid droplets within a gas, or a finely dispersed mist. The formation of a liquid pool, aerosol, or combination of both of these is dependent upon the material and its release characteristics.

During a pressurized release, choked flow may result. This occurs if the pressure differential is sufficiently high that sonic flow occurs (discharge rate can be no greater than the sonic velocity). At internal pressures above the choked flow threshold, the volumetric release rate becomes independent of internal pressure.

A two-phase release may also result from material that is a vapor at ambient conditions, but maintained in the liquid phase via pressure in the containment vessel. When containment fails, the liquid pressure immediately drops to ambient pressure, resulting in sudden vaporization of some or all of the liquid. This phenomenon is known as adiabatic flash. The flash fraction defines the fraction of liquid which flashes to vapor, and the extent of flashing depends upon the storage temperature and physical properties of the material (e.g., normal boiling point and heat of

vaporization). The liquid portion of the release may form an aerosol, a short-lived liquid pool, or both. The tendency for aerosol formation is greater when the material is stored under pressure than when the material is refrigerated since the release energy tends to be relatively high for pressurized releases.

An overview of the fundamentals of two-phase jet releases is provided in Fthenakis (1993). Two-phase flow models are described in more detail in the American Institute of Chemical Engineer's Design Institute for Emergency Relief Systems (DIERS/AIChE, 1992). Leung (1996) provides a simplified method for characterizing flashing and non-flashing two-phase flow assuming no phase slippage and thermal equilibrium between both phases.

A superheated liquid spill (i.e., liquid at a temperature exceeding the saturated-vapor temperature at the given pressure) often leads to aerosol formation because of the rapid expansion of the superheated liquid. The generation of liquid droplets occurs as a result of the reduction in pressure upon release and the cooling of the gas as it expands.

A single-phase gas release may result from a compressed gas or liquefied gas. In this case, no condensation occurs and no aerosol is formed. A gas release will not condense if its pressure is too low to result in subcooling the material during the expansion. Choked flow develops if the release pressure is sufficiently high to reach the choking velocity limitation. Whether one material exhibits the "condensation but no choked flow" combination, or the "no condensation with choked flow" combination is chemical property dependent. If the pressure in the vessel is less than that which would result in condensation or choked flow conditions, a single-phase, unchoked gas release will occur. The release rate in this case is a function of the internal pressure and size of the release point.

Geometry considerations affect the release rate of material to the environment, e.g., horizontal or vertical cylinder, hole/leak size and location. The height of the hole above the ground determines the release height for escaping gas. The height of the hole relative to the height of liquid in the vessel determines the amount of liquid that can be released and the pressure head of liquid available. A release may be from a pipe connected to a vessel, resulting in some resistance to flow depending on pipe condition and size.

Many chemicals have a molecular weight greater than air. These materials may initially form a dense gas cloud, by virtue of their excess density. Dense gas clouds may also form as a result of releases that are colder than the ambient air and/or that contain aerosols formed in the process of a rapid liquid release from a pressurized vessel. A number of criteria exist for assessing whether or not a release will behave as a dense gas. The Richardson number is commonly used. This is the ratio of the initial potential energy of

the vapor cloud to the ambient kinetic energy (see Section 7.3.2). An exact value of the Richardson number, where the transition from dense gas effects to neutrally buoyant behavior occurs, does not exist. However, a value in the range of ~1 to 10 is commonly used to make this determination.

Pressurized releases are often time dependent. The release rate is dependent on the internal pressure in the vessel. As long as this is maintained, a fairly constant release rate will be observed. Once the internal pressure begins to deteriorate, a reduction in the release rate will be observed.

3.3.3 Solid Spills and Resuspension/Sublimation

Solid spills are typically of greater interest if the material is radioactive. Generally, chemical spills are of greater concern for volatile materials. However, there are a few chemicals, such as beryllium and lithium hydride, where solid spills may present a significant hazard. Airborne releases of solid materials are expected to be most significant for material in the powder form. Solid metals and non-metallic or composite solids are generally not of concern from a spill standpoint, although a small release might result from brittle materials that impact an unyielding surface.

There are several contributors to the total source term from a solid spill. These are:

- (1) airborne material generated as a solid falls through a distance;
- (2) airborne material generated as a solid impacts the ground/surface after falling;
- (3) resuspension of material deposited on the ground/surface;
- (4) sublimation of solid material deposited on the ground/surface.

The amount of material made airborne during the fall/impact phase of a spill of powder depends on the balance between the separation forces generated by the event versus the binding forces present in the powder. Separation forces include the shear/drag force encountered by the spilled material as it falls through the air, and the impact force upon encountering a surface. Some parameters that effect binding forces include particle size distribution and moisture content. Bulk density is an indication of initial dispersibility. Fall distance, the mass of spilled material, and bulk density influence the speed and momentum of the falling material and the amount of turbulence created upon impact.

Entrainment and resuspension can occur if the material is exposed to aerodynamic stresses once it has come to rest on a surface. Air passing over a surface or directed onto a surface can induce flow and turbulence that can suspend particles from the surface. Entrainment of particles is a function of the characteristics of the flow, the surface, and the particles.

The entrainment of material is often described by a resuspension factor. This is defined as the ratio between the airborne concentration of a pollutant per cubic meter directly over a contaminated surface and the pollutant surface contamination on the ground. The units are meters⁻¹. In concept, the factor represents the uniform concentration at some height above a contaminated surface. A resuspension rate may also be utilized to characterize the re-entrainment, describing the fraction of initially deposited material made airborne per unit time.

For spilled materials that have a measurable vapor pressure, some amount of the material can become airborne due to sublimation. In most instances, this mechanism will be negligibly small. However, there are some solid materials (e.g., phenol) that do have a significant vapor pressure, and this pathway to the environment should be considered.

3.3.4 Resuspension of Dissolved/Suspended Solid Material from Liquid Spills

Resuspension of dissolved or suspended material from a spilled liquid is generally of greater interest if the dissolved/suspended material is radioactive. The material may become airborne during the spill itself (due to shear and impact forces), it may be resuspended from the liquid once it forms a pool on the ground, or it may be resuspended after the liquid evaporates when the material has been deposited on the ground.

Shear stress at the air-material interface can shed droplets during the fall. Splashing may be a significant mechanism for airborne release of radioactive material dissolved or suspended in a liquid. The quantity of material made airborne by this mechanism is found (empirically) to be dependent on solution density, solution viscosity, and spill height.

Resuspension of dissolved/suspended solid material from spilled liquids has been evaluated in a similar fashion to solid spills using the resuspension factor or a resuspension rate.

3.4 DOE Orders, Guidance, and Other Regulatory Documents

The initial step in the process was to review the DOE and other agency regulatory/ licensing documents, guidance documents, and standards, and to identify from them, specific requirements that would influence the nature of the methodologies that would be considered acceptable for safety analysis. Although the requirements for spill source terms generally were not specific,

an attempt was made to interpret these as specific criteria with respect to code capabilities. The identified requirements/capabilities were further developed into a set of evaluation criteria for spills methodologies, as discussed in the next section. The Spills Working Group reviewed the following documents:

- **Nuclear Safety**
SEN-35-91, Nuclear Safety Policy (note that at the time of preparation of this report, this notice had lapsed)
- **Facility Safety Analysis**
DOE Order 5480.23, Nuclear Safety Analysis Reports
DOE Order 5481.1B, Safety Analysis and Review System
DOE-STD-1027-92, Hazard Categorization and Accident Analysis Techniques for Compliance with DOE Order 5480.23, Nuclear Safety Analysis Reports
DOE-STD-3009-94, Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Analysis Reports
DOE-STD-3011-94, Guidance for Preparation of DOE 5480.22 (TSR) and DOE 5480.23 (SAR) Implementation Plans
- **Process Safety and Risk Management**
29CFR1910.119, Worker Chemical Safety
40CFR68, Risk Management Programs for Chemical Accident Release Prevention
- **Emergency Planning**
DOE Order 5500.3A, Planning and Preparedness for Operational Emergencies Emergency Management Guide, Guidance for Hazards Assessment, 6-26-92
- **Design Requirements**
DOE Order 6430.1A, General Design Criteria
- **DOE Handbooks**
DOE-HDBK-3010-94, Airborne Release Fractions/Rates and Respirable Fractions For Non-Reactor Nuclear Facilities

The approach taken was to review each of the documents listed above, and to identify relevant sections. An attempt to interpret the relevant citations from each document as a requirement for spills methodologies was

then made. These interpretations were summarized, and an overall set of requirements was identified. This formed the basis for the development of a spills model evaluation criteria. Citations and interpretations of the individual documents with respect to spills methodologies are provided in Appendix A.

Given that DOE regulations are in a state of transition, and new Orders, Rules, etc. are being continuously developed and issued, future requirements for safety analysis may differ from those that are followed today. It is therefore prudent to consider reviewing the information in this report with respect to requirements at a future date.

3.5 Outline of this Report

The remainder of this report documents the activities and findings of the Spills Working Group. Section 4 summarizes the requirements that influence the nature of acceptable spills methodologies, presents the evaluation criteria, and describes the problems used in the test problem exercise. In Section 5, the code selection process is provided, along with a summary listing of the codes finally selected for evaluation. Results are given in Section 6 for the code evaluations and for the test problem exercise. The role of hand calculations in spills methodologies is also discussed. Section 7 provides the recommendations of the Spills Working Group, including recommended codes, future development needs, path forward, and best practices. Several appendices are referenced in various sections of this report. Relevant citations from DOE/requirements documents are provided in Appendix A, with an interpretation of the requirements, as they pertain to spills methodologies. The detailed code evaluations are provided in Appendix B. Appendix C gives the test problem results. Appendix D gives supplementary information related to resuspension of spilled material. Listings of important chemicals that should be examined in safety analyses, if present at a facility, are provided in Appendix E.

4. Criteria for Methodology Evaluation

4.1 Summary of Requirements

The initial step in developing criteria for spills methodologies evaluations was to review DOE regulatory/licensing documents, guidance documents, and standards. The documents reviewed are listed in Section 3.4. From the documents, requirements that would influence the nature of the methodologies that would be considered acceptable for safety analysis were identified. The approach taken and documented here was to review each requirement source, and to identify relevant sections. An attempt to interpret the relevant sections from each document as a requirement for spills methodologies was then made. Citations and initial interpretations are provided in Appendix A. Although the requirements for spill source terms were generally vague, an attempt was made to interpret these as specific criteria with respect to code capabilities. These interpretations were then summarized, and an overall set of requirements was identified.

Safety analysis methodologies must be capable of calculating the source term from spill events so that the impact of operations and accidents can be assessed. The SAR is also concerned with the performance of safety-related equipment when exposed to accident conditions that may be detrimental to its function. Thus, an appropriate source term (i.e., conservative, which will lead to a bounding consequence) must be determined so that concentrations of hazardous materials to which workers, equipment, and the public can be potentially exposed are evaluated.

Four sets of requirements were identified, to cover each of the four spill areas being considered by the working group. Based on the review of the requirements documents, analysis methodologies should be capable, at a minimum, of the following:

Liquid Chemical Spills and Evaporation

- determining rate of release/duration of release
- including site-specific conditions
- including physical features/properties (e.g. process equipment and conditions)
- including chemical properties
- modeling mixtures/solutions
- characterizing the initial vapor cloud (e.g. temperature, density, size)
- including materials with vapor pressures above 10 mmHg (@20 °C)

Pressurized Liquid/Gas Releases

- determining rate of release/duration of release
- determining vapor fraction (flash fraction)

- including site-specific conditions
- including physical features/properties (e.g. process equipment and conditions)
- including chemical properties
- characterizing the initial vapor cloud (e.g. temperature, density, size)

Solid Spills and Resuspension/Sublimation

- determining release fraction/rate
- including site-specific conditions
- including physical features/properties (e.g. process equipment and conditions)
- including chemical properties
- including particle size distribution
- being applicable to both chemicals and radionuclides

Resuspension of Dissolved/Suspended Matter from Liquid Spills

- determining release fraction/release rate/release duration
- including site-specific conditions
- including physical features/properties (e.g. process equipment and conditions)
- including particle size distribution
- being applicable to both chemicals and radionuclides

The methodologies should cover a range of levels of sophistication, so that the capability to do more sophisticated analyses where the hazard level and/or complexity dictate, is available. This may range from hand calculations (e.g. screening level analysis, hazards analysis documents, BIO) to very sophisticated analyses considering all of the above listed capabilities (e.g. Category 2 facility SAR).

4.2 General Criteria

The requirements identified by review of applicable DOE/regulatory documents were further developed into evaluation criteria, knowing the types of materials that might be encountered, and the types of accidents that might require analysis. This included general and specific evaluation criteria. The general criteria contain top-level information about each code, its availability, its applicability, its limitations, etc. The general criteria were the same for all four categories of spill-type events. They are summarized below. The evaluations of each of the codes against the general criteria can be found in Appendix B.

- (1) Capabilities: A brief summary of code capabilities, special features, and other general information about the code is given.

- (2) Sponsor/Developing Organization: The organization that developed the code, and the sponsor, if different, are provided.
- (3) Current Custodian: Information on who currently retains the code is listed. This can include a name of an individual, address, phone, fax, email, etc.
- (4) Genealogy: A brief history of the code development is given, including other codes that the code of interest may have been based on, previous versions of the code, etc.
- (5) User's Manual Reference: A citation for the user's manual is provided.
- (6) Model Description Summary: A brief description of the models used in the code is provided. Unique features of the code are highlighted here.
- (7) Model Description References: Citations that contain details on the models used in the code are given.
- (8) Hardware Requirements: The hardware requirements for running the code, including platform, graphics needs, memory requirements, etc. are listed.
- (9) Quality Assurance Documentation: Any references documenting benchmarks, source code verification, or validation against experimental data are provided here.
- (10) Input Summary: The input needed to run the code is briefly described. This would include parameters that need to be specified or any material data required.
- (11) Output Summary: The information calculated by the code and provided as output is summarized.
- (12) Summary of Limitations: Any code limitations or restrictions are listed. This includes types of applications for which the code is not suited.
- (13) Summary of Strengths: Key features that the code offers are highlighted.

- (14) Range of Applicability: The types of scenarios and applications for which the code was developed are listed.
- (15) Comments on User Friendliness: Comments are provided on how easily the code can be used. This would include whether or not the code is menu driven, how easy it is to set up input files, how easy it is to read output files, etc.
- (16) Comments on Error Handling Capabilities and User Feedback: It is noted if the code provides diagnostics messages for errors or warnings, and how easily these can be interpreted.
- (17) Source Code and/or data bases can be modified: Any aspects of the code that can be modified by the user are listed.
- (18) Execution time for typical problem: Estimated run time for a typical problem is provided, either in CPU or real time.
- (19) Acquisition format: The manner in which the code can be acquired is noted. This may include diskette, tape, email, download from bulletin board, etc.
- (20) Cost: The current cost in dollars, if any, for obtaining the code is given.
- (21) First Order evaluation against DOE requirements: Comments are provided here as to whether the code generally appears to be acceptable for supporting DOE safety analysis documentation.
- (22) Comments on Graded Approach applicability: Comments are provided as to whether the code appears to be suited to analyses for a wide range of facility hazard levels, if it is more suited to conservative screening analyses for lower hazard facilities, or if it is better applied to more hazardous facilities that may require more sophisticated analyses.
- (23) Future Enhancements Planned: Any further code developments, either in progress or planned, are noted.
- (24) Additional Information: Any additional information about the code not already provided in response to the other criteria is provided.

4.3 Specific Criteria

Specific evaluation criteria were developed for each of the four spill-type events. These were developed from the requirements identified, as well as the group's knowledge about the phenomena involved in the various types of spill event, and the various factors that affect those phenomena. The specific criteria focus on the details of the models used in the codes evaluated, with the goal of providing a better understanding of the capabilities of the different codes. The Specific Criteria are summarized in Table 1.

In the evaluations, the response to the criteria would be yes or no, with some explanation. Any limitations would also be mentioned. For the liquid chemical spills and evaporation and pressurized liquid/gas releases, the code performance in the test problem exercise was noted. Details on the test problems used, code responses, and insights are provided in Sections 4.4 and 6.2. The evaluations of the codes against these criteria are provided in Appendix B.

4.4 Description of Test Problems

A test problem exercise was performed, with the purpose of testing the capabilities of the codes, rather than for the purpose of comparing final results. From the test problems evaluated, the group hoped to learn which codes can handle the problems of interest, the ease with which the codes handle the problems, and how reasonable the answers seem. The group adopted some previously established test problems provided in Hanna and Strimaitis (1989). The test problems selected were those focusing on source term calculations. These sample problems applied to only two of the four types of spill accidents: liquid chemical spills and evaporation, and pressurized liquid/gas releases. The codes for the other two types (solid spills and resuspension/sublimation, and resuspension of particulate matter from liquid spills) were not evaluated through a sample problem. This was because the available codes are few in number, fairly simple, and based on empirical correlations. There appeared to be little benefit from developing a test problem for these cases.

Table 1: Specific Evaluation Criteria Used for Spill Categories

Liquid Chemical Spills and Evaporation	Pressurized Liquid/Gas Release	Solid Spills and Resuspension/ Sublimation	Resuspension of Dissolved/Suspended Material from Spilled Liquids
Determination of pool size	Determination of release rate	Determination of release fraction	Determination of release fraction
Consideration of pool depth	Determination of initial characteristics of vapor cloud	Consideration of ambient and/or site-specific conditions	Determination of release rate during evaporation
Determination of release rate	Consideration of ambient and/or site-specific conditions	Geometry considerations	Determination of initial concentration
Consideration of ambient and/or site-specific conditions	Geometry considerations	Consideration of resuspension	Consideration of ambient and/or site-specific conditions
Determination of initial characteristics of vapor cloud	Time dependency of rate calculation	Applies to both chemicals and radionuclides	Applies to both chemicals and radionuclides
Time dependency of rate calculation	Temperature dependency/ thermal effects	Time dependency of rate calculation	Time dependency of rate calculation
Temperature dependency/ thermal effects	Consideration of critical flow	Consideration of particle size distribution	Consideration of particle size distribution
Time dependent spill to pool	Consideration of two-phase flow	Temperature dependency/ thermal effects	Temperature dependency/ thermal effects
Consideration of heat transfer from substrate	Consideration of water reactivity	Extensive data base provided	Extensive data base provided

Consideration of chemical reaction with substrate	Extensive data base provided	Some data/properties must be user specified	Some data/properties must be user specified
Consideration of insolation	Some data/properties must be user specified	All data/ properties must be user specified	All data/ properties must be user specified
Consideration of water reactivity	All data/ properties must be user specified	Special features	Special features
Consideration of multi-component mixtures/ solutions	Special features	Linked to transport model	Linked to transport model
Extensive data base provided	Linked to transport model	Other	Other
Some data/properties must be user specified	Test problem evaluation	Graded Approach applicability	Graded Approach applicability
All data/ properties must be user specified	Other		
Special features	Graded Approach applicability		
Linked to transport model			
Test problem evaluation			
Other			
Graded Approach applicability			

Problem #1: Pressurized Liquid Release of Anhydrous Ammonia (from Hanna and Strimaitis, 1989)

This scenario describes the ground level release of anhydrous ammonia from: (a) a nozzle failure and (b) a line rupture near the bottom of a 40 mT storage tank at ambient temperature (298 K) and 8.9 bar (i.e. at saturation pressure). The 1.5 in. ID nozzle is very near the tank and the line rupture is on a 1.5 in. ID line at a distance of 150 in. from the tank. This scenario is illustrated in Figure 2.

Figure 2: Pressurized Liquid Release of Anhydrous Ammonia

Problem #2: High Pressure Gas Release of Carbon Monoxide (from Hanna and Strimaitis, 1989)

This scenario describes the release of high pressure¹ CO from a horizontally directed valve with a valve seat diameter of 1.27 cm and a discharge pipe diameter (initial jet diameter) of 10.2 cm. This combination of valve seat diameter and discharge pipe diameter will ensure that the pipe exit velocity is less than or equal to the sonic velocity. The duration of the release is assumed to be 5 min. This scenario is illustrated in Figure 3.

Figure 3: High Pressure CO Release of Carbon Monoxide

¹Note that in the original reference, the CO pressure is given as 2230 psig. The ALOHA code cannot accept input pressures above 1000 psig. Thus, for the ALOHA runs, the scenario pressure was taken to be 999 psig.

Problem #3: Pressurized Liquid Release of Chlorine (from Hanna and Strimaitis, 1989)

This scenario involves the release of liquid chlorine from a valve failure (0.3 in. ID) on the lower pigtail of a 1 ton cylinder at a temperature of 303 K. The spill occurs on an undiked surface consisting of wet soil. Vapor, aerosol (at various proportions), and a liquid pool must be considered. Figure 4 illustrates this scenario.

Figure 4: Pressurized Liquid Release of Chlorine

Problem #4: Liquid Spill of Acetone (from Hanna and Strimaitis, 1989)

A spill of liquid acetone from a 2 in. nozzle connection near the base of a cylindrical tank of height 25 ft. and diameter 25 ft. occurs over a 30 min. period into a concrete bermed area of height 3 ft. and diameter 72 ft. The chemical is stored at ambient pressure and temperature (303 K). Figure 5 illustrates this scenario.

Figure 5: Liquid Spill of Acetone

A summary of the test problem scenarios and their release conditions is provided in Table 2. For each code that was run through the sample problems, documentation of the code's response to the problems, indicating any concerns or limitations found, is provided in Section 6.2. Detailed code output from the sample problem runs is given in Appendix C.

Table 2: Summary of Test Problems (Hanna and Strimaitis, 1989)

Scenario Description	Release Conditions
#1. Ground level release of liquid anhydrous ammonia from ambient temperature storage (40 mT) by: (a) catastrophic failure in 1.5-in. connecting orifice and (b) catastrophic failure of 1.5-in. line ~ 150 in. from vessel.	Ammonia stored at 8.9 bar and 25 °C. Ambient at 25 °C, 80% RH. Release duration = 30 min.
#2. Release of high-pressure carbon monoxide from relief valve (10.2 cm diameter initial jet).	Relief valve discharge horizontally at 21 °C. Burst pressure of 2230 psig (999 psig for ALOHA). Release duration= 5 min.
#3. Ground level release of liquid chlorine from 0.3-in. i.d. valve failure on a 1-ton cylinder. Consider variable aerosol fractions (0 and 50%). Include secondary pool source term.	Liquid chlorine saturated at 30 °C. Spill occurs on wet soil undiked surface. Ambient at 30 °C, 80% RH. Release duration - until cylinder is empty.
#4. Ground level release of acetone from 2-in. nozzle connection from 25 ft diameter x 25 ft high storage within a concrete bermed area of height 3 ft and diameter 72 ft.	Acetone stored at 30 °C and ambient pressure. Ambient at 30 °C, 50% RH. Release duration = 30 minutes ^a .

^a For this scenario, calculations of the source term were made for a surface roughness of 0.03 and 0.30 m, for stability class F (with wind speed 2 m/s), and for stability class D (with wind speeds 2 and 5 m/s).

5. Codes Evaluated

5.1 Code Selection Process

An initial listing of spill source term codes was provided to the Spills Working Group by the Executive Committee (O'Kula, 1994). The working group reviewed this list, and eliminated several codes because they did not have source term models, were not in use and are no longer supported, were not in the public domain, or could not be located. This list was supplemented by reviewing existing lists of safety analysis-related codes, such as that prepared by the EFCOG Computer Codes Subgroup (EFCOG, 1993) and by SCAPA (SCAPA, 1993).

The Spills Working Group ultimately evaluated 11 codes. This is a reduced set from the initial set of 24. The initial set is provided in Table 3, along with the reasons why many of the codes were not evaluated. A summary list of the codes evaluated is provided in Table 4. This table categorizes the codes according to the type of source term it can generate (i.e. which of the four specific spill-type scenarios it is designed for). It is clear that most of the codes considered apply to analysis of spilled liquids/evaporation or releases of pressurized liquids/gases. Codes modeling spills of solid material, or resuspension of materials contained in spilled liquids are limited.

5.2 Summary of Codes Selected

To follow is a brief summary of each of the codes evaluated. Information provided includes code capabilities, code limitations and recommended use. Additional details are provided in Appendix B, which contains the detailed evaluations of all of the codes.

Code Name: ADAM (Airforce Dispersion Assessment Model) (U.S. Airforce)

Code Capabilities: ADAM is a heavy gas, Gaussian puff dispersion model, that includes source term models for pressurized and non-pressurized liquid and gas releases. Potential reactions of the released chemicals with water vapor can be modeled. N_2O_4 - NO_2 , HF, and NH_3 chemistry are modeled. Eight chemicals are included in the ADAM database; others can be added by the user.

Limitations: While chemicals can be added to the ADAM database, it is not a trivial exercise to do. Pipe releases are not modeled. The pool evaporation model neglects transient heat transfer effects and the mass transfer model is

Table 3: Initial Complete List of Codes Considered by the Spills Working Group

Code Name	Action Taken for the Code
ADAM	Evaluated
AFTOX	Not evaluated - precursor to ADAM
ALOHA	Evaluated
ARAC	Not evaluated - does not yet have a source term model
ARCHIE	Not evaluated - not maintained
CASRAM-SC	Evaluated
EMGRES	Evaluated
EPICode	Not evaluated - not in public domain
HGSystem	Evaluated
HOTSPOT/Resuspension	Evaluated
KBERT	Evaluated
LSM90	Incorporated into HGSystem
MISM	Evaluated
MSPEC	Not evaluated - old, not maintained
ORG40/TP10	Evaluated
PAVA	Not evaluated - could not be located; thought to be PAVAN, a code for evaluating X/Q
PEST	Not evaluated - not in public domain
PSpill (originally listed as Spill)	Evaluated
Release (AIChE)	Not evaluated - not in public domain
Release (WSRC)	Not evaluated - code has poor QA, code is simple and uses Mishima data; better to directly use the data
SLAB	Not evaluated - public domain version does not have a source term model
SPILLS	Not evaluated - old, no longer supported, not included in EPA model application guidelines
TScreen	Evaluated
Whazan	Not evaluated - not in public domain

Table 4: Summary of Codes Evaluated by Type

Liquid Chemical Spills and Evaporation	Pressurized Gas/Liquid Releases	Solid Spills and Resuspension/ Sublimation	Resuspension of Particulate Matter from Liquid Spills
ADAM	ADAM	HOTSPOT	HOTSPOT
ALOHA	ALOHA	KBERT	
CASRAM-SC	CASRAM-SC	PSpill	
EMGRES	EMGRES		
HGSystem	HGSystem		
MISM	TScreen		
ORG40/TP10			
TScreen			

based on rocket/jet fuel experimental data. The Fauske-Epstein models are applied in a quasi-steady manner to two-phase releases.

Recommended Use: Although it ostensibly has applicability to a broad range of chemical accident severity assessment situations, ADAM is best used in situations that require consideration of N_2O_4 - NO_2 , HF, and NH_3 chemistry. For more "generic" situations, especially pool evaporation, there are other codes available that contain a larger data base. The code is generally acceptable in applications supporting SAR, BIO, and JCO documents.

Code Name: ALOHA (Areal Locations Of Hazardous Atmospheres)
(EPA/NOAA/NSC)

Code Capabilities: ALOHA can estimate single component source terms generated via the following mechanisms: (1) evaporation from a pool of liquid, (2) liquid release from a tank, (3) gas release from a tank, (4) two-phase release from a tank, and (5) gas release from a pipe. The code is also capable of performing puff and continuous release dispersion calculations for dense gas and neutral gas source terms.

Limitations: The output generated by ALOHA is ill-posed for detailed analysis needs. In addition it does not provide the aerosol mass fraction for two-phase releases.

Recommended Use: ALOHA is applicable to all hazard categories, although its lack of detailed output could potentially make it unsuitable for high hazard analyses where reduction in over-conservatism may be necessary. The code is generally acceptable in applications supporting SAR, BIO, and JCO documents.

Code Name: CASRAM-SC (Chemical Accident Statistical Risk Assessment Model - Single Case) (ANL/DOT/U. Illinois)

Code Capabilities: The CASRAM-SC code is a chemical consequence and risk assessment model applicable to chemical process, storage, handling, and transportation accidents. The model is capable of determining consequence and risk both deterministically (SC) and stochastically (version not reviewed). It contains source algorithms to characterize instantaneous and time varying releases from ruptured storage vessels (pressurized and non-pressurized) and time varying releases from evaporating pools. The model also predicts "discharge fractions", and flash-entrainment quantities used with the

computed emission rates and specified health criteria to estimate chemical hazard population exposure zones.

Limitations: The model is currently not applicable to releases through a pipe leading to a two-phased jet and to chemical mixture influence on multi-component releases. The physics of aerosol formation from a pressurized liquid release is not explicitly treated in the code. This is a common limitation for all of the spill codes evaluated. The model is not capable of simulating dense-gas behavior. The stochastic version of the model (CASRAM) is now only applicable to chemical releases from transportation accidents. It considers the accident frequency and chemical release probability from the transportation of hazardous material containers. Statistics on accident frequencies, release quantities and types, and facility source types are needed for application to fixed facility accidents.

Recommended Use: The model is applicable to a broad range of chemical accident severity assessment situations. However, it is most applicable to assessment of consequences and risks associated with the operation of "high hazard" chemical facilities. These assessments would be recommended to support the preparation of SARs, BIOs, JCOs, and EISs.

Code Name: EMGRES (Ontario Ministry of the Environment)

Code Capabilities: EMGRES is a screening tool for assessing the downwind distance to a selected chemical concentration. The source-term models in the program include release of a pure vapor through an orifice, release of a subcooled liquid from a reservoir, and point source instantaneous and continuous plume gas releases. All source-term models are linked to neutral and heavy gas dispersion models.

Limitations: EMGRES is admittedly a simplistic model and highly conservative. It should only be used as a preliminary screening tool. Although it is intended as an emergency response program, navigating through all the intermediate menus can take somewhat more time than is ideal.

Recommended Use: Use of EMGRES should be limited to low hazard facilities on the basis of the simplicity and conservatism inherent in its computational models.

Code Name: HGSystem (Shell)

Code Capabilities: HGSystem is a general purpose PC-based chemical source-term and atmospheric dispersion model. It is comprised of a number of individuals modules used to simulate source-terms, near-field, and far-field dispersion. The chemical and thermodynamic models available in HGSystem include reactive hydrogen fluoride and non-reactive, two-phase, multi-compound releases. A very brief summary of the modeling capabilities of the code follow:

- Accounts for the HF/H₂O/air thermodynamics and cloud aerosol effects on cloud density.
- Models both pressurized and non-pressurized releases.
- Predicts concentrations over a wide range of surface roughness conditions.
- Predicts concentrations at specific locations for user-specified averaging periods.
- Considers steady-state, time-varying, and finite release duration releases.
- Computes crosswind and vertical concentration profiles.

Limitations:

- HGSystem cannot be used for analyzing releases where there is pipework present between the reservoir and the outlet orifice.
- There are a limited number of pool substrate materials which can be modeled by HGSystem, specifically sand, concrete, plastic, steel, and water.
- It is difficult to extend the physical/chemical data base utility DATAPROP to include additional chemical species. Such modifications would require an extremely good knowledge of the HGSYSTEM program structure and some consultation with the code developers.

Recommended Use: HGSystem was explicitly designed to model water reactivity of HF when it is released to the ambient environment. Use of the code is also valid for other chemicals releases that exhibit both ideal and non-ideal gas behavior in the flow regime of interest. The code is applicable to

single- or multi-component chemical releases resulting from upset conditions in typical process operations. It is recommended for use with facilities of all levels of hazard classification to analyze public, collocated worker, and local worker consequences.

Code Name: HOTSPOT (LLNL)

Code Capabilities: The HOTSPOT Health Physics codes were created to provide Health Physics personnel with a fast, field-portable calculation tool for evaluating accidents involving radioactive materials. The HOTSPOT codes are a first-order approximation of the radiation effects associated with the atmospheric release of radioactive materials. The resuspension program calculates the downwind consequences from an area contamination event.

Limitations: The default resuspension parameters are based on resuspension of plutonium particulate, but the model is generally applicable. The model is conservative with respect to more recent data.

Recommended Use: The resuspension model in HOTSPOT is widely applicable to all hazard categories for contamination events involving radioactive material. The code is generally acceptable in applications supporting SAR, BIO, and JCO documents.

Code Name: KBERT (Knowledge-Based system for Estimating hazards of Radioactive material release Transients) (SNL-A)

Code Capabilities: KBERT calculates doses to in-facility workers from accidental releases of radioactive material using airborne release fractions/release rates specified in the Mishima Handbook (DOE-HDBK-3010-94 (DOE, 1994a)). Calculations take into account specification of the material at risk, air flows between rooms, deposition, filtration, and worker evacuation schemes.

Limitations: The code is still in prototype form, and it has not been verified. It lost sponsorship before being released by DOE. The code lacks user experience.

Recommended Use: The code can be used for evaluation of in-facility worker exposure from accidents in DOE non-reactor nuclear facilities for which release fractions/release rates of aerosolized material at risk are available from the Mishima data base.

Code Name: MISM (Modified Ille-Springer Model) (Airforce)

Code Capabilities: MISM calculates a source term (evaporation rate) from a spill to ground of three rocket propellant fuels (hydrazine, monomethylhydrazine, and unsymmetrical dimethylhydrazine) and downwind, ground level, centerline concentrations using a single-source Gaussian dispersion algorithm.

Limitations: The code that was reviewed is limited to liquids that have limited use, if any, in the DOE complex; generalization to other liquids would require significant additions of pertinent material properties and data. The code is limited to a steady-state analysis and does not attempt to analyze transient behavior. The predicted evaporation rate is proportional to the spill area, which is a user input to the code; this could lead to significant uncertainty or error in situations involving a spill in an undiked area or where a defensible estimate of area is difficult to make.

Recommended Use: In its current form, the code is generally not useful/applicable to DOE facilities.

Code Name: ORG40/TP10 (Army)

Code Capabilities: The code calculates the evaporation rate of a liquid pool, given the physical state variables, wind speed, and diameter of the pool. It computes the molecular diffusivity for a range of substances in a wide molecular weight range for both indoor (i.e. zero wind speed) and outdoor applications.

Limitations: The code is not ready for general use without some recoding, as it is intended as a subroutine and requires a menu for input/output information. The code appears to underpredict compared with other models, but all models appear to overpredict when compared to field data.

Recommended Use: The code can be used to estimate the rate of liquid pool evaporation.

Code Name: PSpill (PNL)

Code Capabilities: The code determines the mass of material that becomes airborne from a spill of solid powder.

Limitations: The code is limited to powder spills, and applies only to bulk spills rather than continuous pours. It does not consider the airborne particulate generated as a result of impact with the ground.

Recommended Use: An electronic version of the code no longer exists, but a listing is available. It is not recommended that the code be regenerated and used. Hand calculations using the algorithms in the code would be acceptable.

Code Name: TScreen (EPA)

Code Capabilities: TScreen is a simple, conservative screening tool for obtaining maximum downwind vapor concentrations at selected receptor locations for releases resulting from a) particulate releases, b) gaseous releases, c) liquid releases, and d) superfund releases. A particular release scenario is selected via input parameters, and TScreen automatically selects and executes the appropriate dispersion model to simulate that scenario. The model to be used and the worst case meteorological conditions are automatically selected.

Limitations: Many of the models are simplistic and extremely conservative both in terms of source-term and subsequent downwind vapor concentration. Models which exhibit the greatest degree of conservatism are superheated flashing releases and unconfined liquid pool evaporation. Furthermore, the program only computes steady-state release rates for ideal fluids. Hence, in the case of a gas reservoir under extreme pressures, for example, the predicted results may be under conservative because ideal conditions no longer apply.

Recommended Use: Use of TScreen should be limited to low hazard facilities where estimation of the potential hazard zones due to the release of a toxic chemical can be adequately represented by a conservative bounding calculation. The code is only intended to model outside releases where the impacts extend to the far field and surface roughness features may be neglected.

6. Model Review and Comparison Results

6.1 Results of Evaluations Against Criteria

The final codes selected by the Spills Working Group were evaluated against the general and specific criteria. Detailed evaluations are provided in Appendix B. Observations from the evaluations are noted in this section. The discussion is broken into 4 parts, focusing separately on each of the four spill-type events.

6.1.1 Liquid Chemical Spills and Evaporation

Eight codes that could generate source terms from liquid chemical spills and evaporation were evaluated. The models have varying degrees of sophistication. Some of the codes require development work in order to be useful for safety analysis purposes. Table 5 summarizes the results of the code evaluations against the specific criteria for liquid chemical spills and evaporation.

Although the Modified Ille-Springer Model (MISM) improves upon the original model version's ability to properly account for solar insolation and stability, its data base is currently limited to three hydrazine-based liquid rocket propellants, which have limited use (if any) in the DOE complex. To make the code more generally applicable, the code would require modification and pertinent data on any new chemicals would have to be collected.

ORG40/TP10 is a subroutine of the D2PC (Army) code, and can currently not be run on its own. Some modification would be required to achieve a stand-alone version. It may be worthwhile to go ahead with these modifications, as the model generates a source term from a spill in still air. ORG40/TP10 appears to be the only code capable of doing this.

TScreen is a fairly simple model, appropriate for use as a screening tool, or for analysis of lower hazard facilities. EMGRES is on a similar level. TScreen appears to have undergone a more thorough QA process than EMGRES, and is endorsed by the EPA. It also contains a near field dispersion model, which may be valuable in many applications. TScreen is limiting in that it only contains 7 chemicals in its data base. However, it is possible to manually enter data into the code. The burden is on the user to provide appropriate data. EMGRES has data for over 800 chemicals.

Table 5: Summary of Specific Criteria Evaluations for Liquid Chemical Spills and Evaporation Codes

Liquid Chemical Spills and Evaporation Code Evaluation Criteria	ADAM	ALOHA	CASRAM-SC	EMGRES	HGSystem	MISM	ORG40/TP10	TScreen
Determination of pool size	Y	Y	Y	Y	Y	N	Y	Y
Consideration of pool depth	Y	Y	Y	Y	Y	Y	N	Y
Determination of release rate	Y	Y	Y	Y	Y	Y	Y	Y
Consideration of ambient and/or site-specific conditions	Y	Y	Y	Y	Y	Y	Y	Y
Determination of initial characteristics of vapor cloud	Y	Y	Y	Y	Y	N	Y	N
Time dependency of rate calculation	N	Y	Y	N	Y	N	N	N
Temperature dependency/thermal effects	Y	Y	Y	N	Y	Y	Y	N
Time dependent spill to pool	Y	Y	Y	Y	Y	N	N	N
Consideration of heat transfer from substrate	Y	Y	Y	N	N	Y	Y	N
Consideration of chemical reaction with substrate	N	N	N	N	N	N	N	N
Consideration of insolation	Y	Y	Y	N	Y	Y	N	N

Consideration of water reactivity	Y	N	N	N	Y	N	N	N
Consideration of multi-component mixtures/ solutions	N	N	N	N	Y	N	N	N
Extensive data base provided	N	Y	Y	Y	Y ⁺	N	Y	N
Some data/properties must be user specified	N	N	N	N	N	Y	Y	N
All data/ properties must be user specified	N	N	N	N	N	N	N	Y
Special features	Y ⁺	N	Y ⁺	N	N	N	Y ⁺	Y
Linked to transport model	Y	Y	Y	Y	Y	Y	Y	Y
Test problem evaluation	Y	Y	Y	N	Y	N	N	Y
Other	N	N	N	N	Y ⁺	N	N	N
Graded Approach applicability	lower hazard	lower hazard	higher hazard	low hazard	higher hazard	not applicable	lower hazard	lower hazard

Y Feature provided in code.

N Feature not provided in code.

* There are some limitations, described in detailed evaluations found in Appendix B.

+ The special features are described in detailed evaluations found in Appendix B.

ALOHA has a substantial data base (800 chemicals), and additional chemicals can be added by the user. Although the models used are fairly sophisticated, the code is fairly easy to use.

ADAM uses an energy balance equation for pool evaporation in a way similar to the original Ille-Springer model (with a simplified estimation of heat transfer within the liquid pool) for non-cryogenic spills. Cryogenic spills are handled using a method described in Raj (1981) to account for the influence on evaporation rate of substantially higher ground to liquid heat transfer rates. In addition to pool evaporation, the model is capable of estimating vessel release rates from several spill types, including direct releases from pressurized liquid and gas storage tanks. ADAM has a physicochemical properties data base that includes eight chemical compounds. To model chemical compounds not already hard-wired into the code, the user must set up chemical data files and perform some code modifications. The very specialized and limited chemical data base incorporated into MISM (noted previously) and the somewhat constrained data base in ADAM tend to limit the application of these models for SAR related work. However, ADAM's ability to handle more common chemicals, such as chlorine and anhydrous ammonia, gives it greater utility.

CASRAM-SC has a fairly sophisticated spill source term model, with a wide range of features. CASRAM-SC's current data base includes over 50 chemicals. There are plans to add data for an additional 70 to 1000 compounds.

HGSystem has a very detailed model for HF reactivity. Recently, the multicomponent spill model from LSM90 (Exxon) was added, and the data base was expanded to include 29 additional chemicals. It is possible to manually enter more chemicals, but the code must be modified to model exotic behavior specific to a chemical (e.g. chemical reactivity), or to include such details as temperature dependent thermodynamic properties.

There is no one code that the working group can recommend to handle all liquid spill scenarios. Instead, the working group recommends the use of the following codes, depending on the situation: TScreen, ADAM, ALOHA, CASRAM-SC, and HGSystem. TScreen is more appropriate for lower hazard facilities, where conservative assumptions and analysis are acceptable. The test problem results show TScreen to almost always give the most conservative result. The other four codes are more sophisticated, and would therefore be useful for higher hazard facilities where it becomes important to reduce conservatisms. There is no reason, however, why they could not also be used for lower hazard facilities. ALOHA and CASRAM-SC may be considered general use codes, because they have an associated substantial data base. The ADAM and HGSystem data bases can be expanded, but this requires some upfront work on the part of the user. Similarly, because of the detailed

modeling in HGSystem of HF chemistry, it should be considered for HF releases. ADAM also models HF chemistry, as well as that associated with the $\text{N}_2\text{O}_4\text{-NO}_2$ and NH_3 systems.

Depending on the scenario, the codes available for source term modeling of liquid spills and evaporation may be adequate. There is some level of confidence associated with the results provided by these codes, and in most applications, the available codes would be acceptable. However, there are some deficiencies in the existing set of codes, as noted below. Any modeling developments should be directed towards these areas:

- (1) Aerosol generation from splashing liquids as they spill and impact surfaces is not well characterized. A model is given in Ballinger (1988) (see Section 6.3.2), but this has not been included in any computer code.
- (2) Multi-component spills are poorly modeled. The models used are simple, and in most cases conservative. The models would be non-conservative for non-ideal solutions showing positive deviations from Raoult's Law.
- (3) Chemical reactivity is generally not included (HF , $\text{N}_2\text{O}_4\text{-NO}_2$ and NH_3 are the exceptions). Consideration should be given to chemical reactions from spills creating mixtures. In some cases, a more hazardous material may be created by the reaction than from either component spilled (e.g. $\text{KCN} + \text{H}_2\text{SO}_4$ produces HCN ; $\text{H}_2\text{SO}_4 + \text{Na}_2\text{S}$ produces H_2S).
- (4) A good model for evaluating the source term from a liquid spill inside a facility was not found. The available codes are generally written for outdoor releases (i.e. evaporation rate is a function of wind speed). ORG40/TP10 can calculate the molecular diffusivity for an arbitrary substance (in still air), but this subroutine needs modification in order for it to be a standalone code.
- (5) The capability to model water reactives would be valuable. Carhart (1995) provides a data base that can be linked to a code, allowing water reactions to be modeled. The data base includes the production of new species as a result of reaction with water. There is a planned upgrade to the CASRAM-SC model, which will incorporate this data on water reactives.

6.1.2 Pressurized Liquid/Gas Releases

Six codes that could generate source terms from pressurized liquid/gas releases were evaluated. The models span a range of levels of sophistication. Table 6 summarizes the results of the evaluations of these codes against the specific criteria for pressurized liquid/gas release.

As noted in the previous section, TScreen and EMGRES are fairly simple codes. These two codes, as well as ADAM, model pressurized releases as steady state releases, based on the initial conditions. They should give conservative results. They do a poor job modeling flash fraction, aerosol entrainment, and two-phase flow. Because of its EPA endorsement, TScreen would probably be the code of choice when compared to EMGRES and ADAM.

As noted in the previous section, ALOHA uses fairly sophisticated models. It can provide a time dependent source term. However, the output provided by the code lacks detail on the source term. This can be particularly frustrating when attempting to obtain time dependent source term information. The results are presented in a rather obscure fashion.

CASRAM-SC does a more sophisticated time dependent assessment of the release. HGSystem also calculates a time dependent mass release rate.

As for the liquid chemical spills and evaporation codes, there is no one code that the working group can recommend to handle all pressurized release situations. Instead, the working group recommends the use of the following codes, depending on the situation: TScreen, ALOHA, CASRAM-SC, and HGSystem.

The codes available for source term modeling of pressurized releases may be adequate. There is a greater degree of confidence associated with the results from the more sophisticated codes (ALOHA, CASRAM-SC, HGSystem). In most applications, the available codes would be acceptable. However, there are some deficiencies in the existing set of codes, as noted below. Any modeling developments should be directed towards these areas:

- (1) The lack of an accurate and reliable aerosol formation model is a real limitation in accurately simulating pressurized liquid releases and subsequent behavior of the formed vapor cloud. The rate and amount of aerosolization has a direct effect on the vapor cloud density and its subsequent behavior. Aerosol formation is an area where the Center for Chemical Process Safety (CCPS) has been conducting research for a number of years (CCPS, 1991). A unified dispersion model (UDM) has been developed that has utilized much of this data in its aerosol formation, evaporation, and rainout algorithm (CCPS, 1995). Although

**Table 6: Summary of Specific Criteria Evaluations for Pressurized Liquid/
Gas Release Codes**

Pressurized Liquid/Gas Release	ADAM	ALOHA	CASRAM- SC	EMGRES	HGSystem	TScreen
Determination of release rate	Y	Y	Y	Y	Y	Y
Determination of initial characteristics of vapor cloud	Y*	Y*	Y	N	Y*	Y*
Consideration of ambient and/or site-specific conditions	Y	Y	Y	N	Y	Y*
Geometry considerations	Y	Y	Y	Y	Y	Y*
Time dependency of rate calculation	N	Y	Y	N	Y	N
Temperature dependency/thermal effects	N	Y	Y	N	Y	Y*
Consideration of critical flow	Y	Y	N	Y	Y	Y
Consideration of two-phase flow	Y	Y	N	N	Y	Y
Consideration of water reactivity	Y	N	N	N	Y	N
Extensive data base provided	N	Y	Y	Y*	Y*	N

Some data/properties must be user specified	N	N	N	N	N	N
All data/ properties must be user specified	N	N	N	N	N	Y
Special features	Y ⁺	N	Y	N	N	N
Linked to transport model	Y	Y	Y	Y	Y	Y
Test problem evaluation	Y	Y	Y	N	Y	Y
Other	N	N	N	N	N	N
Graded Approach applicability	lower hazard	lower hazard	higher hazard	low hazard	higher hazard	lower hazard

Y Feature provided in code.

N Feature not provided in code.

* There are some limitations, described in detailed evaluations found in Appendix B.

+ The special features are described in detailed evaluations found in Appendix B.

proprietary, this model is well documented and should be considered for evaluation by the Spills Working Group as a natural follow-on to address this modeling need.

- (2) Model development is needed in simulating two-phase flow and/or computing flash fractions. There is no detailed pipe/orifice discharge model in which effects such as inter-phase slip, thermal non-equilibrium, and the influence of wall-friction and heat transfer are taken into consideration. Generally, it is assumed that the fraction flashed is instantaneously released. Consequently, the impacts from slower releases modeled in this fashion would be overpredicted. Additionally, the functions used to describe the fraction flashed are underconservative in some cases (e.g. cryogenic releases).

6.1.3 Solid Spills and Resuspension/Sublimation

The computer codes available for calculating the source term from solid spills are few in number. Those that are available are based on empirical models, which are derived from experimental data. Computer codes including resuspension as a secondary source (i.e. resuspension of material deposited on the ground from a plume, rather than resuspension of material deposited on the ground directly from a spill) were not considered here. The interest here was in computer codes/methodologies for generating a primary source term.

There are several contributors to the total source term from a solid spill. These are: (1) airborne material generated as a solid (powder) falls through a distance; (2) airborne material generated as a solid impacts the ground after falling; (3) resuspension of material deposited on the ground; (4) sublimation of solid material deposited on the ground.

The PSpill code can calculate the quantity of airborne material created during a free fall spill in still air. It is based on a correlation developed from experimental data and provides an average airborne release fraction (the bounding value can be obtained by multiplying the average by a factor of 2 (DOE, 1994a)). Only a listing of the code is currently available, and this is provided in Ballinger (1988). The code is short, and can fairly easily be re-created if desired. It is probably easier, however, to simply use the correlation in hand calculations.

DOE (1994a) lists an alternate correlation that can be used in hand calculations for spills of powder in flowing air. KBERT provides an expert user interface to intelligently access all of the data in DOE (1994a). The use of KBERT is recommended (subject to its availability, i.e. when/if it is distributed by DOE).

The group was unable to find any computer code directly modeling the airborne release fraction of a solid resulting from impact to the ground. However, DOE (1994a) does provide an empirical correlation that appears to take this into account (i.e. includes a release fraction due to shear during the fall and due to impact). There is also a correlation that applies to brittle fracture of solid material upon impact (DOE, 1994a). The correlation relates the release fraction of the material aerosolized to the impact energy density as determined from the fall height of small cylinders of pyrex glass. These correlations can be used in hand calculations to estimate the fraction of a material becoming airborne as a result of the fall, or within the framework of KBERT.

Once the solid material has been spilled on the ground, airborne material will continue to be generated as a result of resuspension and/or sublimation. DOE (1994a) provides a review of past studies of resuspension, and provides recommended airborne release values. As part of this working group, a supplemental review of resuspension methodologies was performed. The methodologies reviewed are provided in Appendix D.

HOTSPOT was the only code identified that could model resuspension of solids as a primary source term. The model in HOTSPOT is based on field data taken at the Nevada Test Site (Anspaugh, 1975). The model is conservative with respect to more recent data (see Appendix D). The working group recommends the use of either the HOTSPOT code, DOE (1994a)/KBERT, or the information presented in Appendix D.

Solid sublimation would only be significant for volatile materials. Most solids are not volatile, and hence would not be expected to significantly contribute to an airborne source term. However, there are a few volatile solids that may be present in the DOE complex (e.g. phenol). Some of the codes (e.g., ALOHA,) discussed in section 6.1.1 do have some solids in their data base, and can be used to assess the source term for these materials. However, since there is no specific model for a sublimation-generated source term in the code, the working group does not recommend using the code for this purpose.

For the most part, the methodologies available for source term modeling of solid spills may be adequate. There are few computer codes available to model this type of a spill event. For chemical spills, source terms from solids are generally small relative to other types of releases. This may not, however, be the case for the release of plutonium oxide powder, for example. The main deficiency identified was that there is no code that specifically models solid sublimation. Any modeling development should be directed towards this area.

6.1.4 Resuspension of Dissolved/Suspended Material from Liquid Spills

As with the solid spills, the methodologies available for calculating resuspension of dissolved/suspended material from liquid spills are limited. Empirical models exist for estimating airborne release fractions for free-fall spills (from shear and impact) of liquids (Ballinger, 1988), but no computer codes have been developed to model this phenomenon. HOTSPOT was the only code identified that could model the resuspension as a primary source term once the spilled material is on the ground. HOTSPOT does not, however, distinguish between the resuspension taking place during the evaporation of the solvent, and the resuspension taking place after complete evaporation when only deposited solid material remains on the ground. As noted in the previous section, the model in HOTSPOT is based on field data taken at the Nevada Test Site. Since that time, new data has become available, and additional models have been developed (see Appendix D). Although the models were not developed from data gathered from solid particulate that precipitated from an evaporating liquid, the models available can be applied. The solid material resuspended during the solvent evaporation phase is expected to be small relative to that resuspended once all of the solid has precipitated from the solution and the solvent is no longer present. However, a better understanding of the resuspension process during the evaporation phase would be beneficial.

6.2 Test Problem Results and Insights from the Test Problem Exercise

As previously discussed in Section 4.4, several of the applicable test problems from Hanna and Strimaitis (1989) were solved using the following codes:

- ADAM
- ALOHA
- CASRAM-SC
- HGSystem
- TScreen

In this section, the application of the selected computer codes to the test problems is discussed.

6.2.1 Execution of Test Problems

For all of the codes considered, additional information beyond that provided in the test problems had to be assumed/generated. This

information included tank geometry data and thermophysical property data. Specific assumptions with respect to each of the codes are discussed in the sample problem summaries located in Appendix C. Some of the test problems were not evaluated with some of the codes due to either the inability of the code to handle the problem or time constraints.

6.2.2 Test Problem Results

Table 7 contains a summary of results of the test problems as well as those from the hand-calculations in Hanna and Strimaitis (1989). Note that the hand calculation results should not be considered benchmarks to which the code results can be compared; rather, they are provided only to demonstrate hand-calculation type results. The reader should also realize that due to differences in modeling techniques, a direct comparison of the summary results may be misleading (e.g. comparing steady-state model results to transient model results). The comparability of the test problem results is commented on further in Section 6.2.3, "Insights from the Test Problem Exercise".

Problem #1a: Liquid Anhydrous Ammonia Release via a Failed Connecting Orifice

ADAM, ALOHA, CASRAM-SC, HGSystem, and TScreen all predict that the release will be two-phase, while the hand calculation assumes a priori that the release is 100% liquid. The wide variability in the results of the codes is likely due to assumptions concerning the size and geometry of the ammonia tank, as well as the effective discharge coefficient of the orifice. In addition, CASRAM-SC and HGSystem consider evaporation from a rainout-formed secondary puddle. Note that all of the codes, except CASRAM-SC, use the Fauske-Epstein two-phase equations in either a steady-state or quasi steady-state manner. CASRAM-SC solves a time-dependent mass/energy equation for two-phase flow.

Problem #1b: Liquid Anhydrous Ammonia Release via a Pipe Break

ADAM, CASRAM-SC, and HGSystem do not have a pipe release model; hence they were not used to solve this problem.

The hand calculation and TScreen predicted similar two-phase release rates and flash fractions. The ALOHA result is different from those calculated by TScreen and the hand calculation because the pipe length was increased from 150 inches to 300 inches in order to get ALOHA to solve the problem (ALOHA will not model pipe release calculations for geometries with an L/D of less than 200).

Table 7: Summary Table of Spill Source Term Test Problem Results

Case	Problem 1a: Liquid anhydrous ammonia release via a failed connecting orifice	Problem 1b: Liquid anhydrous ammonia release via a pipe break	Problem 2: Carbon monoxide release via a relief valve	Problem 3: Liquid chlorine release via a failed valve	Problem 4: Acetone release to a diked area
Hand Calculations Hanna & Strimaitis (1989) (a)	21.5 kg/s for 30 minutes liquid release	5.42 kg/s for 123 minutes; two-phase release, $f=0.22$	3.63 kg/s for 5 minutes	1.17 kg/s liquid release	<u>2m/s</u> 0.96 kg/s <u>5m/s</u> 2.10 kg/s
ADAM (b)	23.7 kg/s two phase release, $f=0.19$ (flashed fraction)	no pipe model	case not run	1.35 kg/s two-phase release, $f=0.21$	case not run
ALOHA (c)	3.4 kg/s two-phase release, no flash fraction provided	0.67 kg/s vapor release	0.40 kg/s	0.28 kg/s two-phase release	<u>2 m/s, F-stability:</u> 1.45 kg/s (see note (c)) <u>2 m/s, D-stability</u> 1.19 kg/s (see note (c)) <u>5 m/s, D-stability</u> 2.48 kg/s (see note (c))
CASRAM-SC (d)	21.3 kg/s maximum two-phase release rate (includes flashing, aerosol entrainment, and secondary pool evaporation)	no pipe model	case not run	case not run	<u>2 m/s, F-stability</u> 0.68 kg/s (30 min. avg.) <u>2 m/s, D-stability</u> 0.98 kg/s (30 min. avg.) <u>5 m/s, D-stability</u> 1.67 kg/s (30 min. avg.)
HGSystem (e)	5.3 kg/s maximum two-phase release, $f=0.28$	no pipe model	4.5 kg/s maximum release rate	0.40 kg/s maximum two-phase release rate, $f=0.02$	<u>2m/s</u> 1.03 kg/s (max.) <u>5m/s</u> 1.9 kg/s (max.)
TScreen (f)	21.2 kg/s for 31.4 minutes; two-phase release, $f=0.19$	8.3 kg/s for 80.3 minutes; two-phase release $f=0.19$	3.4 kg/s for 4.9 minutes	1.19 kg/s for 790 seconds; two-phase release, $f=0.21$	<u>2m/s</u> 0.36 kg/s <u>5m/s</u> 0.71 kg/s

Notes:

- (a) - Releases are all modeled as steady-state.
- (b) - Releases are all modeled as steady-state.
- (c) - The reported values are the average release rates for first 1/5 of inventory; see Appendix C for additional source term generation rate data.
- (d) - CASRAM provides time-dependent source terms; see Appendix C for additional source term generation rate data. A surface roughness of 0.1 m was assumed for the acetone release scenario.
- (e) - HGSysstem provides time-dependent source terms; see Appendix C for additional source term generation rate data.
- (f) - Releases are all modeled as steady-state.

Problem #2: Carbon Monoxide Release via a Relief Valve

TScreen and the hand calculation both predict about the same constant release rate. HGSysntem predicts a higher release rate; this is due to its use of a non-ideal gas equation of state. The ALOHA results differ by over an order of magnitude from the rest because the tank pressure had to be reduced from 2230 psig to 999.9 psig (ALOHA returns an error message for pressures above 1000 psig).

ADAM does not contain carbon monoxide in its data base; and while it is possible to add chemicals to the data base it is not a trivial task; hence it was not used to evaluated this problem.

CASRAM-SC was not used to evaluate this problem due to a resource constraint.

Problem #3: Liquid Chlorine Release via a Failed Valve

ADAM, ALOHA, HGSysntem, and TScreen predict that the release will be two-phase, while the hand calculation assumes a priori that the release is 100% liquid. The wide variability in the results of the codes is likely due to assumptions concerning the size and geometry of the chlorine tank, as well as the effective discharge coefficient of the orifice. Note that all of the codes use the Fauske-Epstein two-phase equations in either a steady-state or quasi steady-state manner.

CASRAM-SC was not used to evaluate this problem due to a resource constraint.

Problem #4: Acetone Release to a Bermed Area

The results from the various calculations differed by up to a factor of four. Factors contributing to this variation in the results includes the use of different energy balance and mass transfer models. Some specifics that illustrate this are:

- some of the codes ignore the transient nature of the release (TScreen and the hand calculation);
- the influence of surface roughness on source term generation rate varies from significant (CASRAM-SC [see Appendix C], to very little (ALOHA), to not-modeled (TScreen, and the hand calculation);
- the influence of stability class on source term generation rate varies from significant (CASRAM-SC and ALOHA) to not modeled (HGSysntem, TScreen and the hand calculation).

6.2.3 Insights from the Test Problem Exercise

The initial insight from the test problem exercise is that without experimental data, it is not possible to benchmark the results of the codes in an absolute manner (i.e. determine which code gives answers closest to the "correct" answer). At best, the variability between the code results can be shown, and semi-qualitative conclusions for differences can be drawn (e.g. the results of code x and code y differ by z%, the difference is most likely due to the codes using different pool evaporation models). Results for the anhydrous ammonia and carbon monoxide releases spanned about an order of magnitude; results for the chlorine and acetone releases are within a factor of about three to four.

Even if experimental data were available, it would still be difficult to benchmark the codes. Due to the complex nature of many of the source term algorithms, it is difficult, if not impossible, to discern the causes of differences in the final code results. A model evaluation using standardized performance measures combined with sensitivity analysis would be necessary to determine what might be causing poor correlation with observed values.

Another insight from the exercise is that variability in the specification of the problem had a dramatic impact upon the code results. While some of the problem variability, such as the lack of information about tank geometries, was an artifact of the exercise, other assumptions (e.g. the release is 100% liquid in the anhydrous ammonia release calculation) were typical of those made in SAR analyses.

In addition, modeling differences were also found to have a large impact on the code results. As would be expected, the inclusion or exclusion of a given physical phenomenon in the source term algorithm affected the results (e.g. consideration of rain-out and subsequent pool evaporation, etc.), as did the choice of the specific model used to characterize a given phenomenon (e.g. use of a transient vs. a steady-state pool evaporation model, energy balance methodology, etc.).

The expectation that simpler, more conservative codes give higher source terms was not fully reflected. With the exception of the acetone problem, TScreen gave the most conservative or nearly most conservative results (i.e. highest source term), and ALOHA gave the least conservative result (i.e. lowest source term). In the two cases run with ADAM, it gave the most conservative results. CASRAM-SC and HGSys, the two most sophisticated of the codes, generally gave results in the middle of the range.

In running the test problems, some limitations were encountered with the codes. For example, problem #1b could only be run with ALOHA and TScreen, as the other codes could not model a pipe release. Also, the CO

problem could not be run with ADAM because of a data base limitation. The CO problem had to be modified for ALOHA (gas pressure had to be reduced) due to a hard-wired limitation on input gas pressure.

In summary, the test problem exercise did not act as a benchmarking for the codes. The codes were found to yield different results for ostensibly the same problems. The causes of the differences in the codes results are due to variations in the model assumptions, the code inputs, and the use of different methods to model a given physical phenomenon. In order to draw further conclusions with respect to the veracity of the codes, comparisons and evaluations of the individual models with available field observations should be performed.

6.3 Role of Hand Calculations

In general, it is the group's consensus that hand calculations are always acceptable. However, they may typically only be practical for simple problems. When analysis requires the use of formulations that can readily be done by hand, this approach is recommended. Codes are more suited for repetitive tasks or in situations where complex solutions are required. Codes separate the user from what they are doing, making it possible to lose sight of details or misapply the code. The analyst is more intimate with what is being done when performing hand calculations, and this should reflect a better understanding of the problem being studied.

If an algorithm is simple, the group recommends using hand calculations rather than a code. For example, ARCHIE is an example of a code with very simple algorithms. We did not specifically evaluate this code because it is no longer maintained. However, some algorithms used in the code have merit and it would be acceptable to use them in hand calculations. ORG40/TP10 is also simple, and direct use of the algorithms would be acceptable (particularly since these require development of a user interface to be used as standalone codes). Some useful formulations for hand calculations for various spill phenomena are provided later in this section. It was agreed that spreadsheet-type calculations are essentially equivalent to hand calculations.

It was noted that hand calculations may be particularly useful for problems like resuspension, where there are only a very limited number of codes. Appendix D provides a summary of methodologies that can be used to estimate source terms with hand calculations. Actual data can also be used in these cases.

DOE (1994a) provides an extensive set of experimental data for airborne release fractions and respirable fractions. A knowledgeable analyst can use

this information to generate source terms through hand calculations. A danger exists for mis-application of the information by analysts not fully familiar with the data. In this regard, KBERT, if ever fully developed, would be an excellent tool.

6.3.1 Liquid Evaporation Hand Calculation Model

In the EPA document, Technical Guidance for Hazards Analysis: Emergency Planning for Extremely Hazardous Substances (EPA, 1987), the following equation is provided for use in calculating the rate of release to air for liquids:

$$QR = \frac{0.106 \cdot u^{0.78} \cdot MW^{2/3} \cdot A \cdot VP}{R \cdot (T + 273)}$$

where

QR rate of release to air (lb/min)
u windspeed (m/s)
MW molecular weight (g/gmole)
A surface area of spilled material (ft²)
VP vapor pressure of material at temperature of interest (mm Hg)
R 82.05 atm · cm³/g · mole K
T temperature of interest (°C).

6.3.2 Free-fall Spill of Liquid Hand Calculation Model

An empirical model for the airborne release fraction from a free-fall spill of a liquid has been developed (Ballinger, 1988). This does not account for post-event evaporation, but it includes airborne material created during the spill/impact. In this model, the airborne release fraction is defined by:

$$ARF = 8.9 \times 10^{-10} \cdot Arch^{0.55}$$

$$Arch = \rho_{air}^2 \cdot h^3 \cdot g / \mu^2$$

where

ARF airborne release fraction
Arch Archimedes number
ρ_{air} density of air (g/cm³)
h spill height (cm)
g gravitational acceleration (981 cm/s²)
μ solution viscosity (poise).

6.3.3 Free-fall Spill of Powder Hand Calculation Model

An model for the airborne release fraction from a free-fall spill of a powder has been developed (Ballinger, 1988). In this model, the bounding airborne release fraction is defined by:

$$ARF = 0.2128 \cdot M_o^{0.125} \cdot h^{2.37} / \rho_{BP}^{1.02}$$

where

ARF bounding airborne release fraction

M_o mass of powder spilled (kg)

h spill height (m)

ρ_{BP} bulk density of powder (kg/m³).

6.3.4 Five-Factor Formula

A common approach for estimating the source term for radionuclide releases from non-reactor nuclear facilities is the "five factor formula". The five-factor formula defines the source term as the product of five scenario and material -specific factors:

$$\text{Source Term} = \text{MAR} \cdot \text{DR} \cdot \text{ARF} \cdot \text{RF} \cdot \text{LPF}$$

where

MAR material at risk, the amount of hazardous material available to be acted upon by a given stress

DR damage ratio, the fraction of the MAR actually impacted by a given physical stress from a specific event

ARF airborne release fraction, the fraction of the impacted material (MAR x DR) that can be suspended in air to become available for airborne transport due to a specific set of induced physical stresses

RF respirable fraction, the fraction of the airborne material present in such a form that can be inhaled into the human respiratory system (e.g. particle size < 10 μm aerodynamic equivalent diameter)

LPF the fraction of the airborne material that leaves the confinement barrier after consideration of depletion mechanisms such as precipitation, settling due to gravity of the released particulate material, or due to agglomeration or filtration.

This formula can be utilized to estimate source terms by hand for a variety of scenarios. Although most commonly used for releases of radioactive materials, it is also suitable for non-radioactive materials. The MAR and DR values are dependent on the scenario being studied. An excellent summary of data for ARFs and RFs is found in DOE (1994a). The LPF can be

conservatively set to one, or estimated by various methodologies. These methodologies have been studied in detail by the APAC In-facility Transport Working Group (Spore et al. (1996)).

7. Recommendations

The following subsections summarize the recommendations of the Spills Working Group. The first subsection summarizes the group's recommendations on which models are acceptable for SAR-type analyses. The second subsection lays out the path forward, and provides a set of recommendations for future work. The last subsection provides a set of good practices that an analyst should consider when first addressing an issue in safety analysis.

7.1 Recommended Spills Source Term Evaluation Models

Before selecting a particular code or model for assessing a source term, the objective and constraints of the analysis should be understood. The basis for omitting or including a particular factor in the analysis should be known, so that the best model for the given application can be selected.

Based on the limited review of readily available codes, and the noted limitations of the codes reviewed, the Spills Working Group recommends the codes listed in Table 8 for application to the various spill-type event. Before using any of these codes, the analyst is referred to the code evaluations in Appendix B so that any code limitations are understood.

Table 8 lists the recommended codes for each of the four spill-type of events considered in this work, and for three levels of facility hazard. Codes capable of modeling additional complex phenomena associated with the first two types of spill events have been specifically called out below:

Multi-component spills: CASRAM-SC, HGSystem (models need improvement)

Water Reactives: planned upgrade to CASRAM-SC

Reactive Chemicals: HGSystem (HF), ADAM (HF, N₂O₄-NO₂, NH₃)

Table 8: Spills Working Group Model Recommendations

Facility Hazard Category	Liquid Chemical Spills and Evaporation	Pressurized Liquid/Gas Releases	Solid Spills and Resuspension/ Sublimation	Resuspension of Material from Spilled Liquids
Low/ Category 3	TScreen ADAM ALOHA CASRAM-SC HGSystem	TScreen ALOHA CASRAM-SC HGSystem	HOTSPOT KBERT a	HOTSPOT a
Moderate/ Category 2	ADAM ALOHA CASRAM-SC HGSystem	ALOHA CASRAM-SC HGSystem	HOTSPOT KBERT a	HOTSPOT a
High/ Category 1	CASRAM-SC HGSystem	CASRAM-SC HGSystem	HOTSPOT KBERT a	HOTSPOT a

^a The information in Appendix D can also be used.

7.2 Future Model/Code Development and Path Forward

Possible future work for the Spills Working Group is identified in this section. In addition, development areas identified in the discussion in Section 6.1 are summarized below.

Follow-on Work for Spills Working Group

- (1) The group agreed that it would be valuable to expand and conduct a more thorough search of models available, first in the U.S., and then internationally. This wider search for state-of-the-science models could include private sector codes if certain conditions are met pertaining to documentation and ultimately to licensing fees.
- (2) It was suggested that a performance evaluation of evaporating pool models against as complete a data set as possible should be conducted. A search for spill and evaporation experimental data for comparison with predictions would be valuable. A comparison against measured data would provide insight on model performance.

- (3) A more thorough review of the codes, including understanding why the sample problem results were different, would be beneficial. The review could include a sensitivity/uncertainty analysis. This would provide a better understanding of which parameters have greatest influence on the source term under a variety of spill event conditions. For sensitive parameters, median and bounding values could be identified for use by the safety analyst.
- (4) Some effort should be directed towards providing better guidance on selection of pool depth. The 1 cm depth commonly used appears to be arbitrary. It was suggested by the EPA (1987), but appears to have little basis. It would be possible to use CASRAM-SC to examine a range of different spill scenarios/conditions, onto different surfaces, to get a range of reasonable depths. CASRAM-SC considers surface tension, viscosity, surface roughness, etc. There are complications such as dike areas, overflow into storm drains/other catchments, which are site specific. However, it would be possible to generate a typical depth for an unconfined spill onto typical surfaces with typical roughness.

Model Development

- (1) Improved modeling to handle flash fraction formation properly is needed. The formulations used in existing codes may produce underestimates of potential health and safety consequences in some cases (e.g., cryogenic releases). In addition, two-phase flow in pipes cannot be properly modeled with the codes considered in this study (e.g. frictional losses in pipes are not accounted for).
- (2) Aerosol generation and entrainment is not properly characterized in the codes that were reviewed. The lack of an accurate and reliable aerosol formation model is a real limitation in accurately simulating pressurized liquid releases and subsequent behavior of the formed vapor cloud. The rate and amount of aerosolization has a direct effect on the vapor cloud density and its subsequent behavior.
- (3) A good model for liquid pool evaporation inside a facility does not currently exist. The codes are generally written for outdoor releases (i.e. evaporation rate is a function of wind speed). ORG40/TP10 can calculate the molecular diffusivity for an arbitrary substance in still air. The code needs modification in order for it to be run on its own.
- (4) The capability to model water reactives would be valuable. Carhart (1995) provides a data base that can be linked to a code, allowing water reactions to be modeled. The data base includes the production of new species as a result of reaction with water. With some modest support, the CASRAM-SC model could be easily modified to provide capability to assess the

consequences of spills into waterways or involving mixtures with water on a spill surface.

- (5) Spills involving multi-components or chemical mixtures could pose significant worker or public risks. The models included in the Spills Working Group initial review could not perform multi-component assessments, or did not adequately treat the physics and thermodynamics of the problem. Consideration should also be given to potential chemical reactions that may occur subsequent to a spill.
- (6) A code should be developed to specifically model solid sublimation.
- (7) A better understanding of the resuspension process during the evaporation phase of a spilled liquid containing dissolved/suspended solid material would be beneficial.
- (8) Continued support for the development of KBERT should be provided so that this potentially very useful tool can be released for use by safety analysts.

7.3 Good Engineering and Safety Analysis Practices

Throughout the Spills Working Group activity, a listing of good analysis practices has been developed. This is comprised of a set of recommended approaches, assumptions, and parameter values to be used when estimating source terms from spill-type events. It includes general guidance on best practices for safety analysis, along with more specific guidance related to consistent modeling procedures.

A number of general best practices have been provided by the In-Facility Transport Working Group (Spore et al., 1996), the Chemical Dispersion and Consequence Analysis Working Group (Lazaro et al, 1997), and the Radiological Dispersion and Consequence Analysis Working Group (O'Kula et al., 1997). These recommendations should be considered along with those provided below when performing source term assessments.

7.3.1 General Guidance

- (1) Chemical Lists. The group decided that it would be valuable to provide guidance on which chemicals in particular to look at for source terms. This is particularly important if a facility contains a substantial number of different materials. The lists can be used to reduce the set of chemicals down to a manageable number for analysis, retaining those that

are of greatest concern. There are several lists of chemicals, which have identified specific chemicals as being hazardous for one reason or another. The lists that the group recommends to be consulted include:

- EPA list (40CFR68.130, (CFR1))
- OSHA list (29CFR1910.119 (CFR2))
- DOE-EH list
- Sample list of hazardous chemicals within the DOE complex (from the Chemical Vulnerability Study (DOE, 1994b)).

These lists are provided in Appendix E.

(2) Chemical Selection Criteria. We identified two EPA criteria for its list of Regulated Substances Rule (Final Rule FR January 31, 1994) in support of its Risk Management Program. This should be considered in part when identifying chemical vulnerabilities for hazard assessment in safety analysis work. However, caution is advised that this criterion should not be used exclusively in eliminating chemicals from hazard analysis. Other factors that can play an important role in the potential impact to workers and the public include process operating parameters, such as high temperature and pressure. If the analyst chooses to evaluate chemicals not on the lists provided in Appendix E (and noted above), the EPA criteria noted below can be used as an additional basis for selection.

- include chemicals with vapor pressure above 10 mm Hg (interpreted to be at 20 °C)
- include chemicals in concentrations above 1 %wt.

(3) Consult EPA Documents, where appropriate. An earlier methodology study that was performed for the EPA was identified (EPA, 1993). The study considered three of the codes (ADAM, ALOHA, HGSys) that are evaluated as part of this work (although earlier versions). In addition to the source term models, the EPA study was also interested in the dispersion aspect. One of the key objectives of the work was to define methods to determine input variables used by the various codes. This reference should be consulted when selecting parameter values. Some specific guidance from this report is summarized in Section 7.3.2.

7.3.2 Specific Guidance

(1) Release Diameter or Area. It is important to provide some guidance on the specifics associated with pressurized liquid/gas release scenarios (e.g. size of discharge point). Some guidance, in the absence of better information, is found in Appendix B of "Guidelines for Use of Vapor Cloud Dispersion Models", by Steve R. Hanna and Peter J. Drivas (Hanna and Drivas, 1987). This is summarized below:

Most studies involve examining Largest Practicable and Largest Potential releases. A Largest Practicable release is one with some reasonable potential of occurrence. A Largest Potential release assumes catastrophic rupture of either the storage vessel or large diameter piping. Some typical examples are:

Largest Practicable

- + rupture of small bore piping, 1" maximum
- + partial flange gasket blow-out of large diameter piping (e.g. 50% blowout of a 2" line resulting in an equivalent hole diameter of 1")
- + failure of a 3/4" fusible plug on a 1 ton cylinder
- + generally limited release duration (15 minutes typical based on time required for operator intervention to stop the leak)

Largest Potential

- + rupture of 2" or 3" liquid line
- + tank truck rupture on a highway (3" or 4" assumed hole size typical)
- + typically, entire source vessel inventory spilled

In addition, EPA (1993) provides some additional guidance on release diameter or area. This is summarized below:

Liquid Pool: The release area is simply the area of the pool. In the absence of a pool depth with technical basis, a depth of 1 cm has been used in the past (EPA, 1987).

Jet Releases: Some expansion at the source usually takes place for a jet release. There are two methods that can be used to estimate the post-expansion dimension of a release, depending on the momentum associated with the release:

Low Momentum-

$$D_{rel} = (2 \cdot E / (u_r \cdot \rho_{rel}))^{0.5}$$

where

D_{rel}	release diameter (m)
E	emission rate (kg/s)
u_r	ambient wind speed (m/s)
ρ_{rel}	release density (kg/m ³)

This formulation should be used if the release is unchoked and the exit velocity is of the same order or less than the ambient wind velocity. The exit velocity can be obtained from:

$$v = E / (A \cdot \rho_s)$$

where

v	exit velocity (m/s)
E	emission rate (kg/s)
A	emission area (m ²)
ρ_s	density of the material in the container (kg/m ³)

The low momentum formula should be used if the released volume of an instantaneous release is not known. If the release volume is available, the release diameter can be taken to be the spherical or cylindrical equivalent diameter of the released volume. If the release is at ground level, assume the cloud formed is cylindrical with the base on the ground, and the height equal to the diameter. If the release is not at ground level, assume the cloud is spherical in shape.

Most jets would qualify as high momentum releases. If the release is a choked gas, the high momentum formula should be used but the value of ρ_s should be replaced with the density at choked conditions.

High Momentum-

$$D_{rel} = D_s \cdot (\rho_s / \rho_{rel})^{0.5}$$

where

D_{rel}	release diameter (m)
D_s	hole or stack diameter (m)
ρ_{rel}	release density (kg/m ³)
ρ_s	density at the hole (kg/m ³)

For a continuous release, if the exit velocity is unknown, the smaller diameter calculated from the two formulas should be used. The smaller diameter will minimize the release buoyancy. The smaller the release diameter, the more likely that the release will behave as a denser-than-air release.

(2) Ground Surface Temperature. If ground surface temperature data are not available from routine on-site measurements, EPA (1993) recommends that the ground surface temperature be set to the ambient temperature.

(3) Dense Gas Effects. If a release can be considered denser than air, standard passive dispersion modeling does not apply. To determine if a release is denser than air, the Richardson number should be calculated (Spencer and Havens (1989), NOAA (1992)).

$$R_{io} = g \cdot [(\rho_g - \rho_a) / \rho_a] \cdot V / (D_{rel} \cdot u \cdot u.^2)$$

Where

R_{io}	friction Richardson Number
ρ_g	gas density (kg/m ³)
ρ_a	air density (kg/m ³ , approximately 1.2 kg/m ³ for air)
V	volumetric gas generation rate (m ³ /s, based on spill rate, flash fraction, and gas density)
D_{rel}	initial plume diameter (see section 7.3.2, item (1))
u	velocity (m/s, at 10 m height)
$u.$	friction velocity of the ambient air flow (m/s, approximately equal to $u/16$)

Values of R_{io} in excess of ~ 1 - 10 indicate that heavy gas effects are important (Spencer and Havens (1989), NOAA (1992)).

(4) Consistency in Parameter Selection. The analyst should be consistent in making realistic selection of parameters for a given problem. That is, for example, the material properties used should be at a temperature consistent with the scenario. Or, a turbulent mass transfer coefficient should be used with high wind speed. Additional specific guidance on parameter selection is given below:

(a) Pool area and depth (and spill size) should be related. These should be based on the volume of material spilled and if possible, they should consider the details of the spill site.

(b) The temperature used should be a value that provides bounding impacts, within the context of a given scenario. A spilled fluid should be assumed to be at the operating temperature or ambient; the ground should be suitably factored into the solution to provide a bounding value; the air should be conservatively warm (hot day) to provide a bounding value.

(c) Wind speed should be selected based on the goal of the overall analysis (e.g. if maximum impacts are desired). The overall picture should be considered, from the source term to dispersion in the environment. If the goal is to obtain a bounding impact, this may or may not result from a bounding source term. For example, an outdoor spill of a liquid will have a higher source term for a higher wind speed, but a higher wind speed will result in greater dispersion in the atmosphere. Some source term models are also dependent on stability class (i.e. source depends on vertical

velocity profile/turbulence). As with the wind speed, the parameter selection should be based on the type of ultimate impacts that one is trying to generate. Building wake effects may also affect the source term, as well as dispersion. The convolution of source term and dispersion that gives the desired impact (e.g., bounding result) should be the basis of parameter selection.

(5) Caution for Cryogenic Releases. An instantaneous spill is not always the worst case. For example, when the boiling point of the material is significantly below ambient, an instantaneous release may result in freezing of the ground. This may change the ground thermal conductivity in such a fashion that the source term is not maximized.

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Appendix A: Summary of Requirements

Introduction

As part of the APAC assessment effort, each of the six working groups was tasked with reviewing DOE regulatory/licensing documents, and identifying from them specific requirements that would influence the nature of the methodologies that would be considered acceptable for safety analysis. The spills working group reviewed the following documents:

- **Nuclear Safety**
SEN-35-91, Nuclear Safety Policy
- **Facility Safety Analysis Reports**
DOE Order 5480.23, Nuclear Safety Analysis Reports
DOE Order 5481.1B, Safety Analysis and Review System
DOE-STD-1027-92, Hazard Categorization and Accident
Analysis Techniques for Compliance with
DOE Order 5480.23, Nuclear Safety Analysis
Reports
DOE-STD-3009-94, Preparation Guide for U.S. Department
of Energy Nonreactor Nuclear Facility Safety
Analysis Reports
DOE-STD-3011-94, Guidance for Preparation of DOE
5480.22 (TSR) and DOE 5480.23 (SAR)
Implementation Plans
- **Process Safety and Risk Management**
29CFR1910.119, Worker Chemical Safety
40CFR68, Risk Management Programs for Chemical
Accident Release Prevention
- **Emergency Planning**
DOE Order 5500.3A, Planning and Preparedness for
Operational Emergencies
Emergency Management Guide, Guidance for Hazards
Assessment, 6-26-92
- **Design Requirements**
DOE Order 6430.1A, General Design Criteria

- **DOE Handbooks**

*DOE-HDBK-3010-94, Airborne Release Fractions/Rates
and Respirable Fractions for Non-reactor Nuclear Facilities*

The group attempted to glean requirements from these documents. Although the requirements for spill source terms were generally vague, an attempt was made to interpret these as concrete capabilities. These became our evaluation criteria for spills methodologies.

To cover the wide range of potential spill scenarios, four specific types of spills were identified:

- (1) liquid spills and evaporation
- (2) pressurized liquid/gas releases
- (3) solid spills and resuspension/sublimation
- (4) resuspension of particulate material from liquid spills

We ultimately identified separate evaluation criteria for each different type of spill.

The approach taken and documented here was to review each document, and to identify relevant sections. Citations are provided later in this appendix. An attempt to interpret the relevant citations from each document as a requirement for spills methodologies was then made. These interpretations were then summarized, and an overall set of requirements was identified. The summary is provided below. These were then further developed into more specific evaluation criteria. The evaluation criteria are provided in Sections 4.2 and 4.3 of the main report, and in Appendix B with the code evaluations. Citations and interpretations of the individual documents are provided on the pages to follow.

Summary of Requirements for Spills Methodologies

Safety analysis methodologies must be capable of calculating the source term from spill events so that the impact of operations and accidents can be assessed. The SAR is also concerned with the performance of safety-related equipment when exposed to accident conditions that may be detrimental to their function. Thus, an appropriate source term (i.e., conservative, which will lead to a bounding consequence) must be determined so that concentrations of hazardous material to which workers, equipment, and the public are exposed can be evaluated. The requirements documents were

reviewed, and based on that, analysis methodologies should be capable, at a minimum, of the following:

Liquid Spills and Vaporization

- determining rate of release/duration of release
- including site-specific conditions
- including physical features/properties
- including chemical properties
- modeling mixtures/solutions
- characterizing the initial vapor cloud (e.g. temperature, density, size)
- including materials with vapor pressures above 10 mmHg (@20 °C)

Pressurized Gas/Liquid Releases

- determining rate of release/duration of release
- determining vapor fraction (flash fraction)
- including site-specific conditions
- including physical features/properties
- including chemical properties
- characterizing the initial vapor cloud (e.g. temperature, density, size)

Solid Spills and Resuspension/Sublimation

- determining release fraction/rate
- including site-specific conditions
- including physical features/properties (e.g., process equipment and conditions)
- including chemical properties
- including particle size distribution
- being applicable to both chemicals and radionuclides

Resuspension of Particulate Matter from Liquid Spills

- determining release fraction/release rate/release duration
- including site-specific conditions
- including physical features/properties (e.g., process equipment and conditions)
- including particle size distribution
- being applicable to both chemicals and radionuclides

The methodologies should cover a range of levels of sophistication, so that the ability to do more sophisticated analyses where hazard level and/or complexity dictate, is available. This may range from hand calculations (e.g. BIO) to very sophisticated analyses making use of all of the above listed capabilities (e.g. Category 2 facility).

**Citations and Interpretations from Requirements
Documents for
Spills Working Group**

SEN-35-91, Nuclear Safety Policy

Interpretation of Requirements:

The policy statement is concerned with impacts of facility operation on the surrounding population. Safety analysis methodologies must be capable of calculating the source term from spill events so that the impact of operations can be assessed.

Citations:

P 2, 3. (Safety Goals):

"DOE has adopted two quantitative safety goals to limit the risks of fatalities associated with its nuclear operations. These goals are the same as those established for nuclear power plants by the Nuclear Regulatory Commission (NRC) and, like the NRC goals, should be viewed as aiming points for performance. The goals are:

The risk to an average individual in the vicinity of a DOE nuclear facility for prompt fatalities that might result from accidents should not exceed one-tenth of one percent (0.1%) of the sum of the prompt fatalities resulting from other accidents to which members of the population are generally exposed. For evaluation purposes, individuals are assumed to be located within one mile of the site boundary.

The risk to the population in the area of a DOE nuclear facility for cancer fatalities that might result from operations should not exceed one-tenth of one percent (0.1%) of the sum of all cancer fatality risks resulting from all other causes. For evaluation purposes, individuals are assumed to be located within 10 miles of the site boundary."

DOE Order 5480.23, Nuclear Safety Analysis Reports

Interpretation of Requirements:

This Order provides requirements for nuclear facility safety analysis reports. In the SAR, an accident analysis must be performed to demonstrate that there is reasonable assurance that the DOE operation can be conducted in a manner that will limit risk to the health and safety of workers and the public, and will adequately protect the environment. The analysis must also conform to the graded approach, where more sophisticated analysis is expected for more hazardous/complex facilities or operations. The SAR is also concerned with the performance of safety-related equipment when exposed to accident conditions that may be detrimental to their function. Thus, safety analysis methodologies must be capable of calculating the source term from spill events so that the impacts of accidents can be assessed. The methodologies should cover a range of levels of sophistication, so that the ability to do more sophisticated analyses where hazard level and/or complexity dictate, is available. Generally, conservative (bounding) assumptions should be made, as the operating envelope (i.e. TSRs) is based on these assumptions. Although the Order considers that quantitative risk assessment techniques be used where appropriate, the scope of the working group will be limited to consequence evaluation only.

Citations:

Para 8.:

"The safety basis to be analyzed shall include management, design, construction, operation, and engineering characteristics necessary to protect the public, workers, and the environment from the safety and health hazards posed by the nuclear facility or nonfacility nuclear operations."

Para 8.b.(3)(k):

"Analysis of normal, abnormal, and accident conditions, including design basis accidents; assessment of risks; consideration of natural and manmade external events; assessment of contributory and casual events, mechanisms, and phenomena; and evaluation of the need for an analysis of beyond-design-basis accidents; however, the SAR is to exclude acts of sabotage and other malevolent acts since these actions are covered under security protection of the facility."

Para 8.c.(3):

"Evaluation of Potential Releases. The hazard analysis shall identify energy sources or processes that might contribute to the generation or uncontrolled release of hazardous materials. The hazard analysis shall estimate the consequences of accidents in which the facility or process and/or materials in the inventory are assumed to interact, react, or be released in a manner to produce a threat or challenge to the health and safety of individuals on site and off site."

Att 1, P 2, 3.a.(1)(a) 5:

"Provide analyses of expected releases, exposures, accidents, and consideration of residual risks to furnish the basis for a conclusion that the risks and consequences of operation are acceptable;"

Att 1, P 15-16, 4.f.(1)(b).(c).(d):

Graded Approach: "The essence of the requirement is that the level of effort necessary to create and maintain an SAR, the sophistication of the analyses that go into the preparation of the SAR, and the thoroughness of documentation in the submitted SAR should all be proportioned to three factors:

1. The magnitude of the hazards being addressed;
2. The complexity of the facility and systems being relied on to maintain an acceptable level of risk; and
3. The stage or stages of the facility life cycle for which DOE approval is sought."

"SAR material dealing with greater potential consequences, must be more penetrating, thorough, and well-documented than SAR material dealing with lesser hazards."

"The allocation of emphasis in analysis and documentation should be proportioned to the complexity for each subject in each SAR."

Att 1, P 26, 4.f.(3)(d).5:

"The energy sources and release processes shall be specified to assess the hazards of the facility, and the bounding analyses of potential accidents associated with each type of hazard should be documented."

Att 1, P30, 4.f.(3)(d).11a:

"Safety analyses should include the application of methods such as deterministic safety analysis, risk assessment, reliability engineering, common-cause failure analysis, human reliability analysis, and human factors safety analysis techniques as appropriate to the identification, investigation, elimination, mitigation, or control of vulnerabilities of the facility to accidents and accidental releases."

Att 1, P 31-34, 4.f.(3)(d), 11b.c.d.e.i.j.n:

"The likelihood and consequences of accidents beyond the design basis accidents should be evaluated to provide a complete documented rationale for acceptance or rejection of the operation of the facility, and to estimate the residual risk associated with facility accidents. The safety analysis is to consider beyond-DBAs as to the potential effects to the public health and safety and protection for the workers."

"The range of accident scenarios analyzed in an SAR should be such that a complete set of bounding conditions to define the envelope of accident conditions to which the operation could be subjected are evaluated and documented."

"Based on the material and energy involved, the physical parameters of the immediate environment can be determined. These parameters may include energy density, temperature, humidity, smoke, concentration of toxic and/or corrosive fumes, shrapnel, explosive atmosphere, and so on."

"The accident analyses should demonstrate:

- i. The adequate protection of health and safety for members of the public both on and off the DOE reservation at which the facility is located;
- ii. The health and safety of workers on the DOE reservation not involved in or responsible for the facility or its safety;
- iii. The adequate protection of the environment from accidental contamination by the facility; and
- iv. The adequate protection of facility workers, particularly as necessary to support their reliable function of safety-related activities as well as individual protection."

"Accident analyses should be developed to furnish an objective basis for verifying the adequacy of provisions to both prevent and mitigate accidents. Accident analyses should also provide the basis for evaluating the incentives and priorities for alternatives that may reduce facility risks."

"Accident and incident analyses should be developed as necessary to identify and validate the technical content of skills and abilities catalogs needed for the development of training and operating procedures for normal, abnormal, and emergency conditions."

"Accident analyses should document the derivation of environmental qualification requirements for safety components. This includes establishing the environmental conditions (e.g., radiation levels, humidity, pressure, temperature) that could be created in rooms containing safety components by credible accidents during which those components would be called upon to

function. The analyses would justify the capability of components to withstand these conditions and accomplish their intended function.

Att 1, P 41, 4.f.(3)(d),16a:

"Safety analyses should furnish a logical basis for the comprehensive definition of the acceptable operating envelope for nuclear facilities in compliance with the DOE 5480.TSR (.22), TECHNICAL SAFETY REQUIREMENTS, and the related guidance document."

Att 1, P 44, 4.f.(4):

"...the thoroughness of documentation of each Safety Analysis Report be proportionate with several factors. One of these factors is the hazard level of the facility."

Att 1, P 46, 4.f.(6)(b):

"A conservative, deterministic accident analysis must be performed for hazard classification purposes. It need be no more sophisticated and cover no more scenarios than necessary to identify the hazard classification of the facility."

Att 1, P 47, 4.f.(9)(b)1:

"Deterministic accident analyses consisting of bounding analyses of the consequence of limiting, design basis events, including the postulation of the worst single failure among active engineered safety features ..."

DOE Order 5481.1B, Safety Analysis and Review System

Interpretation of Requirements:

This Order provides requirements for non-nuclear facility safety analysis reports. In the SAR, an accident analysis must be performed to demonstrate that there is reasonable assurance that the DOE operation can be conducted in a manner that will limit risk to the health and safety of workers and the public, and will adequately protect the environment. Thus, safety analysis methodologies must be capable of calculating the source term from spill events so that the impacts of accidents can be assessed.

Citations:

Chp I, 3.a.(5):

"Demonstrate that there is reasonable assurance that the DOE operation can be conducted in a manner that will limit risks to the health and safety of the public and employees, and adequately protect the environment."

Chp II.4.a:

"The safety analysis should address in appropriate detail the following topics to the extent applicable:

- (5) Probability of occurrence and predicted consequences of hazards expressed in qualitative or quantitative terms;
- (7) Potential accidents, including those resulting from natural phenomena;"

DOE Order 5500.3A, Planning and Preparedness for Operational Emergencies

Interpretation of Requirements:

This Order provides requirements for assessments needed for emergency planning purposes. Accidents must be analyzed to identify the extent of emergency planning required. Thus, analysis methodologies must be capable of calculating the source term from spill events so that the impacts of accidents can be assessed. Material release characteristics, such as respirable fraction, particle size distribution, chemical form, energy content, release height, release duration, etc. should be determined. The phenomenology accompanying the release should be factored into the source term calculation.

Citations:

Para 9.d.:

"Hazard assessments provide the technical basis for emergency management programs. The extent of emergency planning and preparedness required for a particular facility directly corresponds to the type and scope of hazards present and the potential consequences of accidents or events. A hazards assessment includes identification of any hazards and targets unique to a facility, analyses of potential accidents or events, and evaluation of potential accident or event consequences. For the most part, hazard assessments used for emergency planning purposes can be derived from DOE assessments of hazards required by DOE 5481.1B and 5630.11. It is understood that not every conceivable situation will be analyzed, and, thus, not every response can be preplanned. However, the existence of an adequate hazards assessment, in combination with effective emergency planning and preparedness, provides the framework for response to virtually any Operational Emergency."

Para 11.b.(2):

"For each potential Operational Emergency considered, the assessment must address the determination of initiating events, accident mechanisms, equipment or system failures, event indications, contributing events, source terms, material release characteristics, topography, environmental transport and diffusion, and exposure considerations."

29CFR1910.119, Process Safety Management of Highly Hazardous Chemicals

Interpretation of Requirements:

This rule provides requirements for preventing or minimizing the consequences of catastrophic releases of toxic, reactive, flammable, or explosive chemicals (including a Process Hazard Analysis, PHA). Accidents must be analyzed to understand the extent of impacts. Thus, analysis methodologies must calculate the source term from spill events so that the consequences of accidents can be provided for the PHA. Varying levels of sophistication of analysis techniques are required so that the appropriate one, commensurate with the complexity of the process, can be used. Note that this rule focuses on worker safety and accident prevention. SAR requirements for worker safety include only a qualitative hazard analysis. Thus calculation of a source term to assess worker impacts is not needed for SARs. Further, the scope of the working group includes only consequence assessment. Thus, accident prevention or likelihood reduction is not included. Consequently, this rule is generally not applicable to SAR analyses.

Citations:

P 366, (e)(1) (Process Hazard Analysis):

"The process hazard analysis shall be appropriate to the complexity of the process and shall identify, evaluate, and control the hazards involved in the process."

P 366, (e)(3)(iv)(Process Hazard Analysis):

"The process hazard analysis shall address:

- (iv) Consequences of failure of engineering and administrative controls;

P 376, Appendix C, 4. (Process Hazard Analysis):

"A PHA is directed toward analyzing potential causes and consequences of fires, explosions, releases of toxic or flammable chemicals and major spills of hazardous chemicals."

P 377-8, Appendix C, 4. (Process Hazard Analysis):

"Consideration should first be given to those processes with the potential of adversely affecting the largest number of employees. This prioritizing should consider the potential severity of a chemical release, the number of potentially affected employees, the operating history of the process such as the frequency of chemical releases, the age of the process and any other relevant factors."

40 CFR68. Risk Management Programs for Chemical Accidental Release Prevention; Proposed Rule

Interpretation of Requirements:

This rule provides requirements for risk management programs at facilities that manufacture, process, use, store, or otherwise handle regulated substances in quantities that exceed specified thresholds. A risk management plan must be developed that includes the consequences of accidents. Thus, analysis methodologies must be capable of calculating the source term from spill events (including size, concentration, and rate of release/duration of release) so that the consequences of accidents can be provided for the PHA. Site specific conditions affecting the release rate should be considered. Physical and chemical properties should be included in the analysis. Consideration should be given to materials with vapor pressures greater than 10 mm Hg (@20 °C).

Citations:

P 54192, II.A.(Risk Management Programs, Clean Air Act Requirements):

"The regulations under this subparagraph shall required the owner or operator of stationary sources at which a regulated substance is present in more than a threshold quantity to prepare and implement a risk management plan to detect and prevent or minimize accidental releases of such substances from the stationary source, and to provide a prompt emergency response to any such releases in order to protect human health and the environment."

"The risk management plans must include a hazard assessment that evaluates potential effects of an accidental release of any regulated substance. The hazard assessment must include an estimate of potential release quantities and downwind effects; including potential exposure to populations. The assessment also must include a five-year release history, including the size, concentration, and duration of releases, and must consider worst-case release scenarios."

P 54192, II.A.(2)(Risk Management Programs, Clean Air Act Requirements):

"The proposed rule would required facilities to do three things:
(2) The hazard assessment would include offsite consequence analyses and a fire-year accident history."

P 54192, II.A.(3)(Risk Management Programs, Clean Air Act Requirements):

"The proposed rule would require facilities to do three things:

(3) Develop and submit to the Chemical Safety and Hazard Investigation Board, the implementing agency, SERC, and LEPC, a risk management plan (RMP) that would document the results of the risks management program including a summary of the offsite consequence analysis, a list of major hazards, steps being taken to address those hazards (i.e., a summary of the facility's prevention program), a five-year accident history, a description of the emergency response program, and a description of the management system that ensures the safety of the facility and the implementation of the required elements."

P 54194, III.D(Discussion of the Proposed Rule, Risk Management Program Elements, Hazard Assessment):

"...The Clean Air Act requires a hazard assessment that includes evaluation of a range of releases including worst-case accidental releases; analyses of potential offsite consequences; and a five-year accident history. The language in the Conference Report suggests a more extensive assessment that would require a formal process hazard analysis (e.g., basis data on the source, identification of potential points of release, review of the efficacy of release and control measures)."

"The proposed rule would require a hazard assessment that examines a range of accidental release scenarios, selects a worst-case accidental release scenario, analyzes offsite consequences for selected release scenarios including worst case, and documents a five-year history of significant accidental releases with the potential for offsite consequences."

"EPA is proposing to define the worst-case release as the instantaneous loss of all of the regulated substances in a process, with failure of all mitigation systems (active and passive)."

"The Agency recognizes that this approach differs from the approach EPA used in its *Technical Guidance for Hazards Analysis* for local planners to assess credible worst-cases releases for purposes of screening out situations with little or no impact. The credible worst case in the guidance assumed that the entire quantity of a substance was released from the largest vessel or group of interconnected vessels. Gases were assumed to be released in 10 minutes while liquids were assumed to be spilled on the ground or in a diked area and allowed to volatilize. Downwind impacts were assessed using conservative meteorological conditions. The Agency still supports this approach for screening, however, the methodology does not fully account for the site-specific conditions that affect the rate of release. For example, gases may be stored in a liquefied state or a liquid may be handled in large quantities at higher than ambient temperatures giving much different release rates. The Agency believes that the worst-case analysis should account for site-specific conditions and physical chemical properties."

"Once the worst-case and more likely significant accidental release scenarios are identified, the facility would be required to analyze the potential offsite consequences associated with these scenarios. The offsite analyses would estimate, using models or other approaches specific to each substance, the possible rate of release, quantity released, and duration of the release, and the distances in any direction that the substance could travel before it dispersed enough to no longer pose a hazard to the public health or environment. Facilities would be required to analyze the releases under average weather conditions, which would be defined as a wind speed of 1.5 meters per second and F stability (moderately stable weather conditions)."

P 54197, III.D(Discussion of the Proposed Rule, Risk Management Program Elements, Process Hazard Analysis):

"The proposed rule would require facilities to conduct process hazard analyses after determining a priority order for the analyses based on the degree of hazard posed by the processes covered by the rule; that is, the facility would have to conduct its analyses on the most hazardous processes first, where the degree of hazard is related to potential offsite consequences, operating history of the process, and the age of the process."

P 54201, III.E(RMP and Documentation):

"The proposed rule would require facilities to submit an RMP that includes the following information:

- o A summary of the offsite consequence analyses including worst-case and other more likely release scenarios:
- o A list of the major hazards defined through the process hazard analysis, the consequences of failure to control each major hazard, the steps management is taking or planning to take to address the hazards, and an implementation schedule for each step listed;"

P 54207, IX(Section by Section Discussion of the Proposed Rule):

"Proposed 68.15 would provide the requirements for the hazard assessment. Facilities would be required to complete a hazard assessment for each regulated substance present in greater than a threshold quantity. For each such substance, a worst-case release scenario would have to be defined. The offsite consequences of a range of release scenarios, including the worst-case and other more likely significant accidental release scenarios, would have to be analyzed. The proposed section specifies a number of scenarios that should be considered and the information that must be included in the offsite consequence analyses."

Part 68 - Accidental Release Prevention Provisions

P 54213, 68.15, (Hazard assessment):

"(a) The purpose of the hazard assessment is to evaluate the impact of significant accidental releases on the public health and environment and to develop a history of such releases.

(b) Hazard assessments shall be conducted for each regulated substance present at the stationary source above the threshold quantity. For each regulated substance, the hazard assessment shall include the following steps:

- (1) Determine a worst-case release scenario for the regulated substance at the stationary source;
- (2) Identify other more likely significant accidental releases for each process where the regulated substance is present above the threshold quantity, including processes where the substance is manufactured, processed, or used, and where the regulated substance is stored, loaded, or unloaded;
- (3) Analyze the offsite consequences of the worst-case release scenario and the other more likely significant accidental release scenarios identified in 68.15(b)(2);"

"(e) For each regulated substance, the offsite consequences of the worst-case of more likely significant accidental release scenarios shall be analyzed as follows:

- (1) The rate and quantity of substance lost to the air and the duration of the event;
- (2) The distance, in all directions, at which exposure to the substance or damage to offsite property or the environment from the release could occur using both worst-case meteorological conditions (i.e. F stability and 1.5 m/sec wind speed) and meteorological conditions most often occurring at the stationary source;"

"(h) The owner or operator shall maintain the following records documenting the hazard assessment and analysis of offsite consequences:

- (1) A description of the worst-case scenario;
- (2) A description of the other more likely significant accidental release scenarios identified in 68.15(b)(2), assumptions used, analyses or worksheets used to derive the accident scenarios, and the rationale for selection of specific scenarios; and
- (3) Documentation for how the offsite consequences for each scenario were determined including:
 - (i) Estimated quantity of substance released, rate of release, and duration of release;
 - (ii) Meteorological data used for typical conditions at the stationary source;
 - (iii) For toxic substances, the concentration used to determine the level of exposure and the data used for that concentration;"

P 54214, 68.24, (Prevention Program - process hazard analysis):

(b)"The owner or operator shall determine and document the priority order for conducting process hazard analyses based on a rationale which includes such considerations as the extent of process hazards, offsite consequences, age of the process, and operating history of the process."

(e)" The process hazard analysis shall address:

(4) Consequences of failure of engineering and administrative controls;

(7) A qualitative evaluation of a range of possible safety and health effects of failure of the controls on public health and the environment."

P 54218, 68.50, (Risk Management Plan):

(c)"The report shall include, for each regulated substance, a summary of the hazard assessment and analysis of offsite consequences and accident history data required by 68.15(i)."

(d) "The report shall include, for the stationary source, a description of the major hazards (e.g., equipment failure, human error, natural phenomena, or other factors or a combination of such factors which could lead to a significant accidental release) identified through the process hazard analyses, a description of the consequences of a failure to control for each identified major hazard, a summary of all actions taken or planned to address these hazards, and how significant accidental releases are prevented or mitigated, or the consequences reduced by these actions."

40 CFR 9 and 68, List of Regulated Substances and Thresholds for Accidental Release Prevention and Risk Management Programs for Chemical Accident Release Prevention, Final Rule and Notice

P 4482, IV.A1.a.(Discussion of Comments and Major Regulatory Changes, List of Substances and Thresholds, Toxic Substances, Listing criteria):

"EPA has decided to set the vapor pressure criterion at the higher level of 10 mm Hg."

P 4484, IV.A1.b.(Discussion of Comments and Major Regulatory Changes, List of Substances and Thresholds, Toxic Substances, Specific substances):

"As stated above, the Agency believes that accident history, as well as toxicity, physical/chemical properties, and current commercial production volume, are all appropriate elements to be considered in determining the substances to be listed. The Agency reserves the flexibility to consider the listed substances in light of a combination of, or all of these criteria elements."

Mixture Exemption, Toxic Substances

"The proposed rule included a de-minimis concentration of one percent by weight for all listed substances present in a mixture; i.e., quantities of a

regulated substance in a mixture did not have to be accounted for purposes of the threshold quantity if the substance were present at concentrations below one percent by weight."

"Other listed toxic substances (other than hydrogen fluoride/hydrofluoric acid and nitric acid) in solution or mixtures must be included in threshold determination if the partial pressure of the substance in the solution or mixture is equal to, or exceeds, 10 mm Hg. If the partial pressure of the regulated toxic substance in the mixture is determined to be below 10 mm Hg under all conditions in process handling or process storage, the solution or mixture need not be considered in the threshold determination."

"The facility will be required to use the one percent de-minimis concentration in determining threshold quantities unless it can measure or estimate, and document, that the partial pressure of the regulated substance in the mixture or solution is less than 10 mm Hg."

Part 68 - Chemical Accident Prevention Provisions

P 4493, 68.115(b) (Threshold Determination):

(1)"*Concentrations of a regulated toxic substance in a mixture.* If a regulated substance is present in a mixture and the concentration of the substance is below one percent by weight of the mixture, the amount of the substance in the mixture need not be considered when determining whether more than a threshold quantity is present at the stationary source."

"... if the concentration of the regulated substance in the mixture is one percent or greater by weight, but the owner or operator can demonstrate that the partial pressure of the regulated substance in the mixture (solution) under handling or storage conditions in any portion of the process is less than 10 mm Hg, the amount of the substance in the mixture in that portion of the process need not be considered when determining whether more than a threshold quantity is present at the stationary source."

(2)"*Concentrations of a regulated flammable substance in a mixture.* If a regulated substance is present in a mixture and the concentration of the substance is below one percent by weight of the mixture, the mixture need not be considered when determining whether more than a threshold quantity of the regulated substance is present at the stationary source. If the concentration of the regulated substance in the mixture is one percent or greater by weight, then, for the purposes of determining whether more than a threshold quantity is present at the stationary source, the entire weight of the mixture shall be treated as the regulated substance unless the owner or operator can demonstrate that the mixture itself does not meet the criteria for

flammability of flash point below 73 °F (22.8 °C) and boiling point below 100 °F (37.8 °C)."

DOE-STD-1027-92, Hazard Categorization and Accident Analysis Techniques for Compliance with DOE Order 5480.23, Nuclear Safety Analysis Reports

Interpretation of Requirements:

This document provides guidance for facility hazard classification and nuclear facility safety analysis reports. It allows the final hazard classification to be based on an unmitigated release of material, with the analysis considering realistic physical and chemical properties associated with the scenario. A detailed rigorous analysis is not expected for hazard classification, but a range of sophistication techniques should be available for safety analysis. Thus, analysis methodologies must be capable of calculating the source term from spill events so that the consequences of accidents can be used to finalize the hazard classification, and to provide consequence estimates for the safety analysis. Physical and chemical properties (e.g. release rate, particle size distribution) should be included in the analysis. The methodologies for safety analysis should cover a range of levels of sophistication, so that the ability to do more sophisticated analyses where hazard level and/or complexity dictate, is available.

Citations:

P 5, 3.1.2 (Final Hazard Categorization):

"The final categorization is based on an "unmitigated release" of available hazardous material. For the purposes of hazard categorization, "unmitigated" is meant to consider material quantity, form, location, dispersibility and interaction with available energy sources, but not to consider safety features (e.g., ventilation system, fire suppression, etc.) which will prevent or mitigate a release. The Hazards Analysis (or other existing safety analyses) provides an understanding of the material which can physically be released from the facility."

"... if the credible release fractions can be shown to be significantly different than these values based on physical and chemical form and available dispersive energy sources, the threshold inventory values for Category 2 in Table A.1 may be divided by the ratio of the maximum potential release fraction to that found on Page A-9."

P 9-11, 4.0 (Graded Approach - Analysis Techniques, Graded Approach Objective):

"In general, a graded approach dictates a more rigorous and more thoroughly documented analysis and evaluation of higher-hazard facilities than lower-hazard facilities, given the potential for more widespread and severe consequences if a higher-hazard facility fails to meet its safety basis requirements."

"The graded approach directs that the effort should be proportional to the complexity of the facility and the safety systems relied on to maintain an acceptable level of risks. Simple facilities would require less sophisticated analysis."

"When modifications are performed or the facility mission is extended or changed, additional detail to support the justification for the design adequacy will be required. For a facility which is partly shut down and is used for only limited functions, the SAR should develop the basis for confidence in the safety of the inactive portions of the facility and the safety basis for the intended operations. The inactive portion of a facility should be evaluated to ensure that the risks from the residual hazards (e.g. contamination, hazardous material inventory) are evaluated and controlled.

All SARs should furnish information about subsequent stages of the facility life cycle beyond that stage for which approval is sought, including end-of-life decontamination and decommissioning. However, SARs need to develop this information only enough to demonstrate that adequate attention is being given to anticipated future safety problems."

P 12, 4.1.1. (Hazard Analysis):

"The objectives of Hazard Analysis are to (1) identify the hazards contained in a facility, (2) perform final hazard categorization in accordance with section 3 and attachment 1, based on hazardous material quantity identified in 4.1.1.a and energy sources and initiating events identified in 4.1.1.b (preventive and mitigative features are not to be considered in hazard categorization), (3) provide an overall assessment of the importance of the various hazards, (4) identify occupational hazards and related DOE prescribed standards, and (5) characterize and analyze the remaining non-routine hazards that are unique and representative hazards to be analyzed in the SAR."

P 12, 4.1.1.b, (Hazard Analysis, Energy Sources and Potential Initiating Events):

"Hazard Analysis then identifies potential energy sources and potential initiating events which could affect the hazardous material and lead to a release of material or other occurrence. Such events include internally initiated events (e.g., explosions and fires), process-initiated events (e.g., spills or improper material transfers), and externally initiated events (e.g., floods or

earthquakes). Inherent energies within the process (e.g., reactivity, temperatures, and pressures) should also be described."

P 16, 4.1.2, (Accident Analysis, Consequence Analysis):

"This step evaluates the effect of the postulated accident on the workers, the public, and the environment. It includes source term evaluation and dose calculations."

P 18, 4.1.2.a (Accident Analysis, Nuclear Hazard Category 3 Facilities, Consequence Analysis):

"A qualitative determination of consequences from the identified accidents is required."

P 23, 4.1.2.b (Accident Analysis, Nuclear Hazard Category 2 Facilities, Sequence Selection):

"1) Operational Accidents - Operational accidents are those that result from processes and activities involved in operating the facility and generally cover many diverse routine or non-routine events with potential adverse consequences to the workers or the public. Fires, explosions, spills, process disturbances, and criticality events are included as operational events."

P 24, 4.1.2.b (Accident Analysis, Nuclear Hazard Category 2 Facilities, Consequence Analysis):

"1) Source Term Analysis - Provide a reasonably conservative analysis by using defensible realistic values of the characteristics of the release from the building. This analysis includes the amount and form of material, the timing of the release, energy, particle size distribution, etc.,"

P A-7 (Exposure Pathways):

"As can be seen from the modified equation, DOE concurred with the NRC's dismissal of the ground contamination pathway. In general, DOE concurred with the dismissal of cloudshine exposure as well because this path accounted for, on average, slightly less than 2% of dose for all radionuclides but the noble gases. Although, for the types of material that DOE handles, it is expected that the values for noble gases will be included in the mixed fission product threshold, DOE decided to retain this exposure pathway in the calculation for completeness."

DOE-STD-3009-94. Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Analysis Reports

Interpretation of Requirements:

This document provides guidance on format and content of nuclear facility safety analysis reports. It requires that the safety analysis include an assessment of accidents, and examine the response of safety-class and safety-significant equipment to accidental environmental conditions. Thus, analysis methodologies must be capable of calculating the source term from spill events so that the consequences of accidents can be used to provide consequence estimates for the safety analysis. Physical and chemical properties (e.g. release rate, particle size distribution) should be included in the analysis to properly model the phenomena. The methodologies for safety analysis should cover a range of levels of sophistication, so that the ability to do more sophisticated analyses where hazard level and/or complexity dictate, is available.

Citations:

Chp3, P 32, (Purpose):

"Expected products of this chapter, as applicable based on the graded approach, include:

- o Accident analysis of DBAs identified in the hazard analysis. The summary of this activity will include, for each accident analyzed, the following:
 - Estimation of source term and consequence."

Chp3, P 33, (Application of the Graded Approach):

"Accident analysis is also inherently graded in terms of the degree of physical modeling and engineering analysis needed to quantify accident consequences and likelihoods. The use of bounding assumptions and less detailed physical modeling in accident analysis is appropriate.

Chp3, P 53, 3.4 (Accident Analysis):

"Whenever possible DBAs are analyzed using the simplest applicable deterministic, phenomenological calculations (e.g., pressure estimates from a simple ideal gas law calculation, hand calculated Gaussian plume dispersions)."

"Accident analysis typically starts with formal descriptions of accident scenarios. Such descriptions may be supported by basic event trees. All major

assumptions in scenarios must be identified. The next step is determination of accident source terms. Source terms for accidents are obtained through phenomenological and system response calculations."

Chp3, P 55, 3.4.1 (Methodology):

"Documentation of methodology should include the following:

- o Methods used to estimate radiological or other hazardous material source terms for DBAs including: (1) basic approach for estimating physical facility damage from DBAs; (2) general basis for assigning material-at-risk quantities not directly derived from hazard identification, if differing values are used; and (3) basis for material release and respirable fractions or release rates used."

Chp3, P 56, 3.4.2 (Design Basis Accidents):

"The major categories are: internally initiated operational accidents (e.g., fires, explosions, spills, criticality); ..."

Chp3, P 57, 3.4.2.X.2 (Source Term Analysis):

"This subsection determines the accidental material or energy released through the pathways of concern. Define all parameters and phenomenological models used to derive the source term. As a minimum, this definition includes the material at risk (as derived from the hazard identification), the release fraction or rate that determines the initial source term, and the overall facility leakpath factors that determine the final source term released external to the facility. The degree of conservatism believed to be present in the calculation needs to be consistent with Evaluation Guideline definitions. Detailed quantification of uncertainty is not required."

Chp4, P 65, 4.3.X.3 (Functional Requirements):

"Functional requirements specifically address the pertinent response parameters or nonambient environmental stresses related to an accident for which the safety function is being relied upon."

Chp4, P 65, 4.3.X.4.(System Evaluation):

"Evaluate the capabilities of the SSC to meet performance criteria."

Chp4, P 67, 4.4.X.3 (Functional Requirements):

"Functional requirements specifically address the pertinent response parameters or nonambient environmental stresses related to an accident for which the safety function is being relied upon."

Chp4, P 67, 4.4.X.4.(System Evaluation):

"Evaluate the capabilities of the SSC to meet performance criteria."

DOE-STD-3011-94, Guidance for Preparation of DOE 5480.22 (TSR) and DOE 5480.23 (SAR) Implementation Plans

Interpretation of Requirements:

This document provides guidance on the contents of the overall plan and schedule for implementation of DOE 5480.22 and 5480.23. It requires that the BIO safety analysis include a conservative assessment of accidents. Little sophistication is expected, and computer codes may not be necessary. Thus, analysis methodologies for a BIO must allow simple calculation of the source term from spill events so that the consequences of accidents can be approximated.

Citations:

P 23, A-3.c. (Safety Assurance via BIO, Safety Analysis):

"For scenarios resulting in a significant impact outside the facility, the extent of detail incorporated in the analysis must ensure that a qualitative or semi-quantitative determination of the consequences and frequencies of the identified scenarios can be made."

P 25, A-3.c. (Safety Assurance via BIO, Safety Analysis):

"Additionally, the analysis should include a gross estimation of the consequences and frequencies of identified accident scenarios."

P 27, A-4. (Safety Acceptance Guidelines):

"The absence of strict accident dose guidelines for BIO acceptance is based on the expectation that the conservative, qualitative, or semi-quantitative methodology employed in the preliminary assessment of facility hazards will not always be sufficient to demonstrate adherence to the safety acceptance guidelines that could be used in an SAR approval process."

P 33, A-9.g. (Format and Content, Safety Analysis):

"The dominant credible accident scenarios should be identified and evaluated qualitatively or semi-quantitatively."

P 36, B-1. (Purpose and Scope):

"Each accident scenario derived from a PHA has an initiating event, subsequent success or failure of preventive or mitigative features and/or operator responses, and gross estimates of a release source term (Or internal consequence), and the frequency and consequence (external) of the scenario. These characteristics can be qualitative or semi-quantitative."

P 37, B-1. (Purpose and Scope):

"Unlike "worst-case", "reasonable worst-case" does not consider every

parameter to be in its most unfavorable state. Thus, if a toxic material is normally handled as a liquid at room temperature during processing, a reasonable worst-case release does not have to consider a spill with the liquid at 130 °F."

P 40, B-2. (Analysis Procedure):

"Consequences are determined based on parameters such as the bounding quantity of hazardous material involved in the accident, the release mechanism associated with the accident, and the release pathway taken by the hazardous material. Judicious use of conservative assumptions should be made in the determination of consequence magnitudes as well. Again, uncertainties in parameter values should be accommodated by erring in the conservative direction from best-estimate values."

"In general, "back-of-the-envelope" calculations are appropriate for estimating numerical quantities. The use of complex models or computer codes is considered to be beyond the level of analytical rigor implied by PHA, and where uncertainties in outcome cannot be resolved by straightforward methods, it is generally acceptable to simply make the conservative assumption. The selection of release fractions used in source term estimation should be well documented in the PHA, since consequence results are particularly sensitive to assumptions made concerning them."

DOE-HDBK-3010-94. Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities

Interpretation of Requirements:

The document provides a range of experimentally derived release fractions, release rates, and respirable fractions. These can possibly be used as input to computer codes, in lieu of computer code analysis, or to benchmark code results.

Relevant Sections:

Chp 2, Materials in the Gaseous State

Chp 3, Liquids

Chp 4, Solids

Emergency Management Guide, Guidance for Hazards Assessment (DOE Order 5500.3A)

Interpretation of Requirements:

The document provides guidance for the preparation of a Hazards Assessment, under DOE Order 5500.3A. Part of the Hazards Assessment requires determination of the source term from accidents. Source term calculations should consider the physical and chemical characteristics of the source material, the type of failure mode (e.g., small leak vs gross failure), varying substrates, time dependency, and weather conditions. Source term methodologies should apply across the range of potential accident severities (low probability-high consequence events and high probability-low consequence events). The guidance suggests considering alternate pathways (aquatic, ground), but the impacts from these pathways are usually dominated by the impacts from the inhalation pathway (note that SAR analyses do not typically consider aquatic or ground pathways, as airborne pathways typically have a more immediate and severe impact). The guidance also suggests considering reactive properties of hazardous materials, and interactions between substances.

Citations:

P 8, D.3.b.(1) (Preparing the Hazards Assessment, Identification and Screening of Hazards, Screening Thresholds):

"The TPQs defined by the EPA Superfund Amendment and Reauthorization Act (SARA) Title III, 40CFR355 Appendix A, may be used as screening thresholds for those chemicals listed.

Chemically toxic materials not listed may be either included on the hazard list for full characterization, or the facility may develop and document a screening quantity based on the physical and toxicological properties of the material and conservative (i.e. tending to yield the largest impact) consequence modeling."

P 10, D.4.a.(3) (Preparing the Hazards Assessment, Hazard Characterization):

"Both radioactive and nonradioactive hazardous materials should be included in a tabulation with the following information on each:

(3) The properties of the material that are needed for determination of source term and consequence analysis, such as the physical form and chemical characteristics of the material (e.g. solid, liquid, gaseous, particle size, flammability, chemical reactivity, density), radiological characteristics, and the

temperature and pressure conditions under which it is stored, processes, used, or transported;"

P 11, D.4.f (Preparing the Hazards Assessment, Hazard Characterization):

"Available information concerning the reactive properties of the hazardous materials should be assessed and the possibility of interactions between substances considered."

P 11, D.5 (Preparing the Hazards Assessment, Development of Event Scenarios):

"When a release to an aquatic or ground pathway could have a near-term effect on the workers or the public (e.g. through a community water supply) then it should be considered in the hazards assessment."

P 12, D.5.a. (Preparing the Hazards Assessment, Development of Event Scenarios):

"It should be noted that SARs typically include analysis results for a limited number of accident scenarios chosen from the relatively narrow range of severity that defines the limit of credible (in the probabilistic sense) accidents. Thus, the SAR analyses are nearly always an incomplete representation of the spectrum of operational emergencies for which emergency planning is required by DOE 5500.3A. Analyses of the higher probability, lower consequence events that must be effectively addressed in the facility emergency plan are absent from SARs."

P 12, D.5.b.(1) (Preparing the Hazards Assessment, Development of Event Scenarios, Identify Primary Barriers):

"Examples of this concept of a primary barrier might be a solid material that releases hazardous vapors or combustion products if heated or ignited, or radioactive gases trapped on a cryogenic charcoal bed. In both examples, the physical form or phase of the material keeps it from being dispersed under normal operating (or storage) conditions."

P 12, D.5.b.(1) (Preparing the Hazards Assessment, Development of Event Scenarios, Identify Failure Modes of Primary Barriers):

"In the example of a tank or container that contains a gaseous or liquid material, possible causes of failure might include corrosion, design or manufacturing flaw, overpressure, external impact (missile, forklift, crane load), operator error, excessive temperature, water-hammer, or sabotage."

P 13, D.5.b.(3) (Preparing the Hazards Assessment, Development of Event Scenarios, Estimate Magnitude of Release from Primary Barrier):

"For each cause of failure, a quantitative estimate of the material release should be made. Considering the nature of the material, such as volatility, viscosity, melting point, and vapor pressure, and the postulated mode of

failure, the fraction of the material inventory that would be released from the primary barrier in a dispersible form should be estimated.

This evaluation step should yield an estimate of the maximum amount of a material that could be released from the primary container as a function of time for each event or failure mode, considering the physical, chemical, and thermodynamic properties of that material."

P 15, D.6.a (Preparing the Hazards Assessment, Estimate Potential Event Consequences):

"Methods and calculational models used in estimating consequences should be documented in such a manner that the analyses and their results can be critically reviewed, understood, and if necessary, reconstructed by independent experts. Detailed descriptions of the methods, assumptions, and models (e.g., dispersion models, dose codes, or other complex calculational methodologies) need not be included in the Hazards Assessment Document, if they are documented elsewhere and appropriately cross-referenced."

P 17, D.6.e. (Preparing the Hazards Assessment, Estimate Potential Event Consequences):

"At least two sets of dispersion conditions should be considered for each receptor location and source term.

(1) The first case should correspond approximately to the 95% worst-case wind speed and stability for the particular site, if this has been determined. If such a determination has not been made for the site, a wind speed of one (1) meter per second with stability class F is acceptable for this "conservative" case for an assumed ground level release.

(2) The second case should approximate a typical set of conditions for the site, such as the average wind speed and most prevalent stability class in the compass sector (i.e., N, NNE, NE) of each particular receptor."

DOE Order 6430.1A, General Design Criteria

Interpretation of Requirements:

This Order presents requirements for the proper design of safety-related structures, systems, and components (SSCs). This includes the requirement that the safety-related SSCs continue to perform their function during normal, abnormal, and accident conditions. The SSCs should be able to withstand the effects of, and the environmental conditions associated with normal operation, abnormal events, or accidents (e.g. acidic environment after a spill). The SSCs of primary concern, when related to the spills/vaporization working group, are ventilation and confinement systems. The safety analysis should demonstrate the adequacy of systems to effectively perform their required functions. Thus, safety analysis methodologies must be capable of calculating the source term from spill events so that the functioning of SSCs under accident conditions can be ascertained (i.e. SSCs can tolerate the accidental conditions they are exposed to) and the adequacy of the SSCs in protecting the personnel and the public can be assessed.

Citations:

P 1-53 (General Requirements, Architectural and Special Design Requirements, Health and Safety, Performance Objectives):

"Health and safety performance objectives to be achieved in the design of DOE facilities include:

- o Protection of the public and all personnel from injury and from exposure to toxic materials, radiation, and other hazards in accordance with DOE requirements and allowable limits"

P 1-54 (General Requirements, Architectural and Special Design Requirements, Health and Safety, Safety Analysis):

"Areas to be addressed in the safety analysis include, but are not necessarily limited to, the following:

- o Principle hazards and risks that can be encountered in facility operation, including potential accidents and predicted consequences of fire, explosion, radiation, toxic exposure, structural failure, wind, flood, earthquake, tornado, operating error, failure of essential operating equipment, and failure of safety systems."

P 1-94 (General Requirements, Structural Design Requirements, Other Loads for Buildings and Other Structures, Fluid and Gas Pressures):

"The design of components of buildings and other structures shall include the effects of fluid and gas pressures, both internal and external."

P 1-100 (General Requirements, Structural Design Requirements, Special Facilities, Non-reactor Nuclear Facilities - General, Explosions, Internal Pressurization, Criticality, and Other DBA Causes):

"Such DBAs typically involve failure of high-speed rotating machinery, cranes, experimental facilities, high-energy fluid system components, or explosives. Structures required to function following such accidents shall be designed to withstand these DBAs."

P 2-2 (Site and Civil Engineering, Site Development, Facility Siting, Radiological Siting Requirements):

"The accidents to be considered are those attributable to both operational events (determined by using a deterministic and/or a probabilistic approach) and natural phenomena as applicable to the facility and the site."

P 2-3 (Site and Civil Engineering, Site Development, Facility Siting, Radiological Siting Requirements, Guidelines):

"When calculating these doses, degraded performance of ESF and administrative controls shall be assumed unless they can be clearly shown to be unaffected by the accident (capable of performing their safety function) by proper design, installation, testing, and maintenance according to prescribed standards."

P 13-3 (Special Facilities, General Requirements, Coverage and Objectives, Objectives):

"The design of special facilities shall:

- o Protect the public and facility personnel from hazards associated with the use of radioactive and other hazardous materials as a result of normal operations, anticipated operational occurrences, and DBA conditions, including the effects of natural phenomena pertinent to the site, and maintain these effects ALARA"

P 13-4 (Special Facilities, General Requirements, Coverage and Objectives, Guidance on Limiting Exposure of the Public, Accidental Releases):

"Releases of hazardous materials postulated to occur as a result of DBAs shall be limited by designing facilities such that at least on confinement system remains fully functional following any credible DBA (i.e. unfiltered/unmitigated releases of hazardous levels of such materials shall not be allowed following such accidents). Facility design shall provide attenuation features for postulated accidents (up to and including DBAs) that preclude offsite releases that would cause doses in excess of the DOE 5400 series limits for public exposures."

13-12 (Special Facilities, General Requirements, Confinement Systems):

"For a specific nuclear facility, the number and arrangement of confinement barriers and their required design features and characteristics shall be determined on a case-by-case basis. Typical factors that affect confinement system design are the type, quantity, form, and conditions for dispersing the hazardous material, including the type and severity of DBAs."

"The number of confinement systems required in different locations of a facility may vary depending on the potential consequences from hazards during normal operation, anticipated operational occurrences, and DBAs."

"The adequacy of the design of these confinement systems to effectively perform their required functions shall be demonstrated by the safety analysis."

13-47: (Special Facilities, Plutonium Processing and Handling Facilities, Confinement Systems, Primary Confinement System):

"The integrity of the primary confinement system shall be maintainable through all normal operations, anticipated operational occurrences, and any DBA the primary barrier is required to withstand. Breaches in the primary confinement barrier that cannot be totally avoided or ruled out (e.g., due to glove or seal failure) must be compensated for by provision of adequate inflow of air or safe collection of spilled liquid."

P 13-79: (Special Facilities, Uranium Processing and Handling, Confinement Systems, Primary Confinement System):

"The integrity of the primary confinement system shall be ensured for all normal operations, anticipated operational occurrences, and for the DBAs it is required to withstand. Breaches of the primary confinement barrier (e.g., due to glove or seal failure) are acceptable if the off-gas treatment system is capable of maintaining an adequate inflow of air for the specified breach size and location."

P 13-89: (Special Facilities, Reprocessing Facilities, Confinement Systems):

"The degree of confinement required in various locations of the facility depends on the potential hazards associated with the process being carried out and shall suit the most restrictive case anticipated. Consideration shall be given to the characteristics of the hazardous material involved such as type, quantities, physical and chemical forms, dispersibility, and energy available for dispersion."

"The effectiveness of each confinement barrier shall be checked analytically against all challenges it is expected to withstand without loss of function. This applies to any form of the hazardous material (gas, liquid, or solid) and its carrying medium (i.e. airborne or spilled liquid)."

P 13-95: (Special Facilities, Uranium Conversion and Recovery Facilities, Confinement Systems):

"The integrity of the primary confinement system shall be ensured for all normal operations, anticipated operational occurrences, and for the DBAs it is required to withstand. Breaches of the primary confinement barrier (e.g., due to glove or seal failure) are acceptable if the off-gas treatment system is capable of maintaining an adequate inflow of air for the specified breach size and location."

P 13-101: (Special Facilities, Liquid Radioactive Waste Facilities, Confinement Systems):

"Spills, overflow, or leakage from storage vessels or other primary confinement structures shall be collected and retained within a suitable secondary confinement structure (e.g., secondary vessel, dike or berm, elevated threshold within a storage or process building, etc.). The secondary confinement structure shall be capable of retaining the maximum radioactive liquid waste inventory that may be released by a spill, overflow, or leak from the primary confinement structure."

P 13-123: (Special Facilities, Fusion test Facilities, Special Design Features):

"When the severity of DBAs require that a containment structure be used, the design pressure and temperature for fusion machine secondary confinement or containment shall be determined considering the effects of energy transport and chemical reactions that may occur following the failure of a fluid system inside the containment. The containment shall be designed to allow periodic leak rate testing. To minimize the release of hazardous materials to the atmosphere, means shall be provided to isolate the primary containment following DBAs that release hazardous material to the containment atmosphere."

P 15-45: (Mechanical, Special Facilities, Nonreactor Nuclear Facilities - General, Confinement Ventilation Systems):

"Air cleanup systems shall be provided in confinement ventilation exhaust systems to limit the release of radioactive or other hazardous material to the environment and to minimize the spread of contamination within the facility as determined by the safety analysis."

Appendix B: Code Evaluations

General Review Criteria

Code Name: ADAM, Airforce Dispersion Assessment Model

1. Capabilities: ADAM (Airforce Dispersion Assessment Model) is a heavy gas, Gaussian puff dispersion model, that includes source term models for pressurized and non-pressurized liquid and gas releases. Potential reactions of the released chemical with water vapor can be modeled. N_2O_4 - NO_2 and HF chemistry are modeled. Eight chemicals are included in the ADAM database; others can be added by the user.
2. Sponsor/Developing Organization:

U.S. Air Force
3. Current Custodian/Phone/Fax/Internet Address:

Captain Michael Jones
AL/EQS
139 Barnes Drive
Tyndall AFB, FL 32403-5319

Phone: 904-283-6002
4. Genealogy: The ADAM code is based on the Air Force AFTOX code. Version 2.1 is evaluated here.
5. User's Manual Reference:

Mullett, C.A. and P. K. Raj (1990) "A User's Manual for ADAM (Air Force Dispersion Assessment Model)," GL-TR-90-0321 (II), ADA236070.
6. Model Description Summary:

Pool Evaporation: The Ille and Springer (1978) model is used for noncryogenic liquid spills. Evaporation of cryogenic spills are modeled as per Raj (1981).

Liquid Release from a Tank: The steady-state Bernoulli's equation is used to determine the leak rate from the tank. Changes in tank pressure and liquid level with time are not accounted for.

Gas Release from a Tank: The 1-d compressible flow equations are used to determine the release rate and temperature of the source term. Changes in tank pressure with time are not accounted for.

Liquid Flash Model: Adiabatic flashing; rain-out of liquid fraction is not modeled.

Turbulent jet: Raj and Morris (1987).

7. Model Description References:

Pool Evaporation:

Ille, G. and C. Springer (1978) "The Evaporation and Dispersion of Hydrazine Propellants from Ground Spills," CEEDO-TR-83-30, ADA059407.

Raj, P. K. (1981) "Models for Cryogenic Liquid Spill Behavior on Land and Water," J. Haz. Mat., 5,111-130.

Turbulent jet:

Raj, P. K. and J. A. Morris (1987) "Source Characterization and Heavy Gas Dispersion Models for Reactive Chemicals," AFGL-TR-88-0003 (I), ADA200121.

8. Hardware Requirements and Software Requirements: Requirements include: an IBM-compatible PC (code will take advantage of a math coprocessor if one is available), EGA graphics card or better, 512 kB RAM.

9. Quality Assurance Documentation:

Benchmarking - Compared against AFTOX results; Kunkel (1992).

Source code Verification - None.

Evaluation ("Validation") against experimental data - None to date.

10. Input Summary (data and parameters):

General Input: pool material, release type, material storage temperature and pressure, presents of a dike and its diameter, time/date/geographic location of spill

Hole in Tank Release Input: volume of material in tank, tank diameter, hole diameter, height of hole above ground level

Short Pipe from Tank Release Input: volume of material in tank, tank diameter, hole diameter, height of hole above ground level

Hole in Pipe Release Input: diameter of pipe, hole diameter, flow speed in pipe

Severed Pipeline Release Input: diameter of pipe, flow speed in pipe

Ground Conditions: ground temperature, ground roughness

Atmospheric Conditions: air temperature, relative humidity, atmospheric pressure, wind speed, height at which wind speed was measured, wind direction, wind stability

Atmospheric Conditions: air temperature, relative humidity, atmospheric pressure

11. Output Summary: Code output includes:

- mass rate of release
- vapor temperature of release
- mass rate of air entrained
- overall density of mixture
- aerosol mass fraction in initial cloud

12. Summary of Limitations: Code limitations include:

- the code only handles single chemical source terms
- the code has a limited chemical database
- source terms are only modeled as steady state releases
- makes use of the Modified Ille-Springer Model (MISM), which is based on empirical correlations derived from spills of rocket propellants

13. Summary of Strengths: Code strengths include:

- menu-driven input
- models HF, N2O4, and NH3 chemical reactions

14. Range of Applicability (situations, sites, sources, etc.): The code applies to pressurized and non-pressurized liquid and gaseous releases for a limited number of materials.

15. Comments on User Friendliness: The code input is menu-driven. The code is user friendly.

16. Comments on Error Handling Capabilities and User Feedback: None.
17. Source code and/or data bases can be modified?: The chemical property database can be modified by the user.
18. Execution time for typical problem (CPU or real time): Execution time is < 10 seconds (real time).
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): The code is available on IBM 3.5" diskettes.
20. Cost: None?
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? ADAM is generally acceptable for supporting SAR documentation.
22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? The suitability of the code declines as the complexity of the analysis increases, therefore it may be unsuitable for high hazard facilities that require relatively complex analyses.
23. Future Enhancements Planned: None known at this time.
24. Additional Information:

Specific Evaluation Criteria

Liquid Chemical Spills and Evaporation

Code Name: ADAM

Feature	Y/N	Description	Limitations or Assumptions
Determination of pool size (i.e. considers area source)	Y	The pool area can be set equal to a fixed diked area or allowed to be a function of amount of spilled material.	The code cannot model dike overflow; pool depth is fixed at 1 cm.
Consideration of pool depth	Y/N	The pool depth is fixed at 1 cm.	Pool depth is fixed at 1 cm.
Determination of release rate	Y	Steady-state mass and energy balance equations are solved.	Transient release behavior is not modeled. The code makes use of the MISM mass transfer model, which is based on empirical correlations derived from spills of rocket propellants, and may not be broadly applicable.
Consideration of ambient and/or site-specific conditions	Y	Site-specific solar flux is calculated. Site-specific meteorology can be used.	Solar flux is assumed constant over the duration of the event.
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y	Temperature, density, and aerosol mass fraction of initial cloud are calculated.	Transient release behavior is not modeled.
Time dependency of rate calculation	N		
Temperature dependency/thermal effects	Y	Steady-state mass and energy balance equations are solved.	Transient release behavior is not modeled.
Time dependent spill to pool	Y/N	The steady-state Bernoulli's equation is used.	The code does not account for time-variation of the release.

Liquid Chemical Spills and EvaporationCode Name: **ADAM**

Feature	Y/N	Description	Limitations or Assumptions
Consideration of heat transfer from substrate	Y	The steady-state heat transfer between the pool and ground is modeled; potential pool convection-enhanced heat transfer is modeled.	Transient behavior is not modeled; convection-enhanced heat transfer is based on correlations.
Consideration of chemical reaction with substrate	N		
Consideration of insolation	Y	Site-specific solar flux is calculated.	The solar flux is assumed constant over the duration of the event.
Consideration of water reactivity	Y	The potential water reactivity of the eight chemicals in the database is considered.	The source code would have to be modified to handle water reactivity of chemicals other than those given in the database.
Consideration of multi-component mixtures/solutions	N		
Extensive data base provided	N	Eight chemicals are provided in the database: anhydrous ammonia, chlorine, fluorine, hydrogen fluoride, hydrogen sulfide, nitrogen tetroxide, phosgene, sulfur dioxide.	Modification of the database is not trivial.
Some data/properties must be user specified	N		
All data/properties must be user specified	N		

Liquid Chemical Spills and Evaporation

Code Name: **ADAM**

Feature	Y/N	Description	Limitations or Assumptions
Special features	Y	The code models water reactivity of ammonia; chemical reactivity of hydrogen fluoride and nitrogen tetroxide is also modeled.	The source code would have to be modified to handle the potential chemical reactions of chemicals other than those given in the database.
Linked to transport model	Y	The code will calculate puff and continuous releases with heavy and neutral gas dispersion.	
Test problem evaluation	Y	See anhydrous ammonia and chlorine spill test case results in Section 6.2 and Appendix C of this report.	
Other			

Graded Approach Applicability: The code is best suited for simple analyses typical for facilities rated moderate hazard or less.

Specific Evaluation Criteria

Pressurized Liquid/Gas Releases

Code Name: ADAM

Feature	Y/N	Description	Limitations or Assumptions
Determination of release rate	Y	The steady-state Bernoulli's eqn. (liquid), 1-d compressible flow eqns. (gas), adiabatic flashing is considered.	The code only models steady-state releases; pipe flow is not modeled; transient release behavior is not modeled.
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y/N	Temperature, density, and aerosol mass fraction of initial cloud are calculated.	Transient release behavior is not modeled.
Consideration of ambient and/or site-specific conditions	Y	Ambient and inventory temperatures and pressures are considered.	Liquefied gases are at saturation conditions.
Geometry considerations e.g. orifice size	Y		Only round orifices are modeled.
Time dependency of rate calculation	N		
Temperature dependency/ thermal effects	N		
Consideration of critical flow	Y	1-d compressible flow eqns. (gas) are used.	This contains limitations inherent in a simplified 1-d approach.
Consideration of two-phase flow	Y	Adiabatic flashing is considered.	Pipe flow is not modeled; rain-out is neglected.
Consideration of water reactivity	Y	The potential water reactivity of the eight chemicals in the database is considered.	The source code would have to be modified to handle water reactivity of chemicals other than those given in the database.
Extensive data base provided	N	Eight chemicals are provided in the database: anhydrous ammonia, chlorine, fluorine, hydrogen fluoride, hydrogen sulfide, nitrogen tetroxide, phosgene, sulfur dioxide.	Modification of the database is not trivial.

Pressurized Liquid/Gas Releases**Code Name: ADAM**

Feature	Y/N	Description	Limitations or Assumptions
Some data/properties must be user specified	N		
Special features	Y	The code models water reactivity of ammonia; chemical reactivity of hydrogen fluoride and nitrogen tetroxide is also modeled.	The source code would have to be modified to handle the potential chemical reactions of chemicals other than those given in the database.
Linked to transport model	Y	The code will calculate puff and continuous releases with heavy and neutral gas dispersion.	
Test problem evaluation	Y	See anhydrous ammonia and chlorine spill test case results in Section 6.2 and Appendix C of this report.	
Other	N		

Graded Approach Applicability: The code is best suited for simple analyses typical for facilities rated moderate hazard or less.

General Review Criteria

Code Name: **ALOHA, Areal Releases of Hazardous Atmospheres (ALOHA)**

1. Capabilities: ALOHA can estimate single component source terms generated via the following mechanisms: (1) evaporation from a liquid pool, (2) liquid release from a tank, (3) gas release from a tank, (4) two-phase release from a tank, and (5) gas release from a pipe. The code also is capable of performing puff and continuous release dispersion calculations for dense gas and neutral gas source terms. ALOHA is widely used by emergency management organizations.
2. Sponsor/Developing Organization:

EPA/NOAA/NSC
3. Current Custodian/Phone/Fax/Internet Address:

Mary Evans

Phone: 206-526-6325

Customer Service: National Safety Council
P.O. Box 558
Itasca, IL 60143-3201
Phone: (800) 621-7619
Fax: (708) 285-0797
4. Genealogy: ALOHA 5.1 (evaluated here) is based on previous versions of the ALOHA code. ALOHA 5.2 was released since this work was completed, and has not been evaluated.
5. User's Manual Reference:

"ALOHA User's Manual", U.S. Environmental Protection Agency, National Oceanic and Atmospheric Administration, June 1995.
6. Model Description Summary:

Pool Evaporation: Conservation of mass and energy are applied to the pool to determine the rate at which material evaporates. An analytical

solution of the steady-state advection-diffusion equation is used to characterize the evaporation mass transfer rate from the pool.

Liquid Release from a Tank: Bernoulli's equation is used to determine the leak rate from the tank. Leaked material forms a pool from which evaporation can subsequently occur (see Pool Evaporation). Puddle growth (but not shrinkage) is modeled. Heat conduction from the tank inventory to the environment and evaporative heat transfer into the tank vapor space are accounted for.

Gas Release from a Tank: The 1-d compressible flow equations are used to determine the release rate and temperature of the source term. A virial equation of state is utilized to handle high-pressure non-ideal gas behavior.

Two-Phase Release from a Tank: The liquid fraction of all two-phase releases is assumed to quickly evaporate, and thus no liquid pool is formed. Releases via a simple hole are modeled using Bernoulli's equation, with modification made to account for the effective height and density of the liquid-gas mixture. Releases from a short pipe are modeled using a simplified form of the homogeneous nonequilibrium model, while those from a long pipe are handled with the simplified homogeneous equilibrium model.

7. Model Description References:

Pool Evaporation:

Brighton, P. W. M. (1985), "Evaporation from a Plane Liquid Surface into a Turbulent Boundary Layer", *Journal of Fluid Mechanics*, Vol. 159, pp. 323-345.

Liquid Release from a Tank:

Briscoe, F. and P. Shaw (1980), "Spread and Evaporation of Liquid", *Progress in Energy and Combined Science*, Vol. 6, No. 2, pp. 127-140.

Gas Release from a Tank/Pipe:

Belore R. and I. Buist (1986), "A Computer Model for Predicting Leak Rates of Chemicals from Damaged Storage and Transportation Tanks", Report EE-75, Environment Canada.

Shapiro, A. H. (1953), The Dynamics and Thermodynamics of Compressible Fluid Flow, Vol. 1, John Wiley & Sons, New York.

Blevins, R. D. (1985), Applied Fluid Dynamics Handbook, Von Nostrand Reinhold, New York.

Hanna, S. R., and D. Strimaitis (1989), Workbook of Test Cases for Vapor Cloud Source Dispersion Models, Center for Chemical Process Safety of the American Institute of Chemical Engineers, New York.

Two-Phase Release from a Tank/Pipe:

Fauske, H. K. (1985) "Flashing Flow: Some Practical Guidelines for Emergency Releases", *Plant/Operations Progress*, Vol. 4, No. 3, pp. 132-134.

Fauske, H. K. and M. Epstein (1988), "Source Term Considerations in Connection with Chemical Accidents and Vapor Cloud Modelling", *Proceeding of the International Conference on Vapor Cloud Modeling*, New York: Center for Chemical Process Safety, American Institute of Chemical Engineers, pp. 251-273.

Henry, R. E. and H. K. Fauske (1971), "The Two-Phase Critical Flow of One-Component Mixtures in Nozzles, Orifices, and Short Tubes", *Journal of Heat Transfer*, May 1971, pp. 179-187.

Leung, J. C. (1986), "A Generalized Correlation for One-Component Homogeneous Equilibrium Flashing Choked Flow", *AIChE Journal*, Vol. 32, No. 10, pp. 1743-1746.

Huff, J. E. (1985), "Multiphase Flashing Flow in Pressure Relief Systems", *Plant Operations*, Vol. 4, No. 4, pp. 191-199.

Fisher, H. G. , et al. (1989), "The Design Institute for Emergency Relief Systems (DIERS) Project Manual, Version IV", AIChE, New York.

Insolation:

Raphael, J.M. (1962), "Prediction of Temperatures in Rivers and Reservoirs," *Journal of the Power Division*, American Society of Chemical Engineers, pp. 157-165.

8. Hardware Requirements and Software Requirements: Requirements include: an IBM-compatible PC 386 (code will take advantage of a math coprocessor if one is available), 1 MB RAM, 2.5 MB HD space; Windows 3.0 or higher.
or
a Macintosh (code will take advantage of a math coprocessor if one is available), 1 MB RAM, 2 MB HD space; runs under Finder or Multifinder.

9. Quality Assurance Documentation:

Benchmarking - None published.

Source code Verification - None.

Evaluation ("Validation") against experimental data - None published.

10. Input Summary (data and parameters):

General Input: geographic location, date & time, chemical, air temperature, wind speed and direction, stability class, relative humidity, cloud cover

Pool Evaporation Input: puddle area, average puddle depth, puddle volume, soil type, ground temperature, puddle temperature

Tank Release Input: tank type, orientation, and dimensions, chemical state/phase, chemical temperature, amount of chemical, opening geometry, puddle constraints

Pipe Release Input: pipe geometry, chemical temperature and pressure

11. Output Summary: Code output includes:

- maximum computed release rate
- average sustained release rate (averaged over one minute or more)
- total amount of material released

12. Summary of Limitations: Code limitations include:

- only handles single chemical source terms
- non-conservative error in ground-to-puddle heat flux model
- output is ill-posed for detailed analysis needs
- does not provide output on aerosol mass fractions from two-phase releases

13. Summary of Strengths: Code strengths include:

- built-in error checking
- user friendly

14. Range of Applicability (situations, sites, sources, etc.): The code is applicable to a range of release mechanisms (see item 1.) and materials.

15. Comments on User Friendliness: The code input is menu-driven. The code is user-friendly.
16. Comments on Error Handling Capabilities and User Feedback: The code has built-in error checking on meteorological and source term inputs; it will flag inconsistent conditions.
17. Source code and/or data bases can be modified?: The chemical property database can be modified by the user, however such modifications may not be handled correctly by the code.
18. Execution time for typical problem (CPU or real time): Execution time is < 1 minute (real time, source term calculation only).
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): The code is available on IBM or Macintosh 3.5" diskettes.
20. Cost: ~\$375.
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? ALOHA was developed for Emergency Management-type uses. However, given the proper conservatism in the input data, it can be used to perform some analyses that support SAR documentation.
22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? The suitability of the code declines as the complexity of the analysis increases, therefore it may be unsuitable for high hazard facilities that require relatively complex analyses.
23. Future Enhancements Planned: Version 5.2 has been released. It was not evaluated here.
24. Additional Information:

Specific Evaluation Criteria

Liquid Chemical Spills and Evaporation

Code Name: ALOHA

Feature	Y/N	Description	Limitations or Assumptions
Determination of pool size (i.e. considers area source)	Y	The code will calculate area based on pool depth and volume.	The code assumes the pool is square; puddle area can only increase.
Consideration of pool depth	Y	The code will calculate depth based on pool area and volume.	The code assumes the pool is square, minimum depth is limited to 0.5 cm.
Determination of release rate	Y	Time-dependent mass and energy balance equations are solved.	Only maximum release rate, average sustained release rate, and 5 time-averaged release rates are output; calculation is limited to 1-hr duration.
Consideration of ambient and/or site-specific conditions	Y	Site-specific solar flux is calculated. Site-specific meteorology can be used.	The solar flux is assumed constant over the duration of the event.
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y/N	The source term output is limited to maximum release rate, average sustained release rate, and total amount of material released; other parameters are calculated internal to the code and passed as necessary to the dispersion module.	Other source term characteristics are not output by the program.
Time dependency of rate calculation	Y	Time-dependent mass and energy balance equations are solved.	Only a maximum release rate, average sustained release rate, and 5 time-averaged release rates are output; calculation is limited to 1-hr duration.
Temperature dependency/thermal effects	Y	Time-dependent mass and energy balance equations are solved; solar flux, long-wave radiation flux, sensible heat transfer, latent heat transfer, and ground conduction are considered.	There is an error in the ground conduction model; it is only valid for constant temperature (boiling) pool.

Liquid Chemical Spills and EvaporationCode Name: **ALOHA**

Feature	Y/N	Description	Limitations or Assumptions
Time dependent spill to pool	Y	Bernoulli's equation is used to determine tank leak rate.	The model contains limitations inherent in a simplified 1-d approach; max. tank dia./length of 1000 m, min. tank length of 0.5 m, min. tank dia. of 0.2 m; 2-phase flow will not rain-out and form a puddle.
Consideration of heat transfer from substrate	Y	Ground conduction (1-d, semi-infinite slab) is considered.	There is an error in the ground conduction model.
Consideration of chemical reaction with substrate	N		
Consideration of insolation	Y	The code uses Raphael (J.M. Raphael, "Prediction of Temperatures in Rivers and Reservoirs," Journal of the Power Division, American Society of Chemical Engineers, pp. 157-165, 1962).	Solar flux is assumed constant over the duration of the event.
Consideration of water reactivity	N		
Consideration of multi-component mixtures/solutions	N	The user can define chemical properties in the database.	Properties in the database cannot be functions of other parameters.
Extensive data base provided	Y		Properties in the database cannot be functions of other parameters; some material entries are not as complete as others.
Some data/properties must be user specified	N		
All data/properties must be user specified	N		

Liquid Chemical Spills and EvaporationCode Name: **ALOHA**

Feature	Y/N	Description	Limitations or Assumptions
Special features			
Linked to transport model	Y	The code will calculate downwind concentrations for puff and continuous releases of heavy and neutral gases.	All heavy gas releases are modeled to occur at ground level; heavy gas continuous releases are modeled as a series of short steady releases.
Test problem evaluation	Y	See anhydrous ammonia, chlorine, and acetone spill test case results in Section 6.2 and Appendix C of this report.	
Other			

Graded Approach Applicability: The code is best suited for simple analyses typical for facilities rated moderate hazard or less.

Specific Evaluation Criteria

Pressurized Liquid/Gas Releases

Code Name: ALOHA

Feature	Y/N	Description	Limitations or Assumptions
Determination of release rate	Y	Bernoulli's eqn. (liquid), 1-d compressible flow eqns. and virial equation of state (gas), homogeneous equilibrium and nonequilibrium eqns. (2-phase) are used.	The model contains limitations inherent in simplified 1-d approach; max. tank dia./length of 1000 m, min. tank length of 0.5 m, min. tank dia. of 0.2 m. Gas pressure is also limited to less than 1000 psig.
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y/N	Source term output is limited to maximum release rate, average sustained release rate, and total amount of material released; other parameters are calculated internal to the code and passed as necessary to the dispersion module.	Other source term characteristics are not output by the program.
Consideration of ambient and/or site-specific conditions	Y	Ambient and inventory temperatures and pressures are considered.	Liquidified gases are at saturation conditions.
Geometry considerations e.g. orifice size	Y	Round and rectangular orifices can be modeled.	Only one orifice allowed.
Time dependency of rate calculation	Y	Steady-state equations are solve in a quasi-steady manner.	The code contains limitations inherent in simplified quasi-steady approach; only a maximum release rate, average sustained release rate, and 5 time-averaged release rates are output; calculation limited to 1-hr duration.
Temperature dependency/thermal effects	Y	Evaporative heat transfer from the liquid inventory and heat transfer between the tank contents and the environment are considered.	Tank walls are 1-cm thick steel.
Consideration of critical flow	Y	1-d compressible flow eqns. (gas) are used.	The model contains limitations inherent in simplified 1-d approach.

Specific Evaluation Criteria

Pressurized Liquid/Gas Releases

Code Name: **ALOHA**

Feature	Y/N	Description	Limitations or Assumptions
Consideration of two-phase flow	Y	Homogeneous equilibrium and nonequilibrium eqns. (2-Phase) are used.	The code contains limitations inherent in simplified 1-d approach; rain-out is neglected.
Consideration of water reactivity	N		
Extensive data base provided	Y	A data base of chemical properties is provided.	Properties in the database cannot be functions of other parameters; some material entries are not as complete as others.
Some data/properties must be user specified	N		
Special features	N		
Linked to transport model	Y	The code will calculate downwind concentrations for puff and continuous releases of heavy and neutral gases.	All heavy gas releases are modeled to occur at ground level; heavy gas continuous releases are modeled as a series of short steady releases; rain-out is neglected.
Test problem evaluation	Y	See anhydrous ammonia, chlorine, and acetone spill test case results in Section 6.2 and Appendix C of this report.	
Other	N		

Graded Approach Applicability: The code is best suited for simple analyses typical for facilities rated moderate hazard or less.

General Review Criteria

Code Name: **Chemical Accident Statistical Risk Assessment Model -
Single Case (CASRAM-SC)**

1. Capabilities: The CASRAM-SC model is used for assessing consequences of chemical accidents associated with hazardous material shipment, processing, handling, and storage. The basic model has two components, a source-term algorithm and a transport and dispersion algorithm. The source-term provides an estimate of an instantaneous discharge fraction, flash-entrainment fraction, and a liquid pool evaporation rate. Discharge fraction and emission rate estimates are for near-surface and surface releases. The dispersion modeling algorithm in CASRAM-SC uses a continuous plume model for releases from evaporating pools and a single-puff model for instantaneous releases. The treatment of atmospheric transport and dispersion is based on modern concepts of atmospheric-boundary-layer physics and is discussed elsewhere (Brown, 1995, 1994).
2. Sponsor/Developing Organization:

 Department of Transportation-Department of Energy/

 Argonne National Laboratory-University of Illinois
 9700 S. Cass, Bldg. 900
 Argonne, IL 60439
3. Current Custodians/Phone/Fax/Internet Address:

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4. Genealogy: The development of the CASRAM code was initiated in late 1992 to support the Department of Transportation's effort identifying initial

isolation and protective action distances for truck accidents involving hazardous chemical releases. This initial effort included development of the meteorological preprocessor and the dispersion model which comprise the working tools of the current CASRAM model. A probability scheme was added in 1993 to incorporate variability in meteorological input data and provide a means to discern appropriate daytime versus nighttime protective action distances. In 1994, both a source model and a Monte Carlo scheme were added. The Monte Carlo scheme was included to incorporate variability in key input parameters pertaining to accident locations, times and spill characteristics. These additions generated the initial version of CASRAM, which can generate distributions of health risk associated with a given set of transportation scenarios. CASRAM-SC, which was reviewed here, was created for deterministic or single case applications. Unlike CASRAM, CASRAM-SC cannot stochastically treat the spill source term.

5. User's Manual Reference: D.F. Brown, W.E. Dunn, and M.A. Lazaro, "CASRAM, The Chemical Accident Stochastic Risk Assessment Model", Beta-Version 0.8, ANL-UIUC Rept No. TD-xxx, April 5, 1996.
6. Model Description Summary: CASRAM-SC is a chemical consequence and risk assessment model applicable to chemical process, storage, handling and transportation accidents. It predicts "discharge fractions", flash-entrainment quantities, and liquid pool evaporation rates used in estimating chemical hazard population exposure zones. Two versions of the code, one for deterministic computations and one for stochastic computations, are or will be available. The stochastic version (CASRAM) is capable of predicting distributions of these hazard zones, which can be used to generate a probability distribution of health risk associated with potential facility or transportation accidents. The deterministic model (CASRAM-SC), can be utilized for deterministic, single case applications.

CASRAM-SC computes chemical release rates for specified chemical spill and/or vaporization scenarios and simulates air contaminant transport and dispersion. The model contains source algorithms to characterize instantaneous and continuous releases from ruptured storage vessels (pressurized and non-pressurized) and from evaporating pools. Health effect threshold concentrations, required for determining hazard-zone estimates, are specified as model input parameters allowing simple adjustment for modeling varying health impacts. CASRAM-SC is also capable of estimating hazard zones from multiple chemical spills, adjusted for the differences in toxicology among chemicals with common cancer and/or other adverse health effect endpoints. Physical property influence on release rates or pool evaporation rates from multi-component spills is not currently addressed by CASRAM-SC.

7. Model Description References:

D.F. Brown, W.E. Dunn, and M.A. Lazaro, "CASRAM: The Chemical Accident Stochastic Risk Assessment Model: Technical Documentation, Beta-Version 0.8", Argonne National Laboratory, 1997.

D.F. Brown, W.E. Dunn, and M.A. Lazaro, "Users' Guide for CASRAM-SC", Argonne National Laboratory, 1997.

D.F. Brown, Dunn, W. E. and A. J. Policastro, 1994: "Statistical Determination of Downwind Concentration Decay for the 1993 Emergency Response Guidebook," University of Illinois, Urbana, Illinois.

D.F. Brown, Dunn, W. E. and A. J. Policastro, 1994: "Application of a Monte-Carlo Model for Transportation Risk Assessment from DOE Facilities," University of Illinois, Urbana, Illinois.

8. Hardware Requirements: The model runs on a 486 or Pentium class PC or any workstation. The deterministic version can run on a 386, but a 486 is recommended. The stochastic version of the code was originally written for a Sun Workstation. A PC version of the full stochastic code is currently being prepared. The IBM version will require at least a 486, 33 MHz machine with a minimum of 10 Mb of free hard disk space.

9. Quality Assurance Documentation:

Benchmarking - Initial comparisons of the full deterministic code with the ALOHA model have shown CASRAM-SC predicted hazard distances fall within 10% of the ALOHA predictions.

Source Code Verification - The source-code has received a through QA by the developers. Independent code verification is planned during the summer or 1995.

Evaluation ("Validation") against experimental data - None to date.

10. Input Summary (data and parameters): CASRAM-SC is currently set up to interface with standard route-generating codes that provide a sequence of discrete route segments with associated latitude, longitude and population density information. Shipment size and container types are also required. For each chemical shipped, at least one concentration threshold, typically a toxicological limit, is required. Up to three concentration thresholds, corresponding to different averaging times, are accepted.

For a fixed-facility analysis, only the location and the concentration thresholds are required. Information on container types may be used if

applicable; however, distribution information on spill fractions is specifically for transportation accidents and may not apply to fixed-facility cases.

Meteorological data necessary for CASRAM-SC are obtained from NWS surface station and upper air observations. The meteorological data are processed using a meteorological preprocessor, separate from the CASRAM-SC model, and are cataloged in a preprocessed meteorological database. This database currently includes data from 64 cities in the United States from 1985-1989. For a single-case analysis, wind speed, temperature, solar angle (or time and location), cloud cover and inversion height are necessary.

Chemical data required for the source model are contained in a separate file and are keyed by CAS number. These data include molecular weight, critical temperature, critical volume, boiling point, liquid density, vapor pressure and heat of vaporization. Temperature dependent property data are accepted and employed where applicable. The data are formatted such that any chemical in the DIPPR database is easily incorporated into the CASRAM-SC chemical data file.

11. Output Summary: With the input data referenced above, CASRAM-SC predicts discharge fractions, flash-entrainment quantities, and liquid pool evaporation rates used as input to the model's dispersion algorithm in estimating chemical hazard population exposure zones. The output of CASRAM-SC, depending on the version employed, is either a deterministic estimate of the hazard zone (which is used to estimate an associated population health risk value) or the probability distributions of hazard-zones (which is used to estimate an associated distribution population health risk).
12. Summary of Assumptions/Limitations: The release of a liquid from an unpressurized container or the liquid fraction from a pressurized release is assumed to be instantaneously spilled on the ground (e.g., Bernoulli's equation is not employed). The initial liquid pool evaporation rate will thus tend to be larger than assuming a finite liquid spill duration. Currently, CASRAM-SC models near-surface material concentrations from near-surface releases.

Spills containing multiple chemicals are treated in CASRAM-SC. In these instances, no interaction between chemicals is considered, but the combined toxicological effects are modeled as outlined in the American Congress of Government and Industrial Hygienists Threshold Limit Value (ACGIH-TLV) documentation.

For stochastic simulations, accident times (year, day of year and hour) and spill fractions are determined by sampling distributions obtained from the HMIRS database. Relative spill coverage areas are sampled from a heuristic distribution formulated using average chemical property and pavement surface data.

13. Summary of Strengths: CASRAM-SC strengths include:
- Sophisticated treatment of vertical dispersion of passive releases that corrects physical inconsistencies associated with Gaussian models.
 - Built-in state-of-the-art meteorological preprocessor that provides Monin-Obukhov length and friction velocity as a function of routinely observed meteorological data.
 - State-of-the-art pool evaporation algorithm for evaluation of evaporative releases.
 - Estimation of hazard zone size from multiple chemicals in the same release.
14. Range of Applicability (situations, sites, sources, etc.): CASRAM-SC is applicable to any near surface releases where plume buoyancy effects are not significant and where chemical interaction does not cause large variations in chemical properties from those of the individual constituents.
15. Comments on User Friendliness: Although a user's guide would be helpful to a new user, the required input is relatively easily obtained, problems are easy to set-up, and model execution is straight forward.
16. Comments on Error Handling Capabilities and User Feedback: The user needs to understand the basic thermodynamics and physics for the problem being assessed. In addition, knowledge of the appropriateness and/or the ranges of model parameters and input data would be helpful.
17. Source code and/or data bases can be modified?: Yes, the chemical physical property and the health criteria toxicological value databases can be modified/supplemented, and source database can be modified/supplemented. If the source code is modified by user or (if a different health criteria is used), the code can not be referenced as CASRAM.
18. Execution time for typical problem (CPU or real time): Single scenario deterministic version runs for approximately 60 to 120 min on 486 PC and stochastic version runs for 3-6 hrs on SUN Workstation.
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): Disk
20. Cost: None
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? The code is generally acceptable in applications supporting SAR, BIO, and JCO documents.

22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? The model is applicable to a broad range of chemical accident severity assessment situations. However, it is most applicable to assessment of consequences and risk associated with the operation of "high hazard" chemical facilities.

23. Future Enhancements Planned:

- o Incorporation of statistical data on accident frequencies and chemical release frequencies and discharge fractions at fixed facilities within the DOE complex.
- o New algorithm to handle risk assessment of chemicals that are water reactive.
- o New algorithm to handle risk assessment of chemical accidents involving flammables, including enhanced near-field plume rise due to intense heat fluxes close to source.
- o Modification of dispersion algorithm to explicitly account for the influence of surface roughness on vertical plume spread (should be available in April 1995).
- o Modification of source algorithm to compute transient, but finite, release rates as a function of container or vessel: rupture size, initial temperature and pressure, and chemical contents and state.
- o Parameterization of data on statistical variability in health endpoints to enhance the computation of hazard area and risk distributions and to provide a more robust uncertainty calculation.
- o New algorithm to handle physical property dynamics of multi-component chemical spills.

24. Additional Information:

Specific Evaluation Criteria

Liquid Chemical Spills and Evaporation

Code Name: CASRAM-SC

Feature	Y/N	Description	Limitations or Assumptions
Determination of pool size or extent	Y	<p>Pool extent and its evolution is determined largely by surface or substrate roughness. Surface roughness is selected stochastically using a log-normal distribution having a geometric mean of 5 mm and a geometric standard deviation of 1.5. The void fraction of the surface element is taken to be normally distributed with a mean of 0.5 and a standard deviation of 0.05. Pool evolution is simulated numerically considering the following factors: (1) the liquid mass spilled into pool from vessel, (2) the hydrostatic pressure head created by the difference in height between the center and the edge of the pool, (3) the viscous and surface tension forces opposing pool spread, and (4) the evaporation of mass from the pool.</p>	<p>The surface is always assumed to be sufficiently rough so that the maximum contact angle between the edge of the pool and the surface is 180^0. This means that pool growth is never limited by surface tension. Momentum in the numerical solution of the pool evolution equation will not be conserved if the pool growth parameter, spill rate, is instantaneous and the pool limiting parameters (e.g., evaporation rate) are variable.</p> <p>Released liquids that are not flashed, or entrained along with the flashed liquids, form a pool on the ground that reaches its maximum size instantaneously. In the case of slow liquid leaks, this assumption tends to overestimate release rates. However, the uncertainties in calculating evolving pool sizes do not justify more advanced treatments. Moreover, detailed analyses require information, such as container hole size or liquid spill rate, that are not known a priori and are difficult to model statistically.</p>

Liquid Chemical Spills and Evaporation

Code Name: **CASRAM-SC**

Feature	Y/N	Description	Limitations or Assumptions
Consideration of pool depth	Y	The initial pool is taken to be conical in shape with a maximum depth equal to 20% of its diameter. The model considers liquid surface tension and viscosity to compute the equilibrium pool depth. By providing this limit on pool depth, a more physically realistic undiked spill pool size can be estimated.	See discussion on limitations and assumptions for the pool size feature.
Determination of release quantity and/or rate	Y	Spill or discharge fractions are determined stochastically using specified release distributions obtained directly from the HMIRS database. Distributions (ratios of the amount spilled to amount shipped) are provided for three container types: cylinders, small, and large drums.	Release distributions are currently limited to transportation spills. The entire discharge fraction spills on the ground instantaneously to form a pool. The vapor above the puncture hole remains trapped in the container.
Consideration of ambient and/or site-specific conditions	Y	Hourly surface and upper air from 61 National Weather Service stations in the continental United States. Hourly mixing heights time integrated values derived from the twice daily observations. This data along with data from the National Solar Radiation Database are fed to a meteorological preprocessor before input to CASRAM-SC. The data are used in the source-term pool evaporation rate and the transport and dispersion simulations.	

Liquid Chemical Spills and Evaporation

Code Name: CASRAM-SC

Feature	Y/N	Description	Limitations or Assumptions
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y	The initial puff size is determined as the product of downwind travel time and the horizontal wind direction fluctuations for horizontal spread and the product of downwind travel time and the vertical wind direction fluctuations for vertical spread. The initial plume temperature is assumed to be the container liquid temperature for flashed liquids and the container vapor temperature for direct vapor releases.	Vapor cloud density is not accounted for in determining initial cloud conditions, since CASRAM is limited to neutrally or positively buoyant releases.
Time dependency release rate to atmosphere from evaporating pool	Y/N	Pool evaporation is determined using a time dependent, energy-balance model which considers heat transfer to and from the pool via radiation, convection, conduction, and evaporation. A time dependent mass evaporation rate is computed. Although not currently accounted for in the current version of the model, an expression (e.g., the classical Bernoulli/Torricelli equation) for time dependent, gravity driven ($P_s - P_a = 0$) flow through a specified hole size will be considered for the next model upgrade.	The model cannot currently handle liquid spills with a finite release duration. Assuming instantaneous pool formation would lead to a slightly more conservative estimates of the initial pool evaporation rate but an overall shorter duration in the time needed to evaporate all the liquid from the pool.
Temperature dependency/thermal effects	Y	The physical property database used for CASRAM-SC has temperature dependent parameters (e.g. viscosity).	

Liquid Chemical Spills and Evaporation

Code Name: CASRAM-SC

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Feature	Y/N	Description	Limitations or Assumptions
Time dependency liquid release rate into pool	Y/N	Pool evaporation is determined using a time dependent, energy-balance model which considers heat transfer to and from the pool via radiation, convection, conduction, and evaporation. A time dependent mass evaporation rate is computed. Although not currently accounted for in the current version of the model, an expression (e.g., the classical Bernoulli/Torricelli equation) for time dependent, gravity driven ($P_s - P_a = 0$) flow through a specified hole size will be considered for the next model upgrade.	The model cannot currently handle liquid spills with a finite release duration. Assuming instantaneous pool formation would lead to a slightly more conservative estimates of the initial pool evaporation rate but an overall shorter duration in the time needed to evaporate all the liquid from the pool.
Consideration of heat transfer from substrate	Y	This is an important part of the numerical solution of the heat conduction equation at the surface. The model uses intermediate meteorological parameters such as bulk aerodynamic resistance, regional ground temperature, and vertical temperature profile into the surface.	Physical properties of a limited number of substrates have been incorporated into the model. These properties are needed for computing the vertical temperature profile into the surface.
Consideration of chemical reaction with substrate	N	Not considered	
Consideration of insolation	Y	Insolation is a component of the energy budget equation used for determining the boundary conditions in solving the heat conduction at the ground. The model accounts for net radiation or insolation, which is the sum of solar, incoming long-wave, and outgoing short-wave radiation.	
Consideration of water reactivity	N	Not currently considered. Water reactive capability will be incorporated in next version.	

Liquid Chemical Spills and Evaporation

Code Name: CASRAM-SC

Feature	Y/N	Description	Limitations or Assumptions
Consideration of multi-component mixtures/solutions	N	Not currently considered.	Interaction between multiple chemicals is not treated. Evaporation of multiple chemicals is treated as if each is in a separate pool.
Extensive data base provided	Y	Physical and chemical property data are incorporated for over 50 compounds. Data for an additional 70 to 1000 compounds are planned.	
Some data/properties must be user specified		The user can add chemicals outside DIPPR. Temperature dependent properties, such as heat of vaporization, vapor pressure, liquid density, are built-in.	
All data/properties must be user specified	N	N/A	
Special features	Y	The code has an option to determine stochastically or deterministically based release quantities.	There is a need to incorporate release statistics for fixed facilities.
Linked to transport model	Y	CASRAM-SC determined emission rates are fed directly to CASRAM-SC's transport-dispersion and consequence/risk assessment algorithm.	
Test problem evaluation	Y	See anhydrous ammonium and acetone spill test case results in Section 6.2 and Appendix C of this report.	

Graded Approach Applicability: The model is applicable to a broad range of chemical accident severity assessment situations. However, it is most applicable to assessment of consequences and risk associated with the operation of "high hazard" chemical facilities.

Specific Criteria

Pressurized Liquid/Gas Releases

Code Name: CASRAM-SC

Feature	Y/N	Description	Limitations or Assumptions
Determination of release rate	Y	Stochastic calculations are based upon distributions derived from the HMRIS data base. Deterministic calculations solve a one-dimensional time-dependent mass/energy conservation equation.	Release distributions are currently limited to transportation spills. The entire discharge fraction spills on ground instantaneously to form a pool. The vapor above the puncture hole remains trapped in container.
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y	The initial puff size is determined as the product of downwind travel time and the horizontal wind direction fluctuations for horizontal spread and the product of downwind travel time and the vertical wind direction fluctuations for vertical spread. The initial plume temperature is assumed to be the container liquid temperature for flashed liquids and the container vapor temperature for direct vapor releases.	Vapor cloud density is not accounted for in determining initial cloud conditions, since CASRAM-SC is limited to neutrally or positively buoyant releases.
Consideration of ambient and/or site-specific conditions	Y	Local meteorology and surface conditions can be included.	
Geometry considerations e.g. orifice size	Y	Geometry considerations are used in computing release rate.	
Time dependency of rate calculation	Y	The code solves a one-dimensional time dependent mass and energy conservation equation to generate mass emission rates as a function of time.	As with most pressurized release models, aerosol formation is not treated explicitly.

Pressurized Liquid/Gas Releases

Code Name: CASRAM-SC

Feature	Y/N	Description	Limitations or Assumptions
Temperature dependency/ thermal effects	Y	The physical property database used for CASRAM-SC has temperature dependent parameters (e.g. partial pressure).	The storage temperature for the shipped chemicals is assumed to be the same as the local pavement temperature. This assumption is justified since a container in a vehicle will experience the same solar heating effects as does the pavement.
Consideration of critical flow	N		
Consideration of two-phase flow	N		
Consideration of flashed and/or entrained fraction	Y	<p>In CASRAM-SC, we use an empirical approach based on the difference between the storage temperature and the normal boiling point. The flashed and associated entrained amounts are determined such that:</p> $f_{fe} = 1 \quad DT > 10$ $f_{fe} = 0.1 DT \quad 10 > DT > 0$ $f_{fe} = 0 \quad DT < 0,$ <p>where f_{fe} is the flashed/entrainment fraction and DT is difference between the storage temperature and the normal boiling point.</p>	Released materials which are flashed, or entrained along with the flashed liquids, are assumed to be discharged instantaneously, thus forming a puff. Though this assumption may overpredicted material concentrations close to the source, concentration averages over the time periods of interest (15–60 min.) are not significantly affected for most release scenarios. However, the impact of slow leaks modeled in this fashion would be significantly overpredicted. This overprediction does not seriously affect the overall distributions of affected areas since slow vapor releases are uncommon and typically involve the release of very small material amounts.

Pressurized Liquid/Gas Releases**Code Name: CASRAM-SC**

Feature	Y/N	Description	Limitations or Assumptions
Consideration of water reactivity	N	This is not considered in the current version of the model.	
Extensive data base provided	Y	DIPPR database is used.	
Some data/properties must be user specified	N		
Special features	Y	The code has an option to determine stochastically or deterministically based release quantities.	There is a need to incorporate release statistics for fixed facilities.
Linked to transport model	Y	CASRAM-SC determined emission rates are fed directly to CASRAM-SC's transport-dispersion and consequence/risk assessment algorithm.	
Sample of test case accident scenarios run?	Y	See anhydrous ammonia spill test case results in Section 6.2 and Appendix C of this report.	

Graded Approach Applicability: The model is applicable to a broad range of chemical accident severity assessment situations. However, it is most applicable to assessment of consequences and risk associated with the operation of "high hazard" chemical facilities.

General Review Criteria

Code Name: **EMGRES, A Portable Computing System for Use in Toxic Gas Emergencies**

1. Capabilities: EMGRES is a screening tool for assessing the downwind distance to a select chemical concentration. The source-term models in the program include release of a pure vapor through an orifice, release of a subcooled liquid from a reservoir, and point source instantaneous and continuous plume gas releases. All source-term models are linked to neutral and heavy gas dispersion models.
2. Sponsor/Developing Organization:

Ontario Ministry of the Environment
Air Resources Branch
3. Current Custodian/Phone/Fax/Internet Address:

Ontario Ministry of the Environment
Air Resources Branch
880 Bay Street, 4th Floor
Toronto, Ontario M5S 1Z8
4. Genealogy: Development of the first version of EMGRES began in 1980's as an adaptation of a more sophisticated simple (neutral) and heavy gas model implement by the Ontario Ministry of the Environment on an IBM mainframe. The initial version was released in 1985. The 1988 release considered in this evaluation includes in addition to the 1985 release, capabilities for modeling an evaporating liquid pool.
5. User's Manual Reference:

Diamond, G.L., W.C. Tam, P.K. Misra, H. Sahota, March 1988, A Portable Computing System for Use in Toxic Gas Emergencies, Ontario Ministry of the Environment, ARB-150-87, ISBN 0-7729-3448-7 (Revised Edition).
6. Model Description Summary: EMGRES is a PC-based source-term and dispersion screening tool designed for obtaining downwind distances to select levels of concern with a minimum of user input and

computational expense. It use is primarily intended as an emergency response tool in the event of a release of a hazardous chemical. The program provides hazardous contaminant information, calculates toxic concentrations at various distances downwind of a release, and displays the information on the screen compared to threshold exposure levels such as the Threshold Limit Values (TLV), Short Term Exposure Limits (STEL), and Immediately Dangerous to Life and Health (IDLH). Finally, in the event the release possess combustible properties, the code gives an estimate of the mass of vapor within the flammable limits.

7. Model Description References: Model description and references are provided in the user's manual. Select references that capture many of the modeling approaches implemented in EMGRES are as follows:

Chong, J. Hazardous Gas Release Model, 1980, Air Resources Branch, Program Documentation, Ontario Ministry of the Environment.

Eidsvik, K.J., 1980, "A Model for heavy Gas Dispersion in the Atmosphere," *Atmospheric Environment*, 14, 769-777.

Fryer, L.S. and G.D. Kaiser, 1979, DENZ - A Computer Program for the Calculation of the Dispersion of Dense Toxic or Explosive Gases in the Atmosphere, United Kingdom Atomic Energy Authority, Report SRD R152.

Opschoor, Ir.G., "Evaporation", Chapter 5 of TNO "Yellow Book", *Methods for Calculation of the Physical Effects of Escape of Dangerous Materials*, 1st Edition, Volume III, February 1978.

Reid, J., January 1980, "Dispersion of Denser-than-Air Gases," Atmospheric Environment Service, Boundary Layer Research Division.

Van Ulden, A.P., "On the Spreading of a Heavy Gas Released Near the Ground," First International Loss Prevention Symposium, The Hague/Delft Elsevier, Amsterdam, 221-226.

8. Hardware Requirements: Requirements include: an IBM PC compatible computer (8086 processor or greater), CGA or greater graphics support, 640 kbytes of RAM, DOS 3.0 or higher with GWBASIC.

9. Quality Assurance Documentation:

Benchmarking - Sample cases using a set of large-scale propane release field experiment data were analyzed using the 1983 version of the code and compared to DEGADIS and SLAB. See the following reference for details:

Kumar, A., j. Lou, and G.F. Bennett, January 1993, "Statistical Evaluation of Lower Flammability Distance (LFD) Using Four Hazardous Release Models," Process Safety Progress, Vol 12, No. 1, pp. 1-11.

Source code Verification - Unknown.

Evaluation (Validation") against experimental data - Sample cases using a set of large-scale propane release field experiment data were analyzed using the 1983 version of the code. See the following reference for details:

Kumar, A., J. Lou, and G.F. Bennett, January 1993, "Statistical Evaluation of Lower Flammability Distance (LFD) Using Four Hazardous Release Models," Process Safety Progress, Vol 12, No. 1, pp. 1-11.

10. Input Summary (data and parameters): The source-term models consist of a gas release from a reservoir, a liquid release from a vessel, and liquid pool evaporation.

Gas release model: requires the molecular weight of the gas, reservoir temperature, specific heat ratio and outlet orifice area.

Liquid release model: requires the height of the liquid column above the outlet orifice (upright cylindrical geometry assumed), initial vessel pressure, liquid density, and outlet orifice area

Pool evaporation model: requires the molecular weight of the vapor, volume of liquid released and the minimum pool depth, saturated vapor pressure at 20 °C, and the ambient wind speed.

11. Output Summary: The source-term models only provide steady-state gas and liquid mass outflow rates and pool evaporation rate. The output values are summarized as intermediate results in an output screen. Most of the output focuses on the results of the downwind dispersion including cloud dimensions, location and concentration as a function of time.

12. Summary of Limitations: EMGRES is admittedly a simplistic model and highly conservative. It should only be used as a preliminary screening tool. Although it is intended as an emergency response program, navigating through all the intermediate menus can take somewhat more time than is ideal.
13. Summary of Strengths: The code possess an extremely large data base of physical/chemical properties commonly required for screening level of analyses.
14. Range of Applicability (situations, sites, sources, etc.): The code is applicable to pressurized and non-pressurized liquid and gaseous releases for a large number of materials.
15. Comments on User Friendliness: The program is somewhat dated in the sense that it requires loading basic, the source object module, and then executing the program. There is no means of "backing out" of select sequence of menu items (by repeatedly using the Esc key, for instance) at specific junctures in the program without first fulfilling the entire input list requirements.
16. Comments on Error Handling Capabilities and User Feedback: Limited error handling capabilities are included in the program. Non-physical values are rejected by the program and the user is prompted for an alternate value.
17. Source code and/or data bases can be modified?: The program is written in standard MicroSoft basic and distributed in object format with the source code. The physical/chemical database may be modified by the user.
18. Execution time for typical problem (CPU or real time): Execution time is extremely rapid (order of several seconds real time).
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): The entire program is contained on a single medium or high-density floppy disk. The user's manual is provided separately (ISBN 0-7729-3448-7).
20. Cost: None.
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? The code is generally acceptable in applications supporting SAR, BIO, and JCO documents. The source models in EMGRES interface with both the near-field dense gas model and the far-field neutrally buoyant

dispersion model. No assessment of environmental consequences is performed. The dense gas model assumes an effectively instantaneous release of air contaminant. The neutrally buoyant dispersion model is not applicable to receptors close to the release source point. Therefore exposures to local workers attributed either to a passive release or a continuous release of a dense gas will not be modeled appropriately by the program.

22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? Use of EMGRES should be limited solely to low hazard facilities due to its inherently conservative source-term and dispersion models. It may serve as a screening tool where the mitigating effects of initial dilution of a gas or vapor jet are neglected. The pool evaporation model often times gives overly conservative estimates for the liquid mass evaporation rate, which hinders its usefulness for subcooled liquid releases.
23. Future Enhancements Planned: Unknown.
24. Additional Information: The pool evaporation model appears to be in error -- the vapor mass emission rates reported by the code for select chemicals are extremely high and do not compare with results obtained from more sophisticated programs or established experimental correlations.

Specific Evaluation Criteria

Liquid Chemical Spills and Evaporation

Code Name: **EMGRES**

Feature	Y/N	Description	Limitations or Assumptions
Determination of pool size (i.e. considers area source)	Y-	Pool area is simply determined by taking the ratio $A_p = V(t)/d$ where $V(t)$ is the liquid volume spilled at time t and d is the pool depth.	Code does not possess the option for entering a pool dike area directly. A pool area may be effectively entered by specifying an initial volume of liquid and minimum pool depth which will give the desired initial pool dimensions. This approach will not be valid on a long time scale as a significant portion of the initial mass inventory has evaporated.
Consideration of pool depth	Y	The user may specify a pool depth or alternatively the program assumes a minimum depth of 0.1 mm.	
Determination of release rate	Y	The evaporation rate is based on an empirical correlation developed by TNO (Ir. G. Opschoor, "Evaporation", Chapter 5 of TNO "Yellow Book", <i>Methods for Calculation of the Physical Effects of Escape of Dangerous Materials</i> , 1st Edition, Volume III, February 1978).	This calculation may be shown to be under-conservative for certain classes of releases (e.g, cryogenic releases).
Consideration of ambient and/or site-specific conditions	Y	Ambient temperature, pressure, and wind speed is considered in the pool evaporation model.	Pool substrate material is assumed to be impermeable.

Liquid Chemical Spills and Evaporation

Code Name: **EMGRES**

Feature	Y/N	Description	Limitations or Assumptions
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y-	The initial temperature of the cloud is set equal to the minimum of the ambient temperature and the boiling temperature of the chemical substance release into the atmosphere.	No true heat transfer between the cloud and the ambient environment is considered. The initial cloud temperature is only used in the dense gas model and solely for the purpose of determining the mass of air necessary to evaporate the liquid component present in the cloud (where applicable). The fraction of a liquid release which may be initially present in the cloud is a parameter entered by the user.
Time dependency of rate calculation	N		
Temperature dependency/thermal effects	N	The pool evaporation rate calculations assume an ambient temperature of 20 °C.	<p>Note: The technical reference manual states that the evaporation rates at temperatures other than 20 °C are computed via the relation</p> $Q_{amb} = Q_{20^{\circ}C} \frac{P_{amb} T_{20^{\circ}C}}{P_{20^{\circ}C} T_{amb}}$ <p>This relationship is physically counter-intuitive -- the evaporation rate should decrease with increasing pressure and increase with increasing temperature. In any event, the code does not perform this calculation.</p>

Liquid Chemical Spills and EvaporationCode Name: **EMGRES**P

Feature	Y/N	Description	Limitations or Assumptions
Time dependent spill to pool	Y-	The pool spill area at any given instant is given by the product of the steady-state liquid release rate and the time since initiation of the release.	The liquid outflow rate from a vessel or reservoir is simply calculated by means of the Bernoulli equation using the initial liquid height. All liquid reservoirs are assumed to be an upright cylinder.
Consideration of heat transfer from substrate	N		
Consideration of chemical reaction with substrate	N		
Consideration of energy balance	N		
Consideration of water reactivity	N		
Consideration of multi-component mixtures/solutions	N		

Liquid Chemical Spills and EvaporationCode Name: **EMGRES**

Feature	Y/N	Description	Limitations or Assumptions
Extensive data base provided	Y	Chemical data of 856 chemicals have been entered into the program database.	The database is limited in the types of physical/chemical data required for relatively simple calculations.
Some data/properties must be user specified	N		
All data/properties must be user specified	N		
Special features	N		
Test problem evaluation	N		
Linked to transport model	Y	The source-term model is linked to a Gaussian plume and puff model as well as an instantaneous dense gas model.	In many instances pool evaporation leads to the formation of a dense cloud. The use of the dispersion models under these conditions should be limited to receptor locations sufficiently far away to ensure that the 'instantaneous' release assumption is a reasonable approximation.
Other	N		

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Graded Approach Applicability: Use should be restricted to low hazard facilities only.

Pressurized Liquid/Gas Releases**Code Name: EMGRESP**

Feature	Y/N	Description	Limitations or Assumptions
Determination of release rate	Y	Model uses the standard equations for choked and unchoked flow of a gaseous fluid out of a orifice, and the Bernoulli equation for liquid outflow.	Assumes ideal gas behavior for all vapor and gas outflow calculations. Neglects changes in enthalpy, reservoir pressure and temperature.
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	N	Cloud temperature is assumed to be ambient at all times. This constraint is a result of the isothermal assumption in the vapor and liquid outflow models.	Under adiabatic conditions (i.e. an insulated vessel or a release over a significantly short time scale, as a vapor reservoir is evacuated, the temperature of the vapor will reduce as the vessel depressurizes.
Consideration of ambient and/or site-specific conditions	N	Ambient conditions are only taken into consideration (implicitly) when the gas reservoir conditions are allowed to reach equilibrium with the ambient temperature (i.e. no thermal control or insulation).	

Pressurized Liquid/Gas ReleasesCode Name: **EMGRES**

Feature	Y/N	Description	Limitations or Assumptions
Geometry considerations e.g. orifice size	Y		The orifice dimensions should be much less (orders of magnitude) than the dimensions of the vessel. The discharge coefficient is fixed in the code and cannot be modified by the user. No capability for modeling the influence of pipework between the reservoir and the outlet orifice.
Time dependency of rate calculation	N	Simple steady-state orifice calculations are performed based on initial tank pressure and temperature conditions.	
Temperature dependency/thermal effects	N	Isothermal conditions are assumed for all gas and liquid releases.	
Consideration of critical flow	Y	Model uses the standard equations for choked and unchoked flow of a fluid out of a orifice.	Assumes ideal gas behavior for all vapor and gas outflow calculations. Neglects changes in enthalpy, reservoir pressure and temperature
Consideration of two-phase flow	N		
Consideration of water reactivity	N		
Extensive data base provided	Y-	Gas molecular weight, specific heat ratio, and liquid density are the only physical properties used in the calculations (provided by the data base).	

Pressurized Liquid/Gas ReleasesCode Name: **EMGRES**

Feature	Y/N	Description	Limitations or Assumptions
Some data/properties must be user specified	N		
All data/properties must be user specified	N		
Test problem evaluation	N		
Special features	N		
Linked to transport model	Y	The source-term model is linked to a Gaussian plume and puff model as well as an instantaneous dense gas model.	In many instances pool evaporation leads to the formation of a dense cloud. The use of the dispersion models under these conditions should be limited to receptor locations sufficiently far away to ensure that the 'instantaneous' release assumption is a reasonable approximation.
Other	N		

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Graded Approach Applicability: Use should be restricted to low hazard facilities only.

General Review Criteria

Code Name: HGSys~~tem~~

1. Capabilities: HGSys~~tem~~ is a general purpose PC-based chemical source-term and atmospheric dispersion model. It is comprised of a number of individuals modules used to simulate source-terms, near-field, and far-field dispersion. The chemical and thermodynamic models available in HGSys~~tem~~ include reactive hydrogen fluoride and non-reactive, two-phase, multi-compound releases. A very brief summary of the modeling capabilities is given below:

- Account for the HF/H₂O/air thermodynamics and cloud aerosol effects on cloud density.
- Model both pressurized and non-pressurized releases.
- Predict concentrations over a wide range of surface roughness conditions.
- Predict concentrations at specific locations for user-specified averaging periods.
- Consider stead-state, time-varying, and finite release duration releases.
- Compute crosswind and vertical concentration profiles.

2. Sponsor/Developing Organization:

Sponsor: Industry Cooperative HF Mitigation/Assessment
Program, Ambient Impact Technical Subcommittee
(20 chemical and petroleum companies)

Developer: Shell Research Limited, Thornton Research Centre,
England

3. Current Custodian/Phone/Fax/Internet Address:

Howard Feldman
American Petroleum Institute
1220 L Street Northwest
Washington, D.C. 20005

Phone: 202-682-8340

Fax: 202-682-8270

4. Genealogy: The first public domain release of HGSystem Version 1.0 was released in November of 1990. Several later versions of the code were developed but not made publicly available. Version 3.0 (evaluated here) is the second public domain version of HGSystem.

5. User's Manual Reference:

L. Post (editor), 1994, HGSystem 3.0 User's Manual, Report No. TNER.94.058, Shell Research Limited, Thornton Research Centre, P.O. Box 1, Chester, England, Shell International Research Maatschappij B.V.

6. Model Description Summary: HGSystem is a computer-based model to calculate the release properties of an accidental release of hydrogen fluoride (HF) including simulation of plume and jet behavior. Three areas which the code explicitly addresses where a great deal of uncertainty existed in previous models are 1) the modeling of the complex thermodynamics of HF/H₂O/air mixtures (including aerosol effects on cloud density), 2) the treatment of a wide range of surface roughness conditions, and 3) jet flow and air entrainment for pressurized release of HF, followed by transition to ground-based dense gas dispersion.

7. Model Description References:

P.N. Clough, D.R. Grist, and C.J. Wheatley, "Thermodynamics of Mixing and Final State of a Mixture formed by the Dilution of Anhydrous Hydrogen Fluoride with Moist Air", Safety and Reliability Directorate, United Kingdom Atomic Energy Authority, Wigshaw Lane, Culcheth, Warrington, Cheshire, England, WA3 4NE, SRD R 396, 1987.

G.W. Colenbrander and J.S. Puttock, "Maplin Sands experiments 1980: interpretation and modelling of liquified gas spills on the sea", in *Atmospheric Dispersion of Heavy Gases and Small Particles*, G. Ooms

and H. Tennekes, editors, Springer-Verlag, Berlin.

Du Pont, "Hydrofluoric Acid, Anhydrous - Technical, Properties, Uses, Storage and Handling", undated bulletin, E.I. du Pont de Nemours & Company, Wilmington, Delaware, 1988.

L. Post (editor), 1994, HGSysstem 3.0 Technical Reference Manual, Report No. TNER.94.059, Shell Research Limited, Thornton Research Centre, P.O. Box 1, Chester, England, Shell Internationale Research Maatschappij B.V.

W. Schotte, "Fog formation of hydrogen fluoride in air", *Ind. Eng. Chem. Res.*, Vol. 26, pp. 300-306, 1987.

W. Schotte, "Thermodynamic Model for HF Fog Formation", letter to C.A. Soczek, dated August 31, 1988, E.I. DuPont de Nemours & Company, du Pont Experimental Station, Engineering Department, Wilmington, Delaware 1988, private communication.

C.E. Vanderzee and W.W. Rodenburg, "Gas imperfections and thermodynamic excess properties of gaseous hydrogen fluoride", *Journal of Chemical Thermodynamics*, Vol. 2, pp. 461-478, 1970.

H.W.M. Witlox, "Thermodynamics model for mixing of moist air with pollutant consisting of HF, ideal gas, and water", Shell Research Limited, Thornton Research Center, TNER.93.021, 1993.

8. Hardware Requirements: The code is primarily intended for compilation under Microsoft FORTRAN Powerstation and execution on a PC, but it is easily adaptable to any platform possessing a standard FORTRAN 77 compiler. The minimum hardware requirements are as follows:

IBM PC compatible with a 80386 processor or greater
4 Mbytes of RAM
2 Mbytes hard disk space
Math coprocessor chip is optional but highly recommended.

9. Quality Assurance Documentation:

Benchmarking - HGSysstem has been benchmarked in comparison to 9 independent dense gas models: DEGADIS, SLAB, AIRTOX, CHARM, FOCUS, GASTAR, PHAST, TRACE, and the Britter & McQuaid model. Details are provided in Hanna, S.R., D.G. Strimaitis, and J.C. Chung, 1993, "Hazardous Gas Model Evaluation with Field Observations," *Atmospheric Environment*, Vol. 27A, No. 15, pp. 2265-2285.

Source code Verification - Unknown.

Evaluation ("Validation") against experimental data - A comparison of code results to large scale field data has been performed with the Burro, Coyote, Desert Tortoise, Goldfish, Hanford Kr⁸⁵, Maplin Sands, Prairie Grass, and Thorney Island data sets. Details are provided in Hanna, S.R., D.G. Strimaitis, and J.C. Chung, 1993, "Hazardous Gas Model Evaluation with Field Observations," Atmospheric Environment, Vol. 27A, No. 15, pp. 2265-2285.

10. Input Summary (data and parameters): Input is provided by means of the NAMELIST feature where a descriptive variable name is equivalenced to a numeric value. Comment statements are also permitted in input files in order to further clarify input entries.

SPILL (time-dependent liquid and vapor discharge rates calculations)

Input File Parameters:

- RESERVOIR Block - parameters describing the reservoir fluid thermodynamic state
- GASDATA Block - initial composition of the reservoir mixture and the relevant thermodynamic data
- PIPE Block - release pipe/orifice-plane conditions
- AMBIENT Block - conditions of the ambient environment
- TERMINAT Block - sets reservoir release termination criteria.

HFSPILL (the HF-specific counterpart of *SPILL*) has a similar input structure:

- RESERVOIR Block
- LIQUID Block - data from which *HFSPILL* determines the vessel equilibrium state when liquid HF is present
- VAPOUR Block - data from which the vessel equilibrium state is determined when only vapor is present
- PIPE Block.

HFFLASH is a HF-specific program used to calculate post-flash temperature and liquid fraction following release of anhydrous hydrogen fluoride. This module requires the RESERVOIR and PIPE data blocks only.

LPOOL simulates the time-dependent evaporation of a multi-component liquid pool on land or water.

- CONTROL Block - parameters for determining maximum simulation time, minimum film thickness of pool, and time step for pool data used to link to dispersion model

- GROUND Block - parameters which describe the ground composition and the dike composition and size (where applicable)
- SPILL Block - parameters which describe the discharge details for a release of liquid from a reservoir
- RESERVOIR Block - includes radius of a cylindrical tank, initial fluid level, equivalent diameter of reservoir orifice, and elevation of the orifice.
- AMBIENT Block - includes relative air humidity, fraction of sky covered by clouds, spill starting time, and times for sunrise and sunset
- FLASH Block - user-specified flash and aerosol fractions
- GASDATA Block.

11. Output Summary: Each source-term module creates a number of different ASCII text output files including intermediate data values, time-dependent source-term results, and data files used by the dispersion analysis modules.

SPILL Time-Dependent Model Output:

- reservoir total mass content (tonnes)
- release mass flow rate (kg/s)
- reservoir absolute pressure (atm)
- reservoir temperature (°C)
- reservoir mixture density (kg/m³)
- reservoir total enthalpy (kJ/kg)
- reservoir mole fraction liquid (%)
- reservoir average molar mass (kg/kmole)
- reservoir liquid density (kg/m³)
- heat flux from ambient to reservoir (kW/m²)
- reservoir fluid state (vapour/two-phase)
- average release rate since release start (kg/s)

LPOOL Time-Dependent Model Output:

- total vapor release rate
- flash rate
- aerosol release rate
- pool evaporation rate
- cumulative mass released from the reservoir
- mass of liquid in the pool
- pool area
- pool temperature

12. Summary of Limitations: Code limitations include:

- HGSysyem cannot be used for analyzing releases where there is pipework present between the reservoir and the outlet orifice.
- There are a limited number of pool substrate materials which can be modeled by HGSysyem, specifically sand, concrete, plastic, steel, and water.
- It is difficult to extend the physical/chemical data base utility DATAPROP to include additional chemical species. Such modifications would require an extremely good knowledge of the HGSysyem program structure and some consultation with the code developers.

13. Summary of Strengths: HGSysyem offers the most rigorous treatments of HF source-term and dispersion analysis available for a public domain code. The code also offers modeling capabilities to other chemical species with complex thermodynamic behavior. Some special features in HGSysyem include:

- Aerosols and multi-component mixtures: Ability to model spillage of a liquid non-reactive compound from a pressurized vessel.
- Time-dependent dispersion: Ability to carry out more efficient simulations of time-dependent dispersion problems by automating the selection of output times and output steps in the HEGADAS-T model. Improve dosage calculations and time averaging (HEGADAS-T/HTPOST). Ability to model dispersion on terrain with varying surface roughness.
- Evaporating pools: Ability to include effects of dike containments (EVAP). General upgrade of evaporating pool model.
- User friendliness of HGSysyem: Upgrading of post-processors HSPOST and HTPOST. Shared input parameter file.
- Sensitivity analyses performed for EVAP, SPILL, AEROPLUME, HEGADAS-S and HEGADAS-T to ensure robustness and correctness of code and to evaluate effect of model parameters on dispersion analysis.
- Concentration predictions: Inclusion of a concentration profile in AEROPLUME that provides smooth transitions with the concentration profiles adopted in PGPLUME for airborne plumes. Re-examination of cross-wind concentrations

formulation in HEGADAS.

14. Range of Applicability (situations, sites, sources, etc.): The code was explicitly designed to model water reactivity of HF when it is released to the ambient environment. Use of the code is also valid for other chemicals releases that exhibit both ideal and non-ideal gas behavior in the flow regime of interest. It is also applicable to single- or multi-component chemical releases resulting from upset conditions in typical process operations.
15. Comments on User Friendliness: The program is run in batch mode using a combination of customized batch files and input data files. Some manual manipulation of the data may be necessary when using results from utility programs such as DATAPROP as input into a successive source-term model. No graphical post-processing utilities are included with the code, but output is suitably output in tabular form such that second party graphics packages can be used with minimal modification of the output format.
16. Comments on Error Handling Capabilities and User Feedback: A variety of diagnostic messages including input data file validation, runtime error messages, numeric convergence information, warning messages, as well as run information detailing the progress of the calculations are provided.
17. Source code and/or data bases can be modified?: Source code modification is possible, but the parameter space of the correlations used in the model as well as overall program logic should be understood VERY WELL prior to modification.
18. Execution time for typical problem (CPU or real time): Execution time is several minutes (real time) maximum.
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): The code is distributed on three floppy diskettes. Documentation is provided separately in a two-volume set.
20. Cost: None.
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? The code is generally acceptable in applications supporting SAR, BIO, and JCO documents. The source-term models are linked to dispersion models, which in turn can predict the level of chemical vapor concentration exposure to a collocated worker or public offsite receptor. Environmental impacts are not assessed by the code (e.g., no vapor

deposition model). The source-term simulation is sufficiently refined in terms of spatial and temporal resolution to support use of near-field models for assessing the impact to individuals located near the chemical source.

22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? HGSysSystem is applicable to low, moderate, and high hazard facilities where the potential exposures to toxic chemicals outside facilities in the ambient environment require analysis. The level of sophistication in the modeling capabilities offered by the code exceed the requirements for most low hazard facilities.
23. Future Enhancements Planned: Version 3.0 was just released prior to completion of the evaluation. Future enhancements are still to be determined.
24. Additional Information:

Specific Evaluation Criteria

Liquid Chemical Spills and Evaporation

Code Name: **HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Determination of pool size (i.e. considers area source)	Y	<p>Equations governing the spread of a vaporizing pool can be found in the following reference:</p> <p>Shaw, P. And F. Briscoe, 1978, "Evaporation from the Spills of Hazardous Liquids on Land and Water", United Kingdom Atomic Energy Authority.</p> <p>The spreading law for releases on water is based on a "dam burst" equation for the leading edge velocity.</p> <p>Pool shape is determined by the presence of a dike. An unconfined pool is assumed to be circular for all time. However, if a dike is encountered during the spreading phase, the pool is modeled as a succession of reforming wedges that eventually fill the region between the tank and the dike if sufficient quantities of liquid are released.</p>	The referenced equations are based on a circular spreading pool of uniform thickness. The implementation in HGSystem uses a modification of the equations where the pool cross-sectional profile is triangular rather than rectangular in the spill phase. The pool growth model is based on the conversion of gravitational potential area to kinetic energy and neglects all viscosity and surface tension effects. The pool growth model may therefore not accurately model highly viscous liquids.
Consideration of pool depth	Y	The user may specify a desired minimum pool thickness (minimum of 0.1 mm).	

Liquid Chemical Spills and Evaporation

Code Name: **HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Determination of release rate	Y	<p>The release rate from the liquid reservoir into the pool is based on the simple Bernoulli equation for non-flashing flows and the Fauske-Epstein equation for two-phase choked flow out of an orifice for flashing liquid releases.</p> <p>The subsequent evaporation rate from a liquid pool is dependent upon the ambient conditions (see "Temperature dependency/ thermal effects" evaluation criteria below) which determines the mass entrainment rate.</p>	<p>The orifice outlet model has not been generalized to include the frictional effects of pipework between the reservoir and the orifice outlet.</p> <p>There is no model for the mass transfer taking place at a two-phase film above the surface of the pool. Such a film may form under high stability, low wind speed conditions and will likely possess different thermodynamic characteristics from that of the bulk liquid. This phenomena occurs most prevalently in the case of cryogenic releases.</p>
Consideration of ambient and/or site-specific conditions	Y	Ambient temperature, pressure, wind speed, relative air humidity, solar radiative heat flux (long and short wave length), ground temperature, and pool substrate material is accounted for in the pool evaporation calculations.	There are a limited number of pool substrate materials from which the user can select: sand, concrete, plastic, steel, and water. Clay or asphalt surfaces, for instance, can not be modeled without significant modification of the program.

Liquid Chemical Spills and Evaporation

Code Name: HGSystem

Feature	Y/N	Description	Limitations or Assumptions
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y	The initial characteristic of the vapor cloud are based on the saturated vapor temperature (which in turn is determined by the bulk liquid pool temperature) and ambient conditions. The liquid evaporation model is interfaced with the transient HEGADAS dispersion model which calculates the heat transfer between the cloud and the entrained ambient air as well as characterizes the cloud size and density as a function of time.	
Time dependency of rate calculation	Y	The pool evaporation simulation is completely time-dependent.	Select thermodynamic variables are assumed to remain constant within an individual time step during the simulation. The computer program automatically adjusts the time step size to satisfy some error criteria. It is not well understood from the user's perspective what that criteria is nor how to gain access to it.
Temperature dependency/thermal effects	Y	The heat transfer processes considered in the code include convective heat transfer, conductive heat transfer (ground and dike when present), heat loss due to evaporation, heat of liquid added (spill phase only), ambient radiative heat transfer (long-wave emissions), solar short-wave radiation, heat conduction through the vessel walls, and sensible heat.	

Liquid Chemical Spills and Evaporation

Code Name: HGSystem

Feature	Y/N	Description	Limitations or Assumptions
Time dependent spill to pool	Y	The release rate from the liquid reservoir into the pool is based on the simple Bernoulli equation for non-flashing flows and the Fauske-Epstein equation for two-phase choked flow out of an orifice for flashing liquid releases.	The orifice outlet model has not been generalized to include the frictional effects of pipework between the reservoir and the orifice outlet.
Consideration of heat transfer from substrate	N	The heat transferred to the pool due to ground conduction is based on the simple analytic expression for heat transfer through a semi-infinite slab.	A more accurate treatment would be to consider the cooling of the substrate as liquid evaporation proceeds. Also, moisture content of the substrate is an important consideration because the thermodynamic properties of the substrate may be significantly changed if freezing of the water occurs such as in the case of cryogenic releases.
Consideration of chemical reaction with substrate	N		
Consideration of insolation	Y	Short-wave solar radiation is modeled.	The radiative heat transfer depends on the time of day (i.e. adjustment for the variation in view factor due to the relative position of the vessel with respect to the sun).

Liquid Chemical Spills and Evaporation

Code Name: HGSystem

Feature	Y/N	Description	Limitations or Assumptions
Consideration of water reactivity	Y	The code models the hygroscopic behavior of HF primarily by means of a combination of first-principles (conservation of equivalent molar flow, mass, and energy) and empirical correlations based on small and large scale tests.	<p>The assumptions and underlying physical principles of the HF/Water/Air interactions are relatively involved. See references:</p> <p>(1) W. Schotte, "Fog formation of hydrogen fluoride in air", <i>Ind. Eng. Chem. Res.</i>, Vol. 26, pp. 300-306, 1987.</p> <p>(2) W. Schotte, "Thermodynamic Model for HF Fog Formation", letter to C.A. Soczek, dated August 31, 1988, E.I. DuPont de Nemours & Company, du Pont Experimental Station, Engineering Department, Wilmington, Delaware 1988, private communication.</p> <p>(3) Du Pont, "Hydrofluoric Acid, Anhydrous - Technical, Properties, Uses, Storage and Handling", undated bulletin, E.I. du Pont de Nemours & Company, Wilmington, Delaware, 1988.</p> <p>(4) C.E. Vanderzee and W.W. Rodenburg, "Gas imperfections and thermodynamic excess properties of gaseous hydrogen fluoride", <i>Journal of Chemical Thermodynamics</i>, Vol. 2, pp. 461-478, 1970.</p> <p>(5) P.N. Clough, D.R. Grist, and C.J. Wheatley, "Thermodynamics of Mixing and Final State of a Mixture formed by the Dilution of Anhydrous Hydrogen Fluoride with Moist Air", Safety and Reliability Directorate, United Kingdom Atomic Energy Authority, Wigshaw Lane, Culcheth, Warrington, Cheshire, England, WA3 4NE, SRD R 396, 1987.</p>

Liquid Chemical Spills and Evaporation

Code Name: HGSystem

Feature	Y/N	Description	Limitations or Assumptions
Consideration of multi-component mixtures/solutions	Y	The code possesses the ability to model the thermodynamic behavior of a multi-component release.	A maximum of 8 different chemical species may be present.
Extensive data base provided	Y-	The physical/chemical data base utility DATAPROP has the capability of generating the temperature-dependent parameters required by the HGSystem source-term models for 30 different chemical species. There is an extensive list of physical and chemical specific thermodynamic properties required for input if the user wishes to model a release of a species not included in the data base.	It is difficult to extend the physical/chemical data base utility DATAPROP to include additional chemical species. Such modifications would require an extremely good knowledge of the HGSystem program structure and some consultation with the code developers.
Some data/properties must be user specified	N		
All data/properties must be user specified	N		
Test problem evaluation	Y	See anhydrous ammonia, chlorine, and acetone spill test case results in Section 6.2 and Appendix C of this report.	
Special features	N		
Linked to transport model	Y	The source model is linked to a variation of the HEGADIS steady-state and transient models for dense gases as well as the Pasquill/Gifford dispersion model for neutrally buoyant releases.	

Liquid Chemical Spills and Evaporation

Code Name: HGSystem

Feature	Y/N	Description	Limitations or Assumptions
Other	Y	Contains a pool evaporation model, EVAPW, (G.W. Colenbrander and J.S. Puttock, "Maplin Sands experiments 1980: interpretation and modelling of liquified gas spills on the sea", in <i>Atmospheric Dispersion of Heavy Gases and Small Particles</i> , G. Ooms and H. Tennekes, editors, Springer-Verlag, Berlin.) that calculates the time-dependent spreading and evaporation of a liquid pool on water.	Assumes the liquid is a cryogenic liquid having a boiling point much below ambient. The evaporation rate is entirely dependent on the heat flux from the water body, which must be specified by the user.

Graded Approach Applicability: Use of the code is appropriate for all hazard levels, but it may be most useful for higher hazard facilities.

Pressurized Liquid/Gas Releases**Code Name: HGSystem**

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Feature	Y/N	Description	Limitations or Assumptions
Determination of release rate	Y	The reservoir release model is based in part on an ensemble of empirical correlations for the efflux of mass and heat from the vessel into the atmospheric environment. The release calculations also must satisfy equations ensuring physical consistency between the state variables, conservation of total reservoir mass, conservation of energy, and conservation of each individual compound mass.	There is no detailed pipe/orifice discharge models in which such effects as inter-phase slip, thermal non-equilibrium, and the influence of wall-friction and heat transfer are taken into consideration. The flow acceleration from reservoir fluid at rest to flow within the discharge pipe is assumed to be governed by the Bernoulli equation for compressible flow (entry losses are neglected).
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y-	Orifice outlet pressure, temperature, vapor mass fraction, and degree of polymerization (HF releases only) are provided as a function of time.	Some of the outlet properties are assumed to be in thermodynamic equilibrium with the corresponding quantities inside the reservoir.
Consideration of ambient and/or site-specific conditions	Y	Ambient temperature, pressure and wind speed are user-specified.	Radiative heat flux on the vessel, the surface area of the vessel, and the emissivity of the vessel material may be user-specified.
Geometry considerations e.g. orifice size	Y	An effective orifice diameter is specified by the user.	A fixed loss coefficient for wall orifice releases is assumed.

Pressurized Liquid/Gas Releases**Code Name: HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Time dependency of rate calculation	Y	The time-dependency of the following state variables are considered: Mass release rate, reservoir total mass content, reservoir absolute pressure, reservoir temperature, reservoir mixture density, reservoir total enthalpy, reservoir mole fraction liquid, reservoir average molar mass, reservoir liquid density, heat flux from ambient to reservoir, reservoir fluid state, average release rate since release start.	The orifice size is assumed to be sufficiently small that the assumption of thermal equilibrium through the reservoir is valid. Effects of highly transient depressurization such as bulk flashing, liquid boil-off, and near homogeneous two-phase conditions with the reservoir must be neglected in order to preserve consistency with requirements of the near-field jet dispersion model.
Temperature dependency/thermal effects	Y	Reservoir internal enthalpy, pressure, temperature, and vapor-to-liquid mass fraction is computed as a function of time following initiation of the release.	All reservoir release calculations assume adiabatic invariance.
Consideration of critical flow	Y	Critical flow is based on standard orifice calculations for choked flow.	The possibility of droplet flow resulting from condensation within the vapor phase is neglected. Furthermore, the model takes no account of in-wall or pipe wall friction in estimating the mass discharge rates and choke pressures at the point of release. On the other hand, the code does account for the non-ideal behavior of gases under extreme pressures.

Pressurized Liquid/Gas ReleasesCode Name: **HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Consideration of water reactivity	Y	The code models the hygroscopic behavior of HF primarily by means of empirical correlations based on small and large scale tests.	<p>The assumptions and underlying physical principles of the HF/Water/Air interactions are relatively involved. See references:</p> <p>(1) W. Schotte, "Fog formation of hydrogen fluoride in air", <i>Ind. Eng. Chem. Res.</i>, Vol. 26, pp. 300-306, 1987.</p> <p>(2) W. Schotte, "Thermodynamic Model for HF Fog Formation", letter to C.A. Soczek, dated August 31, 1988, E.I. DuPont de Nemours & Company, du Pont Experimental Station, Engineering Department, Wilmington, Delaware 1988, private communication.</p> <p>(3) Du Pont, "Hydrofluoric Acid, Anhydrous - Technical, Properties, Uses, Storage and Handling", undated bulletin, E.I. du Pont de Nemours & Company, Wilmington, Delaware, 1988.</p> <p>(4) C.E. Vanderzee and W.W. Rodenburg, "Gas imperfections and thermodynamic excess properties of gaseous hydrogen fluoride", <i>Journal of Chemical Thermodynamics</i>, Vol. 2, pp. 461-478, 1970.</p> <p>(5) P.N. Clough, D.R. Grist, and C.J. Wheatley, "Thermodynamics of Mixing and Final State of a Mixture formed by the Dilution of Anhydrous Hydrogen Fluoride with Moist Air", Safety and Reliability Directorate, United Kingdom Atomic Energy Authority, Wigshaw Lane, Culcheth, Warrington, Cheshire, England, WA3 4NE, SRD R 396, 1987.</p>

Pressurized Liquid/Gas Releases

Code Name: **HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Consideration of two-phase flow	Y	The mass flow rate correlations developed by Fauske and Epstein are implemented for two-phase flow. Mass flux is governed by conditions at choke formation or attainment of ambient pressure according to $\frac{dm}{dt} \bigg _{exit} = (A_p u) \bigg _{vena contracta}$	The Fauske and Epstein equations do not take into account frictional losses for pipe flow. This is one of the major reasons why a pipe outflow model is not included in HGSystem.
Extensive data base provided	Y-	The physical/chemical data base utility DATAPROP has the capability of generating the temperature-dependent parameters required by the HGSystem source-term models for 30 different chemical species. There is an extensive list of physical and chemical specific thermodynamic properties required for input if the user wishes to model a release of a species not included in the data base.	It is difficult to extend the physical/chemical data base utility DATAPROP to include additional chemical species. Such modifications would require an extremely good knowledge of the HGSystem program structure and some consultation with the code developers.
Some data/properties must be user specified	N		
All data/properties must be user specified	N		
Response to test problem	Y	See anhydrous ammonia, carbon monoxide, and chlorine spill test case results in Section 6.2 and Appendix C of this report.	
Special features	N		

Pressurized Liquid/Gas Releases**Code Name: HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Linked to transport model	Y	The source model is linked to AEROPLUME (high-momentum jet and elevated plume model), HFPLUME (AEROPLUME version specifically for hydrogen fluoride), and HEGABOX (dispersion of an instantaneous heavy gas release).	
Other			

Graded Approach Applicability: Use of the code is appropriate for all hazard levels, but it may be most useful for higher hazard facilities.

Pressurized Liquid/Gas Releases - Liquid Aerosol Model**Code Name: HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Determination of release fraction (initial)	Y	External flashing of a pressurized superheated liquid is calculated.	The saturated vapor pressure of a multi-component ideal liquid release is based on Raoult's Law (in the presence of an aerosol, the ratio of the mole fraction of the compound in the vapor and the mole fraction of the compound in the aerosol equals the ratio of the partial vapor pressure for the compound and the total vapor pressure). A generalization of Dalton's Law and the Peng-Robinson equation of state is used for aerosol formation when the superheated liquid exhibits non-ideal behavior.
Determination of release rate (during evaporative phase)	N	Evaporation of the airborne aerosol component is modeled by means of heat transfer with the water content of the air entrained into the cloud and heat transfer from the ground substrate. The evaporation of the unflashed portion of a superheated release must be modeled in a separate computer run.	There is some confusion of how the modeling of saturated vapor in the jet or plume is performed. Furthermore, the model assumes all components of the jet are homogeneously mixed and moving with the same bulk speed. In reality, the aerosol component of a release may behave much differently than the vapor component both in terms of mechanical flow and thermodynamic interactions.

Pressurized Liquid/Gas Releases - Liquid Aerosol Model**Code Name: HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Determination of initial concentration	Y	The component makeup of the release (vapor to liquid ratio, initial dilution due to air entrainment around the edges of the jet) is computed immediately following the flashing zone.	Many of these parameters are interfaced with the jet and plume models in such a way that it is difficult to extract them for individual analysis.
Consideration of ambient and/or site-specific conditions	Y	Ambient temperature and wind speed is user specified.	Direction of the wind with respect to the initial jet orientation is neglected. This directional dependency is an important factor in wind shear.
Applies to both chemicals and radionuclides	N	The model applies only to chemical releases.	
Time dependency of rate calculation	Y	The flashing contribution is proportional to the rate of liquid or two-phase release.	Computation of the flashing fraction is accomplished as follows: 1) It is assumed that the mixture liquid-vapor composition does not change during the acceleration phase as the liquid passes through the orifice, 2) the new thermodynamic state of the mixture is then calculated using the full aerosol algorithm assuming that the pressure decreases from the orifice pressure to the ambient pressure. The post-flashover change in liquid-vapor composition are then calculated.
Consideration of particle size distribution	N		

Pressurized Liquid/Gas Releases - Liquid Aerosol Model**Code Name: HGSystem**

Feature	Y/N	Description	Limitations or Assumptions
Temperature dependency/ thermal effects	Y	Temperature distributions are modeled in a "Top-Hat" fashion.	A model based on similarity theory with some radial and azimuthal dependence in the jet or plume may be more accurate.
Extensive data base provided	Y-	The physical/chemical data base utility DATAPROP has the capability of generating the temperature-dependent parameters required by the HGSystem source-term models for 30 different chemical species. There is an extensive list of physical and chemical specific thermodynamic properties required for input if the user wishes to model a release of a species not included in the data base.	It is difficult to extend the physical/chemical data base utility DATAPROP to include additional chemical species. Such modifications would require an extremely good knowledge of the HGSystem program structure and some consultation with the code developers.
Some data/properties must be user specified	N		
All data/properties must be user specified	N		
Special features	N		
Linked to transport model	Y	The source model is linked to AEROPLUME (high-momentum jet and elevated plume model), HFPLUME (AEROPLUME version specifically for hydrogen fluoride), and HEGABOX (dispersion of an instantaneous heavy gas release).	
Other			

Graded Approach Applicability: Use of the code is appropriate for all hazard levels, but it may be most useful for higher hazard facilities.

General Review Criteria

Code Name: HOTSPOT/Resuspension Model

1. Capabilities: The HOTSPOT Health Physics codes were created to provide Health Physics personnel with a fast, field-portable calculation tool for evaluating accidents involving radioactive materials. HOTSPOT codes are a first-order approximation of the radiation effects associated with the atmospheric release of radioactive materials. The codes are designed for short-term (less than 24 hours) release durations. HOTSPOT consists of four main programs: Plume, Explosion, Fire, and Resuspension, which calculate the downwind consequences following the release of radioactive material resulting from a continuous or puff release, explosive release, fuel fire, or an area contamination event. The resuspension program is the subject of this assessment. Also included in the HOTSPOT package are programs dealing with: (1) the release of plutonium, uranium, and tritium to expedite an initial assessment of accidents involving nuclear weapons; (2) the dose commitment from the inhalation of any one of the radionuclides listed in the data base of radionuclides; (3) calibration of a radiation survey instrument for ground-survey measurements; and (4) screen plutonium uptake in the lung.

2. Sponsor/Developing Organization:

Lawrence Livermore National Laboratory
P.O. Box 808
Livermore, CA 94551

3. Current Custodian/Phone/Fax/Internet Address:

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4. Genealogy: Development of HOTSPOT began in the mid-1980's, with the first version, 1.0, being released in 1985. The codes have been under continuous development since then. The most recent release is version 8.0 (evaluated here).
5. User's Manual Reference:

"HOTSPOT Health Physics Codes for the PC," Lawrence Livermore National Laboratory, UCRL-MA-106315, March 1994.
6. Model Description Summary: HOTSPOT models the resuspension from an area contaminated with solid particulate. An upwind virtual source term is used to model the initial airborne distribution of material; the virtual source is located at the point which results in σ_y at the center of the zone equal to 50% of the input radius for the contamination zone. The resuspension factor is a function of both time and wind speed.
7. Model Description References:

"HOTSPOT Health Physics Codes for the PC," Lawrence Livermore National Laboratory, UCRL-MA-106315, March 1994.

Anspaugh, L.R., Shinn, J.H., and Phelps, P.L., "Resuspension and Redistribution of Plutonium in Soils", Lawrence Livermore National Laboratory, UCRL-76419, 1975.
8. Hardware Requirements: The software is IBM compatible and will run on an IBM PC XT, AT, or compatible, with a minimum of 512 kbytes of RAM, and a single floppy disk drive. The programs, however, run more efficiently when they reside on a hard disk. MS DOS version 3.0 or later is required. HOTSPOT can also run on the HP 100 LX Palmtop. High-resolution (300-dpi) output to printers and also to graphics files (.PCX and .BMP files) can also be supported.
9. Quality Assurance Documentation:

Benchmarking - HOTSPOT uses the Anspaugh model, which is based on field data taken at NTS years ago (Roller Coaster series of experiments).

Source code Verification - The code has been developed over the past ten years, and is currently used world-wide (i.e. it has gained credibility). WSRC recently did an reviewed of the code and associated documentation as part of their configuration management and QA requirements. The assessments are documented in documents below:

Marc L. Nadeau, "Transmittal of Software Management and QA package for the HOTSPOT Codes" (HOTSPOT version 7.01, Fidler version 7.0), Westinghouse Savannah River Company, ECS-EST-95-0077, August 1995.

Marc L. Nadeau, "Evaluation of the HOTSPOT Computer Codes (HOTSPOT version 7.01, Fidler version 7.0), Westinghouse Savannah River Company, S-CLC-G-00080, August 1995.

Marc L. Nadeau, "Operation and Management of the HOTSPOT Computer Codes (HOTSPOT version 7.01, Fidler version 7.0), Westinghouse Savannah River Company, TP-95-003, August 1995.

Evaluation ("Validation") against experimental data - HOTSPOT uses an empirical model based on experimental data. The model is conservative with respect to more recent information (Reeks-Hall model) from the Chernobyl accident.

10. Input Summary (data and parameters): The Resuspension model requires the following inputs: initial ground contamination level, initial resuspension factor (provides default value), size of contaminated area, contamination age, wind speed, and stability class.
11. Output Summary: The Resuspension model provides the source term as intermediate output (Ci/s). The source is fed into a dispersion model.
12. Summary of Limitations: The default resuspension parameters are based on resuspension of plutonium particulate, but the model is generally applicable.
13. Summary of Strengths: HOTSPOT is straightforward, easy to use, defensible, and well documented.
14. Range of Applicability (situations, sites, sources, etc.): The code is widely applicable.
15. Comments on User Friendliness: The code is very user friendly and easy to use.
16. Comments on Error Handling Capabilities and User Feedback: The code provides feedback to the user on inappropriate input values. For example, the user is warned if an alphabetic character is provided when a number is sought, or if a number is thought to be outside the reasonable range. A glossary of terms is provided, along with an

onboard information system.

17. Source code and/or data bases can be modified?: The source code is not available (for control reasons). The data base can be modified.
18. Execution time for typical problem (CPU or real time): The code runs very quickly, typically on the order of one second (real time).
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): The code is available on a single, high-density 1.44 Mb disk (3.5").
20. Cost: The code is currently available at no charge from LLNL. It is now also available from the Radiation Shielding Information Center (RSIC) or the Office of Scientific and Technical Information (OSTI) to government or educational institutions for a fee of \$250.
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? The code is generally acceptable in applications supporting SAR, BIO, and JCO documents.
22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? The resuspension model in HOTSPOT is widely applicable to all hazard categories.
23. Future Enhancements Planned: No enhancements are currently planned. However, as the need arises or as new information is available, the developer would be enthusiastic about further developing the code.
24. Additional Information:

Specific Evaluation Criteria

Solid Spills and Resuspension/Vaporization

Code Name: HOTSPOT/Resuspension

Feature	Y/N	Description	Limitations or Assumptions
Determination of release fraction	Y/N	Although the release fraction is not specifically evaluated, it is implicitly determined through the resuspension factor and resuspension rate. The HOTSPOT codes evaluate a 50-year committed effective dose equivalent based on a one-hour residence time.	
Consideration of ambient and/or site-specific conditions	Y	The resuspension factor is a function of the user specified wind speed: $S = S (u/3)^2$ for $u > 3 \text{ m/s}$ $S = S$ for $u \leq 3 \text{ m/s}$ S defined below stability class plays a role, as σ_y is set to match the spill radius, which is then used to locate the virtual source.	
Geometry considerations e.g. spill height	Y	The spill area or area covered by contamination is a required input.	
Applies to both chemicals and radionuclides?	N	The code is specific to radionuclides, although the model could be applied to non-radioactive particulate (e.g. set to infinite half-life).	
Consideration of resuspension (provides release rate)	Y	The Anspaugh model is used to determine the resuspension factor: $S = S_i \exp (-0.15 t^{0.5}) + 10^{-9} \text{ m}^{-1}$ with t in days since initial deposition.	The model based on resuspension of plutonium particulate.

Solid Spills and Resuspension/VaporizationCode Name: **HOTSPOT/Resuspension**

Feature	Y/N	Description	Limitations or Assumptions
Any time dependency?	Y	The resuspension factor is time dependent (i.e. a resuspension factor corresponding to age of deposited material at time of resuspension is used.)	The source term is not time dependent.
Consideration of particle size distribution	Y	The code assumes a log-normal distribution, with activity mean aerodynamic diameter of 1 μm , and a standard deviation of 3.	
Temperature dependency/ thermal effects	N		
Consideration of external heat sources outside the ambient environment	N		
Extensive data base provided	N		
Some data/properties must be user specified	N		
All data/properties must be user specified	Y	The code requires only a few inputs (deposition velocity, resuspension factor, initial ground contamination level, radius of contaminated area, contamination age, wind speed, stability class).	
Special features			
Linked to transport model	Y	The resuspension model feeds into the HOTSPOT gaussian dispersion model, which evaluates impacts at downwind locations.	
Other			

Graded Approach Applicability: The model is fairly simple, but nothing more detailed is available. It should be suitable for a wide range of hazard levels.

Specific Evaluation Criteria

Resuspension of Particulate Matter from Liquids

Code Name: **HOTSPOT/Resuspension**

Feature	Y/N	Description	Limitations or Assumptions
Determination of release fraction (initial)	Y	Although the release fraction is not specifically evaluated, it is implicitly determined through the resuspension factor and resuspension rate. The HOTSPOT codes evaluate a 50-year committed effective dose equivalent based on a one-hour residence time.	
Determination of release rate (during evaporative phase)	N		The presence of an evaporating liquid does not play a role in determining the quantity of particulate that becomes airborne.
Determination of initial concentration	Y	The initial airborne concentration above the contaminated area is determined from the product of the ground contamination (C_i/m^2) and the resuspension factor (m^{-1}).	
Consideration of ambient and/or site-specific conditions	Y	The resuspension factor is a function of the user specified wind speed: $S = S (u/3)^2$ for $u > 3 \text{ m/s}$ $S = S$ for $u \leq 3 \text{ m/s}$ S defined below stability class plays a role, as σ_y is set to match the spill radius, which is then used to locate the virtual source.	
Applies to both chemicals and radionuclides?	N	The code is specific to radionuclides, although the model could be applied to non-radioactive particulate (e.g. set to infinite half-life).	

Resuspension of Particulate Matter from LiquidsCode Name: **HOTSPOT/Resuspension**

Feature	Y/N	Description	Limitations or Assumptions
Any time dependency?	Y	The resuspension factor is time dependent (i.e. a resuspension factor corresponding to age of deposited material at time of resuspension is used.)	The source term is not time dependent.
Consideration of particle size distribution	Y	The code assumes a log-normal distribution, with activity mean aerodynamic diameter of 1 μm , and a standard deviation of 3.	
Consideration of external heat sources outside the ambient environment	N		
Extensive data base provided	N		
Some data/properties must be user specified	N		
All data/properties must be user specified	Y	The code requires only a few inputs (deposition velocity, resuspension factor, initial ground contamination level, radius of contaminated area, contamination age, wind speed, stability class).	
Special features			
Linked to transport model	Y	The resuspension model feeds into the HOTSPOT gaussian dispersion model, which evaluates impacts at downwind locations.	
Other			

Graded Approach Applicability: The model is fairly simple, but nothing more detailed is available. It should be suitable for a wide range of hazard levels.

General Review Criteria

Code Name: **KBERT, Knowledge-Based System for Estimating Hazards of Radioactive Material Release Transients**

1. **Capabilities:** The current prototype version of the code calculates doses and consequences to in-facility workers from accidental releases of radioactive material. This calculation includes: specifying material at risk and worker evacuation schemes, and calculating airborne release, flows between rooms, filtration, deposition, concentrations of released materials at various locations and worker exposures.

2. **Sponsor/Developing Organization:**

Sponsor: DOE/EH

Developing Organization: Sandia National Laboratories

3. **Current Custodian/Phone/FAX/Internet Address:**

Dr. S.K. Sen
U.S. Department of Energy
Office of Environment, Safety, and Health, EH-34
19901 Germantown Road
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20874-1290

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P.O. Box 5800
Albuquerque, NM
87185

Phone: 505-844-0231
Fax: 505-844-3296
e-mail: kewashi@sandia.gov

4. Genealogy: KBERT was developed from basic models and the Jofu Mishima data base (later published as DOE-HDBK-3010-94) for use in a PC/Windows environment as a menu driven routine. It is written in Microsoft Visual C++.
5. User's Manual Reference:

"User's Guide for the KBERT 1.0 Code", SAND95-1324, Sandia National Laboratories, June 1995.
6. Model Description Summary: KBERT can be used for qualitative or quantitative risk analyses. Facilities are modeled as a collection of rooms connected by flowpaths (including HVAC ducts). To simulate the accidental release inside the facility, the Mishima database is incorporated as a relational electronic database inside KBERT. Databases on material properties and dosimetry are also included in KBERT. Mechanistic models of air transport inside the facility, given user input flow rates, are used in KBERT. Aerosol removal mechanisms are currently limited to gravitational settling. Additional deposition mechanisms could be implemented. Filters that mitigate exposures can be modeled in any flowpath. Evacuation plans for individual workers or groups of workers can be specified. Radiological dose models include cloudshine, inhalation, groundshine, and skin contamination pathways. Protective equipment effects can be modeled. Output from KBERT includes airborne and surface concentrations of released material throughout the facility and whole-body and organ-specific worker doses. To begin a simulation, materials at risk and events are specified in an Event dialogue box to represent a facility accident. An Intuitive dialogue box interface with the Mishima database provides either a one time airborne release fraction or a continuous airborne release rate and respirable fractions for materials that have been subjected to various accidents such as fires, explosions, and spills. The developers claim that an important feature of the code is that "only realistic combinations" of release data, materials at risk, and stresses due to the accident can be utilized in a simulation.
7. Model Description References:

KBERT is described in "User's Guide for the KBERT 1.0 Code", SAND95-1324, Sandia National Laboratories, June 1995.

The release fractions of aerosolized material at risk is from:
J. Mishima, "Recommended Values and Technical Bases for Airborne Release Fractions (ARFs), Airborne Release Rates (ARRs), and Respirable Fractions (RFs) for Materials from Accidents in DOE Fuel

Cycle, Ex-Reactor Facilities," Revision 2, Draft DOE report, April 21, 1993.

The Aerosol Deposition is from T.J. Heames and J.E. Brockmann, "Aerosol Deposition in Leak Paths," Sandia National Laboratories, June, 1994.

Dosimetry is from : D. Monroe, "Calculation of Doses and Consequences for KBERT", Sandia National Laboratories, June, 1994.

8. Hardware Requirements: The code requires: an IBM compatible PC with 80386 processor or higher, 80486 processor highly recommended, Microsoft Windows 3.1, VGA graphics display (SVGA recommended), a mouse or compatible pointing device, and a hard disk with at least 10 MB free space.

9. Quality Assurance Documentation:

Benchmarking - Not available at this time.

Source Code Verification - Not performed at this time.

Evaluation ("Validation") against experimental data - KBERT makes use of experimental data for source terms. However, the overall code has not been evaluated against experimental data.

10. Input Summary (Data and Parameters):

Facility: room sizes; ventilation - ducting, airflow, filtration; doorways; temperatures, pressures, etc.

Event: material form (powder, liquid, etc.), type of event (drop, thermal stress), material at risk (radioisotope(s), initial mass). Access to the Mishima database is through an Event dialog box, which includes an event name, materials category (e.g. solid-powder), event type (e.g. explosion), allows the user to choose the MAR (material at risk from a materials database), and under a section entitled "Airborne Release", guides the analyst to values of ARF/ARR/RF and a Mishima reference (i.e. where in Mishima document the numbers for this type of event/materials are located and/or documented).

Workers: distribution of workers throughout the facility including time for evacuation and movement.

Selection of nominal parameters or minimum and bounding parameters from the Mishima database.

11. Output Summary: Code output includes:
- How much material was released, its location and concentration at the end of the simulation (amount in filters, on floors, in building air, etc).
 - Location of workers.
 - Dose to each worker followed.
 - Expected consequence.
12. Summary of Limitations: Code limitations include:
- The code is still in prototype form. It has lost sponsorship and has not been released.
 - The code has not been verified.
 - Each problem is run separately. It is not obvious at this time if "batch" running of the code is available for large number of runs with differing parameters. Sensitivity studies or generation of uncertainty distributions presently require individual runs.
 - The code assumes that released material is mixed instantaneously in a room, so concentration gradients are not available. However a room can be broken into smaller volumes to get around this.
 - Aerosols settle only by gravitational settling without agglomeration. The manual indicates, however, that other deposition mechanisms can be "readily" implemented.
 - The user's manual refers to the draft (1993) version of Mishima's report, not the DOE Handbook (1994 version).
13. Summary of Strengths: This program was designed to be an integrating tool. Other than the dynamics of the air flow and settling of material, the program makes heavy use of data bases for information concerning characteristics of releases, health effects and health models. Therefore, in principle this program is not technically limited to the release of radioactive material but could be expanded to include the effects of chemical releases. The program is menu driven with easy change of input and default parameters. Modeling of a facility is relatively easy and the facility model can be stored. Once a facility has been modeled, part of it can be used for any particular accident scenario.
14. Range of Applicability: As it stands, this program can calculate the expected worker dose from an accidental release of radioactive material within the confines of a facility.
15. Comments on User Friendliness: Based on demonstration, this should be an extremely easy to use program.

16. Comments on Error Handling Capabilities and User Feedback: There is not enough user experience at this time to comment in this area.
17. Source Code and/or Data Bases Can be Modified?: Much of the data base information can be overridden by any individual analysis. There is not enough experience with the code yet to know if it can be permanently modified. Availability of the source code is not known at this time.
18. Execution Time for Typical Problem (CPU or real time): Execution time is seconds to tens of seconds (real time), depending on the size of the facility modeled. For a complete model of a large facility, it is unknown how much time would be required.
19. Aquisition Format (tape, disk, email, bulletin board, etc.): KBERT is available on two installation disks from the developers.
20. Cost: Not known.
21. First Order Evaluation Against DOE Requirements, i.e., is the code generally acceptable for supporting SAR documentation?: The code is generally acceptable for supporting SAR documentation, within the limitations discussed in item 12. Note that it does not presently include any type of sensitivity analysis other than through running the program for each individual parameter change.
22. Comments on Graded Approach Applicability: Is the code more suited for one hazard category than another? In principle, the program can calculate the hazards from a release of radioactive material over a large dynamic range.
23. Future Enhancements Planned: These would depend on future funding and include:
 - extension of the code to incorporate toxic chemicals
 - more sophisticated aerosol agglomeration, deposition and distribution models
 - inclusion of fire sprays
 - calculation of doses outside the facility
 - Monte Carlo sensitivity analysis.

There are no current plans by DOE/EH to provide more funding.

24. Additional Information:

Specific Evaluation Criteria

Solid Spills and Resuspension/Vaporization

Code Name: **KBERT**

Feature	Y/N	Description	Limitations or Assumptions
Determination of release fraction	Y	ARR/ARF/RF are provided by the Mishima database.	The user can override the Mishima values if desired.
Consideration of ambient and/or site-specific conditions	Y	KBERT models release and transport inside a room and includes the ambient conditions in the room.	The current prototype version does not perform transport outside the facility.
Geometry considerations, e.g., spill height	N	Geometry is considered only to the extent that this effect on the release is already included in the Mishima database.	
Consideration of resuspension (provides release rate)	Y	This data is from the Mishima database.	
Applies to both chemicals and radionuclides	N		The current prototype version only includes radionuclides.
Any time dependency	Y	Time dependency can be user input as far as release rate is concerned. Flow rates are also user input.	
Consideration of particle size distribution	Y	Particle size dependence is used to calculate gravitational settling.	
Temperature dependency/thermal effects	Y	Air (and any other gases) is assumed to follow the ideal gas law. Heat and mass transfer within the facility are evaluated through first order equations.	
Consideration of external heat sources outside the ambient environment	N		

Solid Spills and Resuspension/VaporizationCode Name: **KBERT**

Feature	Y/N	Description	Limitations or Assumptions
Extensive data base provided	Y	Besides Mishima, KBERT includes data on filter efficiencies, materials, dose factors, and health effects.	
Some data/properties must be user specified	Y		
All data/properties must be user specified	N		
Special features	Y	The code is an interactive program, which allows the analyst to create a complete simulation of the facility on the screen.	
Linked to transport model	N		Only transport within the facility is considered in the current prototype version.
Other			

Graded Approach Applicability:

This program is very flexible. One can start with a very simple single room with a ventilation system and expand the model to an entire facility.

General Review Criteria

Code Name: **MISM, Modified Ille-Springer Model**

This evaluation is based on information contained in the report, "The Evaporation and Dispersion of Hydrazine Propellants from Ground Spills," G. Ille and C. Springer, CEEDO-TR-780-30, August 1978.

1. Capabilities: The MISM model is an evaporation and dispersion model for hydrazine (N_2H_4), monomethylhydrazine (MMH) and unsymmetrical dimethyl hydrazine (UDMH) ground spills. The evaporation rate is computed as a function of soil temperature, solar insolation, air temperature, wind speed, and spill area. A single-source Gaussian dispersion algorithm calculates the downwind, ground level centerline concentration based on dispersion coefficients in Turner's Workbook of Atmospheric Dispersion estimates (EPA, Publication No. AP-26, 1970). The code also computes the crosswind dimension of a hazard corridor based on a user-selected concentration limit.
2. Sponsor/Developing Organization:

Department of Defense, Civil and Environmental Engineering
Development Office, Tyndall Air Force Base, Panama City, Florida, 32403.
3. Current Custodian/Phone/Fax/Internet Address: Trying to locate a current custodian and phone.
4. Genealogy: The evaporation rate model is based on the approach of D. Mackay, (D. Mackay and R.S. Matsugo, "Evaporation Rates of Liquid Hydrocarbon Spills on Land and Water," Can. J. Ch. Eng., 51, 434-39, 1973). The evaporation rate is computed as a function of concentration driving force as determined from vapor pressure, mass transfer rate as determined by wind-generated turbulence and diffusive properties of the liquid-air interface.
5. User's Manual Reference:

"The Evaporation and Dispersion of Hydrazine Propellants from Ground Spills," Gerhard Ille and Charles Springer, CEEDO-TR-78-30, August 1978.
6. Model Description Summary: The rate of evaporation of a liquid spill into the atmosphere is necessary input to modeling the release of a toxic, flammable or explosive material. This code predicts the rate of evaporation

from a pool of spilled liquid by estimating a mass transfer rate. The mass transfer rate is determined from the vapor pressure of the pure liquid, the diffusive properties of the vapor at the air-liquid interface, and the wind generated turbulence over the pool. The model assumes: the spill occurs without atomization; the spill is adiabatic and the liquid is chemically stable; the spill occurs onto a flat non-porous surface; evaporation occurs at a steady-state pool temperature; the spill is a pure liquid; and ideal gas behavior of the vapor film. The steady-state pool temperature is determined from an energy balance that equates heat inputs (convective heating from the ground and atmosphere, solar insolation and radiative heat transfer from the atmosphere) with heat losses (radiative emission from the pool and evaporative cooling). A steady-state pool temperature that satisfies the energy balance is found through iteration. This temperature establishes the equilibrium vapor pressure of the liquid. The separation of this equilibrium vapor pressure from the steady-state vapor concentration that develops at the pool interface establishes the concentration driving force for evaporation. A mass transfer coefficient equates the driving force to the mass transfer rate. The mass transfer coefficient is a complex function of the wind speed, the degree of atmospheric turbulence, and the pool diameter. The properties of the evaporating vapor enter into this expression through the inclusion of the Schmidt number. A derivation of the model and examples of input development are given in Appendix A to the user manual. A simple, point source Gaussian model without any buoyancy or plume rise effects is used to calculate dispersion and downwind concentration of the releases. The dispersion coefficients, σ_y and σ_z , are based on Turner's EPA Workbook.

7. Model Description References:

G. Ille and C. Springer, "The Evaporation and Dispersion of Hydrazine Propellants from Ground Spills", CEEDO-TR-78-30, Air Force Systems Command, Tyndall Air Force Base, Panama City, Florida 32403, August 1978.

Kunkel, B.A., "A Comparison of Evaporative Source Strength Models for Toxic Chemical Spills", AFGL-TR83-0307, ADA139431, 1983.

D. Mackay and R.S. Matsugo, "Evaporation Rates of Liquid Hydrocarbon Spills on Land and Water", Can J Ch Eng, 51, pp. 434-439, 1973.

E. Schmidt and P. Silveston, "Natural Convection in Horizontal Layers", Heat Transfer, Vol 55 (20), American Institute of Chemical Engineers, Chicago, 1959.

R.B. Bird, W.E. Stewart, and E.N. Lightfoot, Transport Phenomena, John Wiley and Sons, New York, 1966.

D.B. Turner, Workbook of Atmospheric Dispersion Estimates, Technical Information and Publications, Office of Air Programs, Publication No. AP-26, Environmental Protection Agency, Research Triangle Park, NC, 1970.

8. Hardware Requirements: The manual does not discuss hardware requirements. However, the code is written in approximately two hundred lines of Fortran and should run on most available computers including the current generation of personal computers.

9. Quality Assurance Documentation:

Benchmarking - No discussion of inter-code comparison for calculation of the evaporation rate is presented in the code manual. The code manual does state that "this model will significantly improve predictions" by perhaps an order of magnitude in contrast to models that do not consider heat gain and losses to the evaporating pool.

Source Code Verification - Not discussed in code manual.

Evaluation ("Validation") against experimental data - Manual states that code estimates compared with experimental results "... show good agreement for initial (first hour average) evaporation rates." However, these comparisons indicated the failure of the model to predict a decreasing evaporation rate with time. Absorption of and chemical reaction with carbon dioxide and water vapor by the hydrazine propellants appear to cause the discrepancy.

10. Input Summary: Input includes: air temperature, wind speed, diameter of spill, area of spill, ground roughness factor and temperature profile in the atmosphere, solar insolation rate, liquid propellant type, ground temperature at depth of 10 cm, depth of pool.
11. Output Summary: The code supplies the predicted steady-state pool temperature (°C) and evaporation rate (kilograms per hour). Steady-state values of the heat flow which comprise the energy balance are also provided in the code output.
12. Summary of Limitations: The code reviewed considers only three liquid rocket propellants. (While not thoroughly explored) the usage of large amounts of these materials within the DOE complex is not likely, although two sites (ANL and Hanford) have listed possession of hydrazine. The code could be modified and/or generalized to treat other liquids. This would require changes to the code, e.g., properties like the heat of evaporation of hydrazine are hardwired within the code, and generalization to other liquids would require the collection of pertinent material(s) data to support the analysis.

The model is limited to a chemically non-reactive, volatile, pure liquid below its boiling points. Since atomization is not considered, the code cannot treat a pressurized liquid spill where atomization during initial ejection from container can be expected to result in the generation of a significant aerosol release to the environment. The code does not attempt to predict the transient behavior including pool formation or the evaporation rate during potential initial pool cooling and/or heating. The latter may be important in a case where the liquid spill is from a process that is carried out at a temperature above or below ambient temperature.

The manual states that the predicted evaporation rate is directly proportional to spill area, which is a user input to the code. If a spill is not confined to a well determined area, e.g., such as that determined by a tank berm, then the analyst must provide a defensible estimate of this area. Sensitivity analyses reported in the manual indicate that an error in the spill area results in a directly proportional error in the evaporation rate. The manual points out that "since irregular spill areas may be difficult to measure, assessment of this parameter may result in the largest error to the evaporation rate."

13. Summary of Strengths: The model is relatively simple and could be generalized to treat a wide variety of liquids. The necessary material data should in general be available in the literature, or, where it is unavailable, it may be estimated in many cases by application of thermodynamics and the kinetic theory of gases.
14. Range of Applicability (situations, sites, sources, etc.): The code in its current form (and without modification) has very limited applicability. Suitably modified, it may treat a substantial variety of pure liquid spills, e.g., benzene and chlorinated hydrocarbons.
15. Comments on User Friendliness: This program is a batch type FORTRAN program: not interactive, no on-line prompting or help.
16. Comments on Error Handling Capabilities and User Feedback: None.
17. Source Code and/or Data Bases Can Be Modified: Modification of both the source code and the data base is possible.
18. Execution Time for Typical Problem (CPU or real time): Execution time is not stated in the code manual. Although the reviewer has not executed the code, it is believed the code will execute in seconds or a few tens of seconds (real time) on a 486-based machine.
- 19.. Acquisition Format (tape, disk, e-mail, bulletin board, etc.): The manual provides a source code listing.

20. Cost: None.
21. First Order Evaluation Against DOE Requirements, i.e., is the code generally acceptable for supporting SAR documentation?: The code is not applicable, since it is limited to chemicals which are not (or appear not to be) of interest in the DOE community.
22. Comments on Graded Approach Applicability: Is the code more suited for one hazard category than another? The code is generally not applicable to DOE facilities.
23. Future Enhancements Planned: None known at this time.

Specific Evaluation Criteria

Solid Spills and Resuspension/Vaporization

Code Name: MISM

Feature	Y/N	Description	Limitations or Assumptions
Determination of pool size (i.e., considers area source)	N	Pool (spill) Area and Diameter is user input.	Any error in spill area input causes proportional error in the evaporation rate calculation.
Consideration of pool depth	Y	Pool depth is user input.	This is user input, not calculated.
Determination of release rate	Y	Steady-state rate is calculated.	The code does not treat pressurized releases.
Consideration of ambient and/or site-specific conditions	Y	Ambient air and ground (0.1 m depth) temperatures are user inputs.	
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	N		
Time dependency of rate calculation	N	Iterative, equilibrium, steady-state model.	The code only provides steady-state evaporation rate.
Temperature dependency/thermal effects	Y	The code considers the full energy balance, including heat transfer with air and ground and solar radiative input.	
Time dependent spill to pool	N		
Consideration of heat transfer from substrate	Y	The model includes 5 distinct modes of heat transfer from ground to pool.	Values of heat transfer coefficient based on experimental studies; accuracy is not discussed in the manual.
Consideration of chemical reaction with substrate	N		The model assumes the liquid is chemically inert.

Solid Spills and Resuspension/Vaporization**Code Name: MISM**

Feature	Y/N	Description	Limitations or Assumptions
Consideration of insolation	Y	Solar insolation explicitly taken into account.	Solar insolation current user input.
Consideration of water reactivity	N		
Consideration of multi-component mixtures/solutions	N		The code assumes a pure liquid is spilled.
Extensive data base provided	N	The code is limited to three hydrazine liquids.	The code treats only three hydrazines.
Some data/properties must be user specified	Y	Spill area, pool depth/diameter, ground roughness factor, solar insolation rate, air temp, ground temp (0.1 m depth), atmos temp profile, wind speed, are user input.	
All data/properties must be user specified	N	Material properties of the hydrazines are hardwired into the code.	
Special features	N		
Linked to transport model	Y	A point-source Gaussian model is provided to estimate dispersion and to calculate downwind concentrations.	Dispersion coefficients based on Turner's EPA Workbook.
Other	N		

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Graded Approach Applicability: The code is generally not applicable to DOE facilities because of its limited data base.

General Review Criteria

Code Name: Army ORG-40/TP10 (part EVAP4.FOR of D2PC)

1. Capabilities: The subroutine calculates an evaporation rate from a pool of spilled liquid in presence of wind (ORG-40), or in still air (TP-10).
2. Sponsor/Developing Organization:

U.S. Army Chemical Research and Development Engineering
Center, Aberdeen, Maryland.
3. Current Custodian/Phone/Fax/Internet Address:

Commander, U.S. Army CRDEC,
Aberdeen Proving Ground, MD
21010-5423.
4. Genealogy: The code was developed by U.S. Army for downwind hazard prediction following release from smoke munitions and chemical agents. It was part of the D2PC Code and functioned as a Fortran subroutine (EVAP4.FOR). The physics of the spill estimation method is discussed in the D2PC User's manual, and came from references showing that the spills methods were produced by two organizations: TP-10 and ORG-40; hence the names of the methods.
5. User's Manual Reference:

Whitacre, C.G., J.H. Griner, M.W. Myirski, and D.W. Sloop (1987), "Personal Computer Program for Chemical Hazard Prediction (D2PC)", Technical Report CRDEC-TR-87021, U.S. Army Munitions Command, Aberdeen Proving Ground, MD 21010-5423.
6. Model Description Summary: The code calculates the evaporation rate of a liquid pool, given the physical state variables, wind speed, and diameter of pool. ORG-40 and TP-10 models are coded as a Fortran 77 subroutine, EVAP4.FOR, in D2PC.
7. Model Description References: See User's Manual Reference, pp 38-43.

Also see reference: Hanna, S.R. and P.J. Drivas (1987) Guidelines for Use of Vapor Cloud Dispersion Models, published by Center for Chemical Process Safety, American Institute of Chemical Engineers, New York, 177 pages.

8. Hardware Requirements: The code requires an IBM/PC. (Coded in Fortran 77, EVAP4.FOR consists of 126 lines of code, but first 31 lines need replaced by menu selections).

9. Quality Assurance Documentation:

Benchmarking - The subroutine was compared with 4 other models by Kunkel and seemed to underpredict rate by factor of 2 from consensus, but also was compared with five models against field tests by McNaughton et al, and they all appeared to overpredict. See discussion in above reference: Hanna and Drivas (1987).

Source code Verification - The source code listing is in the User's Manual Reference. The dispersion model compares to a classical Gaussian dispersion in the limit.

Evaluation ("Validation") against experimental data - A comparison by McNaughton et al with 4 field tests of nitrogen tetroxide spills showed all models overpredict source rate.

10. Input Summary (data and parameters): The user is required to input: mole weight, mole volume, boiling point, 3 vapor pressure constants, freezing point, pool diameter, wind speed, temperature, and pressure.
11. Output Summary: The output consists of a vapor generation rate in kg/s.
12. Summary of Limitations: The code is not ready for general use without some recoding--the code is intended as a Fortran 77 subroutine and needs a menu for Input/Output information. The model appears to underpredict compared with other models, but all models appeared to overpredict compared with field validation. The code needs a substrate heat balance to make an improvement.
13. Summary of Strengths: The code is very short and efficient. It has a method of computing molecular diffusivity for a range of substances in a wide mole weight range for both indoor and outdoor applications. It is comparable to other simple spill codes in its class.
14. Range of Applicability (situations, sites, sources, etc.): The code applies only to liquid pool evaporation.

15. Comments on User Friendliness: The code is not ready for general use without some recoding--the code is intended as a Fortran 77 subroutine and needs a menu for Input/Output information. It could be adapted to spread sheet use, as well.
16. Comments on Error Handling Capabilities and User Feedback: No feedback is provided.
17. Source code and/or data bases can be modified?: The source code is written in Fortran 77 and can be modified, in fact, must be modified to be of general use. The units are metric but not standard SI units.
18. Execution time for typical problem (CPU or real time): Execution time is typically a few minutes (real time) on an IBM/PC 486 machine.
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): An electronic version of the code is not available.
20. Cost: None.
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? The models should be verified before use in SAR work.
22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? The code is so simple, it should be easily and generally used as a screening tool for lower hazard facilities.
23. Future Enhancements Planned: No enhancements are currently planned.
24. Additional Information:

Specific Evaluation Criteria

Liquid Chemical Spills and Evaporation

**Code Name: Army ORG-40/TP-10
(part EVAP4.FOR of D2PC code)**

Feature	Y/N	Description	Limitations aor Assumptions
Determination of pool size (i.e. considers area source)	Y	The user must input the downwind diameter of the pool.	The code needs an Input/Output menu; recoding.
Consideration of pool depth	N		
Determination of release rate	Y	The code calculates the vapor generation rate.	There is no consideration of heat exchange.
Consideration of ambient and/or site-specific conditions	Y	Ambient temperature is considered.	
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y	Temperature and vapor pressure of the initial cloud are determined.	
Time dependency of rate calculation	N		
Temperature dependency/thermal effects	Y	Ambient temperature is considered but steady state is assumed.	
Time dependent spill to pool	N		
Consideration of heat transfer from substrate	Y	The code considers ambient air temperature only.	The code lacks heat exchange with substrate.
Consideration of chemical reaction with substrate	N		
Consideration of insolation	N		

Liquid Chemical Spills and Evaporation

Code Name: **Army ORG-40/TP-10**
(part EVAP4.FOR of D2PC code)

Feature	Y/N	Description	Limitations aor Assumptions
Consideration of water reactivity	N		
Consideration of multi-component mixtures/solutions	N		
Extensive data base provided	Y	The data base includes chemical agent and munitions data.	The data is not applicable to chemical spills.
Some data/properties must be user specified	Y	Physical state and ambient variables must be provided.	There are no subsurface considerations.
All data/properties must be user specified	N		
Special features	Y	The code can calculate molecular diffusivity, D.	The code calculates D for arbitrary substances.
Linked to transport model	Y	It links to a dispersion code.	
Other	N		

Graded Approach Applicability:

The model is fairly simple, and therefore better suited for lower hazard facilities. Some development work is required before ORG-40/TP-10 can be used as a stand-alone code.

General Review Criteria

Code Name: PSpill

1. Capabilities: The PSpill code determined the mass airborne from a spill of solid powder.
2. Sponsor/Developing Organization:

Pacific Northwest Laboratory
P.O. Box 999
Richland, WA 99352
3. Current Custodian/Phone/Fax/Internet Address:

Marcel Ballinger,
Pacific Northwest Laboratory,
P.O. Box 999
Richland, WA 99352

Phone: (509) 373-6715
4. Genealogy: The original code was developed as part of an NRC sponsored effort to provide methods for determining the consequences of postulated accidents for safety analyses and Environmental Impact Statements. This took place in the mid-1980s. The electronic version of the original code is no longer available, but a print-out is. The listing is short, so the source code could easily be recreated.
5. User's Manual Reference:

M.Y. Ballinger et al., 1988, "Methods for Describing Airborne Fractions of Free Fall Spills of Powders and Liquids", Pacific Northwest Laboratory for the U.S. Nuclear Regulatory Commission, NUREG/CR-4997, January 1988.
6. Model Description Summary: The code models the shearing effect of the air on the powder as it falls. The shearing effect is enhanced by the lengthening of the spill column caused by the acceleration of gravity. The mass of material that becomes airborne from a spill of powder is assumed proportional to the drag force on the powder as it falls. The growth rate of the powder front is constant and can be characterized by

an angle of dispersion. The diameter of the powder front at the start of the spill is equal to the diameter of the container from which it was spilled. The model assumes that any airborne material created as a result of impact with a surface is negligible.

7. Model Description References:

"Methods for Describing Airborne Fractions of Free Fall Spills of Powders and Liquids," Pacific Northwest Laboratory NUREG/CR-4997, January 1988.

8. Hardware Requirements: The original code was written in fortran, to run on a VAX minicomputer. It could easily be rewritten to run on most any platform.

9. Quality Assurance Documentation:

Benchmarking - The model is based on experimental data of Sutter et al., ("Aerosols Generated by Free Fall Spills of Powders and Solutions in Static Air", NUREG/CR-2139, 1981) and Ballinger and Hodgson ("Aerosols Generated by Spills of Viscous Solutions and Slurries", NUREG/CR-4658, 1986).

Source code Verification - Not performed.

Evaluation ("Validation") against experimental data - The code uses an empirical model, based on experimental data.

10. Input Summary (data and parameters): The user is required to input: mass of material spilled, spill height, bulk density of powder, density of air, viscosity of air.

11. Output Summary: The output consists of an estimate of the total mass of material made airborne by the spill.

12. Summary of Limitations: The model ignores airborne particulate generated as a result of impact. The model applies only to powders for bulk spills, not continuous pours.

13. Summary of Strengths: PSpill is simple.

14. Range of Applicability (situations, sites, sources, etc.): The code is applicable to powder spill situations.

15. Comments on User Friendliness: The user must be familiar with fortran.

16. Comments on Error Handling Capabilities and User Feedback: No feedback is provided.
17. Source code and/or data bases can be modified?: The source code is not available, but it can easily be recreated, and therefore modified.
18. Execution time for typical problem (CPU or real time): This is not known, but is presumably very fast.
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): An electronic version of the code is not available.
20. Cost: None.
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? The methodology would be acceptable for SARs.
22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? The methodology is widely applicable to all hazard categories.
23. Future Enhancements Planned: No enhancements are currently planned.
24. Additional Information:

Specific Evaluation Criteria

Solid Spills and Resuspension/Vaporization

Code Name: PSpill

B-115

Feature	Y/N	Description	Limitations or Assumptions
Determination of release fraction	Y	The maximum airborne fraction is determined based on the shearing effect of the air as the powder falls, according to the following: $ARF = 0.2128 \cdot M_o^{0.125} \cdot H^{2.37} / \rho^{1.02}$ $M_o = \text{mass of powder spilled (kg)}$ $H = \text{spill height (m)}$ $\rho = \text{bulk powder density (kg/m}^3\text{)}$ for an air density of 1.18 kg/m ³ and an air viscosity of 1.85x10 ⁻⁵ Pa · s.	The model does not consider the effect of impact; it applies only to bulk powder spills, not continuous pours.
Consideration of ambient and/or site-specific conditions	N		
Geometry considerations e.g. spill height	Y	Spill height plays a role in determining the release fraction. See above.	
Consideration of resuspension (provides release rate)	N		
Applies to both chemicals and radionuclides?	Y	Only the density of the material is required to be known, so whether or not the material is radioactive is irrelevant.	
Time dependency of rate calculation	N		
Consideration of particle size distribution	N	A method is provided for calculating the particle size distribution in the supporting documentation.	

Solid Spills and Resuspension/VaporizationCode Name: **PSpill**

Feature	Y/N	Description	Limitations or Assumptions
Temperature dependency/ thermal effects	N		
Extensive data base provided	N		
Some data/properties must be user specified	N		
All data/properties must be user specified	Y	The code requires only a few inputs (mass of material spilled, spill height, bulk density of powder, density of air, viscosity of air).	
Special features	N		
Linked to transport model	N		
Other			

Graded Approach Applicability: The model is fairly simple, but nothing more detailed is available. It should be suitable for a wide range of hazard levels.

General Review Criteria

Code Name: TScreen

1. Capabilities: Tscreen is a simple, conservative screening tool for obtaining maximum downwind vapor concentrations at select receptor locations for releases resulting from a) particulate releases, b) gaseous releases, c) liquid releases, and d) superfund releases. A particular release scenario is selected via input parameters, and Tscreen automatically selects and executes the appropriate dispersion model to simulate that scenario. The model to be used and the worst case meteorological conditions are automatically selected.
2. Sponsor/Developing Organization:

Sponsor: United States EPA
Developer: Pacific Environmental Services, Inc
5001 So. Miami Blvd, Suite 300
P.O. Box 12077
Research Triangle Park, NC 27709
(919) 941-0333
3. Current Custodian/Phone/Fax/Internet Address:

Jawad Touma, Project Officer
US EPA, OAQPS, TSD (MD - 14)
Source Receptor Analysis Branch
Research Triangle Park, NC 27711

Phone: (919) 541-5381
4. Genealogy: This is the first version of code.
5. User's Manual Reference:

EPA-454/B-94-023, July 1994
(Revised EPA-450/4-90-013).
6. Model Description Summary: Tscreen is a computerized ensemble of simple screening techniques for estimating ambient concentrations due to various toxic/hazardous pollutant releases. The screening techniques are simplified calculational procedures designed with sufficient conservatism to allow a determination of whether a source

a) is clearly not an air quality threat or b) poses a potential threat which should be examined with more sophisticated estimation techniques or measurements. Further details on the models may be found in the following EPA guide:

TScreen provides a computerized implementation of the Work Book of Screening Techniques for Assessing Impacts of Toxic Air Pollutants.

7. Model Description References:

EPA-454/R-92-024, December, 1992, Work Book of Screening Techniques for Assessing Impacts of Toxic Air Pollutants.

8. Hardware Requirements: Requirements include: an IBM PC compatible computer with an 80286 processor or greater, 570 Kbytes of RAM, 2 Mbytes of free hard disk space. A math coprocessor chip is optional but recommended.

9. Quality Assurance Documentation:

Benchmarking - No benchmarking has been performed.

Source code Verification - Unknown.

Evaluation ("Validation") against experimental data - No validation has been performed.

10. Input Summary (data and parameters): Tscreen has a front-end control program that drives a series of on-screen menus requesting input parameters for defining a release scenario. Context-sensitive help is available throughout the input process. Once the input is completed, Tscreen automatically saves the input to a file that can be retrieved and viewed or edited at a later time. Menu selections can be made by clicking a mouse, moving the highlight bar with the arrow keys and pressing <Enter>, or pressing the letter of a menu item. Once the user has specified the initial form of the release (particulate, gaseous, liquid, and superfund), a list of possible types of release scenarios is provided for selection. Once the scenario has been selected, unique data entry screens will appear for that scenario.

11. Output Summary: The source-term output from Tscreen is very terse, because the program is intended primarily for obtaining worst-case downwind vapor concentrations. Output parameters unique to the release scenario generally consist of source emission rate and duration, and the vapor fraction of the release and associated exit temperature.

12. Summary of Limitations: Many of the models are simplistic and extremely conservative both in terms of source-term and subsequent downwind vapor concentration. Models which exhibit the greatest degree of conservatism are superheated flashing releases and unconfined liquid pool evaporation. Furthermore, the program only computes steady-state release rates for ideal fluids. Hence, in the case of a gas reservoir under extreme pressures, for example, the predicted results may be under conservative because ideal conditions no longer apply.
13. Summary of Strengths: The code offers a high degree of user-friendliness, short execution times, and a chemical data base which can be modified and supplemented by the user.
14. Range of Applicability (situations, sites, sources, etc.): Use of Tscreen should be limited to low hazard facilities where estimation of the potential hazard zones due to the release of a toxic chemical (particulate, liquid, or gas) can be adequately represented by a conservative bounding calculation. The code is only intended to model outside releases where the impacts extend the far field and surface roughness features may be neglected.
15. Comments on User Friendliness: Tscreen is generally easy to use and offers context-sensitive online help. Invalid numerical entries are immediately flagged upon entry so that errors may be more easily located and corrected.
16. Comments on Error Handling Capabilities and User Feedback: The program prompts the user when an invalid value for a parameter has been entered and forces the user to enter a proper value or exit the menu. Sometimes the program aborts the input session after preliminary calculations with a message there exists an invalid combination of input parameters. Probably the parameter space has been violated, but no guidance is provided to resolve the problem.
17. Source code and/or data bases can be modified?: Modification is possible. The source code is a combination of (FoxPro®) menu interfaces, Microsoft C®, FORTRAN®, and BASIC®.
18. Execution time for typical problem (CPU or real time): Execution time is several seconds to 1 minute (real time) on a 80386 processor.
19. Acquisition format (tape, disk, e-mail, bulletin board, etc.): The code can be obtained from the EPA automated bulletin board, data line phone number 919-541-5742. Once logged onto the bulletin board system, proceed to the following succession of menus (in order):

<T>	Gateway to TTN Technical Areas
<C>	SCRAM - Regulatory Air Models/Information
<M>	Models, User's Guides and Model change Bulletins
<A>	Air Quality Models
<S>	Screening Procedures

The code (executable and source) will be distributed among several ZIP files, as will the documentation in WP5.1 for DOS format.

20. Cost: None.
21. First Order evaluation against DOE requirements, i.e. is the code generally acceptable for supporting SAR documentation? Tscreen can perform far-field dispersion calculations, where the combination of meteorological conditions (wind speed and stability class only) are automatically chosen to achieve maximum concentration at a given receptor location. Environmental impacts are not assessed, but rather the introduction of a pollutant into the atmosphere is estimated for ongoing superfund activities. The code links the source-term estimate with the Britter & McQuaid model for near-field dispersion, choosing the meteorological conditions in the same manner as described above for public and collocated workers.
22. Comments on Graded Approach applicability. Is the code more suited for one hazard category than another? The code is only applicable to low hazard facilities where bounding conservative calculations may be used in determining potential zones of impact.
23. Future Enhancements Planned: Unknown.
24. Additional Information:

Specific Evaluation Criteria

Liquid Chemical Spills and Evaporation

Code Name: TScreen

Feature	Y/N	Description	Limitations or Assumptions
Determination of pool size (i.e. considers area source)	Y	Pool size is determined by dividing the total volume of liquid released by the pool depth (instantaneous release only).	The pool are calculation assumes a pool depth of 1 cm for instantaneous low volatility releases. Low volatility continuous releases assume the evaporation rate is equal to the liquid emission rate (highly conservative), and the pool area is estimated by solving the Clewell evaporation correlation for the pool area term.
Consideration of pool depth	Y-	Pool depth is assumed to be 1 cm for instantaneous low volatility, unconfined liquid releases. In no other instance is pool depth explicitly used in boiling/evaporation calculations.	Pool boiling and evaporation is largely driven by heat transfer from the ground substrate. When the depth of the pool is increased, the amount of heat transfer to the free surface of the pool is reduced significantly and hence pool evaporation is mitigated. None of these considerations are incorporated into the model.
Determination of release rate	Y	The liquid release rate from containment is based on conventional mass balance orifice calculations.	
Consideration of ambient and/or site-specific conditions	Y	The ambient temperature and wind speed are used to estimate the pool evaporation rate.	Many other ambient parameters influence the rate at which a liquid pool evaporates: solar radiation heat flux, temperature of the ground, thermal properties of the pool bed, permeability and water content of the ground surface, etc.

Liquid Chemical Spills and Evaporation

Code Name: TScreen

Feature	Y/N	Description	Limitations or Assumptions
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	N		The initial temperature of the vapors emitted from the liquid pool are assumed to be equal to the minimum of the storage and ambient temperature (not true in many cases: e.g. cryogenic releases), and initial dilution of the vapor is neglected.
Time dependency of rate calculation	N		All calculations are based on instantaneous or steady-state release rates.
Temperature dependency/thermal effects	N		
Time dependent spill to pool	N		
Consideration of heat transfer from substrate	N		
Consideration of chemical reaction with substrate	N		
Consideration of insolation	N		
Consideration of water reactivity	N		
Consideration of multi-component mixtures/solutions	N		
Extensive data base provided	N	The chemical data base has limited data on the following substances: anhydrous ammonia, benzene, chlorine, ethylene oxide, hydrogen chloride, hydrogen fluoride, and sulfur dioxide.	

Liquid Chemical Spills and Evaporation**Code Name: TScreen**

Feature	Y/N	Description	Limitations or Assumptions
Some data/properties must be user specified	N		
All data/properties must be user specified	Y	Data input is entered interactively through a screen menu system.	
Special features	Y	Evaporation from surface impoundments and superfund sites (air strippers only).	Model is oversimplified.
Test problem evaluation	Y	See anhydrous ammonia, chlorine, and acetone spill test case results in Section 6.2 and Appendix C of this report.	
Linked to transport model	Y	The liquid emission models are linked to the Britter & McQuaid model, gaussian 'complex' and simple terrain models, or a gaussian puff model, depending on the release duration, location of receptors, and the presence of buildings.	
Other	N		

Graded Approach Applicability: The code should be used for analyses of lower hazard facilities only.

Specific Evaluation Criteria

Pressurized Liquid/Gas Releases

Code Name: TScreen

Feature	Y/N	Description	Limitations or Assumptions
Determination of release rate	Y	Release rates for steady-state single and two-phase vapor releases are computed for both critical and subcritical conditions. Specific release classes include direct leaks from a vessel, a stack, a short length of pipe attached to a reservoir, and a long length of pipe attached to a reservoir with options for several elbows.	Temperature and pressure changes in a tank or reservoir are neglected. Therefore, the orifice size must be sufficiently small so that a relatively small percentage of the vessel contents are lost over the time span of interest. Furthermore, when the release source is a pipe, the reservoir conditions should be taken from an upstream location when the orifice area exceeds 20% of the pipe cross-sectional area.
Determination of initial characteristics of the vapor cloud (temperature, density, size, etc.)	Y-	Initial temperature and density of the vapor release are estimated. All episodic releases are treated as point sources with the exception of a multiple-source fugitive release.	All aerosol component as well as saturated residual (unflashed) liquid is assumed to evaporate immediately at the source location. This assumption is extremely over-conservative except in cases of cryogenic releases (e.g. anhydrous ammonia).
Consideration of ambient and/or site-specific conditions	Y-	Ambient temperature is the only input variable.	A more sophisticated model would consider the effects of relative humidity and wind shear on the initial characterization of the release.

Pressurized Liquid/Gas ReleasesCode Name: **TScreen**

Feature	Y/N	Description	Limitations or Assumptions
Geometry considerations e.g. orifice size	Y-	One model for two-phase flow from a pipe attached to a reservoir implicitly assumed. Furthermore, the model for pipe leak emissions estimates the frictional losses inside the pipe as a function of pipe length and the number of elbows.	
Time dependency of rate calculation	N	All releases are assumed to be steady-state or instantaneous.	
Temperature dependency/thermal effects	Y-	A majority of the release calculations make use of adiabatic expressions for mass release rate, and therefore implicitly assume some temperature dependence.	The temperature dependence in the release calculations is implicitly contained in the calculations and cannot be explicitly extracted for use in subsequent dispersion analysis.
Consideration of critical flow	Y	The standard model for choked flow from a small orifice is used.	
Consideration of two-phase flow	Y	Standard expressions from sources such as Perry's and Fauske & Epstein are used for the two-phase calculations.	
Consideration of water reactivity	N		
Extensive data base provided	N	The chemical data base has limited data on the following substances: anhydrous ammonia, benzene, chlorine, ethylene oxide, hydrogen chloride, hydrogen fluoride, and sulfur dioxide.	
Some data/properties must be user specified	N		

Pressurized Liquid/Gas Releases**Code Name: TScreen**

Feature	Y/N	Description	Limitations or Assumptions
All data/properties must be user specified	N		
Test problem evaluation	Y	See anhydrous ammonia, carbon monoxide, and chlorine spill test case results in Section 6.2 and Appendix C of this report.	
Special features	N		
Linked to transport model	Y	The gas/liquid pressurized release models are linked to the Britter & McQuaid model, gaussian 'complex' and simple terrain models, or a gaussian puff model, depending on the release duration, location of receptors, and the presence of buildings.	
Other	N		The vapor phase of the released material is assumed to be an ideal gas at the reservoir conditions and following release to the atmosphere. The physical behavior of many saturated liquids, however, is not well approximated by the ideal gas model.

Graded Approach Applicability: The code should be used for analyses of lower hazard facilities only.

Appendix C: Test Problem Results

ADAM

Test Problem Evaluations

Introduction

The ADAM computer code was used to evaluate test problems 1(a) and 3, as described in Section 6.2 of this report (taken from Hanna and Strimaitis (1989)). The other problems were not evaluated because ADAM does not model pressurized liquid releases from long pipes, and does not have carbon monoxide or acetone in its database, respectively.

The following section gives an overall discussion of using the ADAM code to solve the sample problems, along with separate discussions pertaining to the specifics of the individual problems.

General Information:

In order to evaluate the problem using ADAM, parameters in addition to those given in Hanna and Strimaitis (1989) had to be specified. A list of those parameters required in all of the sample problems and their assumed values are given below:

time: 1200 hours

date: July 4, 1995

geographic location: Aiken, SC (Lat: 33, Lon: 82)

Three sets of wind speed and stability class are given in the sample problems (2 m/s, F-stability; 2 m/s, D-stability; and 5 m/s, D-stability), along with two ground roughness length scales (3 cm and 0.3 cm). These parameters will only impact the source term generation rate in cases where evaporation occurs from a liquid pool however, ADAM always requires them as part of its input. Default values of 2 m/s, D-stability, and 3 cm were used in the sample problems without pool evaporation.

The ADAM output data file contains an input echo, and the following output data:

- the source term release rate (steady-state),
- the temperature of the source term,
- the mass of air entrained by the release,
- the overall density of the source term, and

- the source term aerosol fraction

Data relating to the dispersion of the source term is also given in the output file.

Problem 1(a): Pressurized Liquid Release of Anhydrous Ammonia (nozzle failure)

This problem considers a pressurized liquid release of anhydrous ammonia (at saturated conditions; 25 C and 8.9 bar) via a 1.5 inch tank orifice.

ADAM required the diameter of the tank from which the release occurs as an input, therefore it was assumed that the tank was 5.25 meters in diameter. Also, it had to be specified at what location the release occurred and whether the release occurred from a short pipe/valve or directly from the tank; at the bottom and short pipe/valve were assumed, respectively.

ADAM predicts this release to be two-phase; in Hanna and Strimaitis this release is modeled as a liquid release.

Problem 1(a)

OUTIN.dat, created by OUTIN.for (called from INCK).

This file contains data read from the user by
the input panels.

=====

TEST DATA	TITLE
1	MENU1
AMA	CH (from ^)

2	IREL 1=inst, 2=cont
1	ISOUR
1	ITYPE2

5.2500	DTANK
0	IDIKE
9.663	PSTOR
298.0000	TSTOR
66.70	VCH
20.0000	DDIKE

2	MENU42
1	IHOLE
0	IPIPE
0	IHOLPIP
.0380	DHOLE
.0000	HHOLE
.0500	DPIPE
34.5000	FPIPE

298.0000	TG
.03000	Z0
.03000	Z0MT
80.0000	RH
298.0000	TA1
2.0000	UW
.0000	WD
10.0000	ZW
0	ISIGTH
15.0000	SIGTH
10.0000	WAVGTIM
1	IATM
.2500	CLDFRC
.5000	sp
.2600	TOW
N	IWET
N	ISNOW
101325.0	PATM

33.0000	LAT
82.0000	LON
95	ACYEAR
7	ACMONTH
4	ACDAY
12	
0	
0	
25	
14.3656	TIME
12.0001	TIMESP

30.0	CLIMIT
15.0000	CAVGTIM
.0	DLIMIT
0	IWINDIR
0	IDOSE

100.0000	MCH
290.0000	TCH
.2000	FLI
200.0000	MAIR
.00	WHALF
.00	HI
.00	QI
.00	X0
.00	V0
2.0000	U10
.2000	USTAR
.2300	R
.6500	ALPHA
.1000	GCOEFF
298.0000	TAIR

SOURCE CALCULATION RESULTS

CHEMICAL: AMMONIA

----- DATA CALCULATED (OR READ IN) BY SOURCE MODELS -----

Mass Chemical Released or Release Rate from Source.....: 23.73 kg or kg/s
 Chemical Temperature Upon Release.....: 239.84 K
 Mass of Air Entrained Initially During Release.....: 2395.52 kg
 Plume or Puff Half-Width at End of Source Calculations...: 58.53 m
 Overall Density of Mixture.....: 1.193 kg/m³
 Liquid Aerosol Mass Fraction in the Initial Cloud.....: .8050
 Fraction of the Liquid After Flash Which is Entrained....: 1.0000

----- DATA CALCULATED (OR READ IN) BY ATMOSPHERIC MODELS -----

Horizontal Stability Parameter.....: .5000
 Vertical Stability Parameter.....: .5000
 Wind Friction Velocity (U*).....: .1734 m/s

DISPERSION CALCULATION RESULTS

85 = # of Points

Contour for Concentration = 30.000000 ppm

Time Since Release	Distance From Source	Velocity of Plume or Puff	Peak Concentration	Peak Dose	Contour Width
(s)	(m)	(m/s)	(ppm)	(ppm-s)	(m)
55.17	80.01	1.6781	16467.	.0000	58.53
55.47	80.50	1.6775	16390.	.0000	61.08
55.96	81.32	1.6766	16263.	.0000	61.76
56.69	82.55	1.6753	16078.	.0000	62.77
57.71	84.27	1.6735	15828.	.0000	64.18
59.10	86.59	1.6712	15505.	.0000	66.08
60.93	89.64	1.6683	15107.	.0000	68.55
63.31	93.60	1.6647	14631.	.0000	71.70
66.35	98.65	1.6604	14074.	.0000	75.70
70.21	105.0	1.6555	13430.	.0000	80.67
75.07	113.1	1.6500	12463.	.0000	112.0
81.17	123.1	1.6438	10639.	.0000	127.0
88.78	135.5	1.6371	8207.6	.0000	144.6
98.26	151.0	1.6301	5903.7	.0000	164.9
110.0	170.1	1.6228	4076.3	.0000	185.9
124.6	193.6	1.6156	2751.1	.0000	209.5
142.6	222.6	1.6086	1831.6	.0000	241.8
164.8	258.2	1.6021	1209.4	.0000	274.1
192.2	301.9	1.5966	794.18	.0000	310.4
226.0	355.5	1.5869	526.68	.0000	348.5
267.3	421.2	1.5871	346.00	.0000	386.5
317.7	501.6	1.5977	224.89	.0000	422.8
379.0	600.1	1.6077	147.64	.0000	455.2
440.6	700.1	1.6228	103.42	.0000	475.1
444.9	708.7	2.0000	102.03	.0000	474.7
449.2	717.4	2.0000	100.14	.0000	473.6
453.5	726.0	2.0000	98.298	.0000	472.4
457.9	734.6	2.0000	96.510	.0000	471.2
462.2	743.3	2.0000	94.772	.0000	470.0
466.5	751.9	2.0000	93.082	.0000	468.7
470.8	760.6	2.0000	91.438	.0000	467.3
475.1	769.2	2.0000	89.837	.0000	465.9
479.4	777.8	2.0000	88.279	.0000	464.5
483.8	786.5	2.0000	86.761	.0000	463.0
488.1	795.1	2.0000	85.281	.0000	461.4

492.4	803.8	2.0000	83.840	.0000	459.8
496.7	812.4	2.0000	82.433	.0000	458.2
501.0	821.0	2.0000	81.062	.0000	456.5
505.4	829.7	2.0000	81.451	.0000	458.3
509.7	838.3	2.0000	79.377	.0000	455.0
514.0	846.9	2.0000	77.373	.0000	451.7
518.3	855.6	2.0000	75.437	.0000	448.3
522.6	864.2	2.0000	73.565	.0000	444.7
527.0	872.9	2.0000	71.754	.0000	441.1
531.3	881.5	2.0000	70.004	.0000	437.4
535.6	890.1	2.0000	68.309	.0000	433.6
539.9	898.8	2.0000	66.668	.0000	429.7
544.2	907.4	2.0000	65.080	.0000	425.8
548.6	916.1	2.0000	63.541	.0000	421.7
552.9	924.7	2.0000	62.051	.0000	417.4
557.2	933.3	2.0000	60.606	.0000	413.1
561.5	942.0	2.0000	59.205	.0000	408.7
565.8	950.6	2.0000	57.847	.0000	404.2
570.1	959.2	2.0000	56.530	.0000	398.8
574.5	967.9	2.0000	55.252	.0000	392.7
578.8	976.5	2.0000	54.011	.0000	386.5
583.1	985.2	2.0000	52.807	.0000	380.2
587.4	993.8	2.0000	51.638	.0000	373.8
591.7	1002.	2.0000	50.503	.0000	367.2
596.1	1011.	2.0000	49.400	.0000	360.5
600.4	1020.	2.0000	48.328	.0000	353.7
604.7	1028.	2.0000	47.287	.0000	346.7
609.0	1037.	2.0000	46.275	.0000	339.5
613.3	1046.	2.0000	45.290	.0000	332.2
617.7	1054.	2.0000	44.333	.0000	324.6
622.0	1063.	2.0000	43.403	.0000	316.9
626.3	1072.	2.0000	42.497	.0000	309.0
630.6	1080.	2.0000	41.617	.0000	300.8
634.9	1089.	2.0000	40.759	.0000	292.3
639.3	1097.	2.0000	39.925	.0000	283.6
643.6	1106.	2.0000	39.112	.0000	274.6
647.9	1115.	2.0000	38.322	.0000	265.2
652.2	1123.	2.0000	37.551	.0000	255.5
656.5	1132.	2.0000	36.801	.0000	245.3
660.9	1141.	2.0000	36.070	.0000	233.8
665.2	1149.	2.0000	35.358	.0000	221.1
669.5	1158.	2.0000	34.664	.0000	207.7
673.8	1167.	2.0000	33.988	.0000	193.4
678.1	1175.	2.0000	33.329	.0000	178.0
682.4	1184.	2.0000	32.686	.0000	161.2
686.8	1192.	2.0000	32.059	.0000	142.4

691.1	1201.	2.0000	31.447	.0000	120.8
695.4	1210.	2.0000	30.852	.0000	93.22
699.7	1218.	2.0000	30.270	.0000	52.84
701.8	1222.	2.0000	29.702	.0000	.0000

Problem 3: Pressurized Liquid Release of Chlorine

This problem considers a pressurized liquid release of chlorine (at saturated conditions; 30 C and 1 atm) via a 0.3 inch valve.

ADAM required the diameter of the tank from which the release occurs as an input, therefore it was assumed that the tank was 5.25 meters in diameter. Also, it had to be specified at what location the release occurred and whether the release occurred from a short pipe/valve or directly from the tank; at the bottom and short pipe/valve were assumed, respectively.

ADAM predicts this release to be two-phase; in Hanna and Strimaitis this release is modeled as a liquid release.

ADAM predicts this release to be two-phase; in Hanna and Strimaitis this release is modeled as a liquid release.

Problem 3

OUTIN.dat, created by OUTIN.for (called from INCK).

This file contains data read from the user by
the input panels.

=====

PROB4	TITLE
2	MENU1
CLX	CH (from ^)

2	IREL 1=inst, 2=cont
1	ISOUR
1	ITYPE2

.7500	DTANK
0	IDIKE
8.726	PSTOR
303.0000	TSTOR
.65	VCH
20.0000	DDIKE

1	MENU42
1	IHOLE
0	IPIPE
0	IHOLPIP
.0076	DHOLE
.0000	HHOLE
.0500	DPIPE
34.5000	FPIPE

298.0000	TG
.01000	Z0
.01000	Z0MT

80.0000	RH
298.0000	TA1
2.0000	UW
.0000	WD
10.0000	ZW
0	ISIGTH
15.0000	SIGTH
10.0000	WAVGTIM
0	IATM
1.0000	CLDFRC
.5000	sp
.5000	TOW
Y	IWET
N	ISNOW
101325.0	PATM

33.0000	LAT
82.0000	LON
95	ACYEAR
7	ACMONTH
4	ACDAY
12	
0	
0	
79	
12.7372	TIME
12.0002	TIMESP

30.0	CLIMIT
15.0000	CAVGTIM
.0	DLIMIT
0	IWINDIR
0	IDOSE

100.0000	MCH
290.0000	TCH
.2000	FLI
200.0000	MAIR
.00	W HALF
.00	HI
.00	QI
.00	X0
.00	V0
5.0000	U10
.5000	USTAR
.2300	R
1.0000	ALPHA
.1000	GCOEFF
298.0000	TAIR

SOURCE CALCULATION RESULTS

CHEMICAL: CHLORINE

----- DATA CALCULATED (OR READ IN) BY SOURCE MODELS -----

Mass Chemical Released or Release Rate from Source.....: 1.35 kg or kg/s
 Chemical Temperature Upon Release.....: 239.18 K
 Mass of Air Entrained Initially During Release.....: 333.13 kg
 Plume or Puff Half-Width at End of Source Calculations...: 36.67 m
 Overall Density of Mixture.....: 1.180 kg/m³
 Liquid Aerosol Mass Fraction in the Initial Cloud.....: .7910
 Fraction of the Liquid After Flash Which is Entrained....: 1.0000

----- DATA CALCULATED (OR READ IN) BY ATMOSPHERIC MODELS -----

Horizontal Stability Parameter.....: .5000
 Vertical Stability Parameter.....: .5000
 Wind Friction Velocity (U*).....: .1407 m/s

DISPERSION CALCULATION RESULTS

69 = # of Points

Contour for Concentration = 30.000000 ppm

Time Since Release	Distance From Source	Velocity of Plume or Puff	Peak Concentration	Peak Dose	Contour Width
(s)	(m)	(m/s)	(ppm)	(ppm-s)	(m)
33.33	42.01	1.3511	1642.9	.0000	36.67
33.70	42.50	1.3512	1635.8	.0000	37.64
34.31	43.32	1.3513	1624.0	.0000	37.89
35.21	44.55	1.3515	1606.7	.0000	38.26
36.48	46.27	1.3519	1582.9	.0000	38.78
38.20	48.59	1.3523	1551.7	.0000	39.47
40.43	53.03	1.9910	1555.1	.0000	39.47
42.67	57.48	1.9910	1525.5	.0000	39.50
44.90	61.93	1.9910	1410.7	.0000	47.80
47.13	66.37	1.9910	1246.7	.0000	49.82
49.37	70.82	1.9910	1084.7	.0000	51.75
51.60	75.27	1.9910	943.82	.0000	53.57
53.83	79.71	1.9910	826.08	.0000	55.24
56.06	84.16	1.9910	728.59	.0000	56.77
58.30	88.60	1.9910	647.59	.0000	58.09
60.53	93.05	1.9910	579.68	.0000	59.03
62.76	97.50	1.9910	522.13	.0000	59.87
65.00	101.9	1.9910	472.80	.0000	60.65
67.23	106.4	1.9910	430.07	.0000	61.37
69.46	110.8	1.9910	392.70	.0000	62.03
71.70	115.3	1.9910	359.78	.0000	62.64
73.93	119.7	1.9910	330.57	.0000	63.20
76.16	124.2	1.9910	304.51	.0000	63.71
78.40	128.6	1.9910	281.18	.0000	64.17
80.63	133.1	1.9910	260.20	.0000	64.58
82.86	137.5	1.9910	241.27	.0000	64.94
85.10	142.0	1.9910	224.16	.0000	65.26
87.33	146.4	1.9910	208.64	.0000	65.53
89.56	150.9	1.9910	194.54	.0000	65.75
91.80	155.3	1.9910	181.70	.0000	65.92
94.03	159.7	1.9910	169.99	.0000	66.04
96.26	164.2	1.9910	159.28	.0000	66.12
98.49	168.6	1.9910	149.47	.0000	66.15
100.7	173.1	1.9910	140.48	.0000	66.14
103.0	177.5	1.9910	132.21	.0000	66.08

105.2	182.0	1.9910	124.60	.0000	65.97
107.4	186.4	1.9910	117.58	.0000	65.82
109.7	190.9	1.9910	111.10	.0000	65.62
111.9	195.3	1.9910	105.11	.0000	65.37
114.1	199.8	1.9910	99.554	.0000	65.07
116.4	204.2	1.9910	94.402	.0000	64.72
118.6	208.7	1.9910	89.616	.0000	64.33
120.8	213.1	1.9910	85.163	.0000	63.88
123.1	217.5	1.9910	81.014	.0000	63.37
125.3	222.0	1.9910	77.144	.0000	62.81
127.5	226.4	1.9910	73.529	.0000	62.19
129.8	230.9	1.9910	70.149	.0000	61.50
132.0	235.3	1.9910	66.984	.0000	60.76
134.2	239.8	1.9910	64.016	.0000	59.94
136.5	244.2	1.9910	61.232	.0000	59.06
138.7	248.7	1.9910	58.615	.0000	58.10
140.9	253.1	1.9910	56.155	.0000	57.05
143.2	257.6	1.9910	53.838	.0000	55.91
145.4	262.0	1.9910	51.655	.0000	54.68
147.6	266.5	1.9910	49.595	.0000	53.35
149.9	270.9	1.9910	47.650	.0000	51.91
152.1	275.3	1.9910	45.812	.0000	50.35
154.3	279.8	1.9910	44.073	.0000	48.66
156.6	284.2	1.9910	42.426	.0000	46.82
158.8	288.7	1.9910	40.866	.0000	44.81
161.0	293.1	1.9910	39.386	.0000	42.61
163.3	297.6	1.9910	37.982	.0000	40.18
165.5	302.0	1.9910	36.648	.0000	37.48
167.7	306.5	1.9910	35.379	.0000	34.44
170.0	310.9	1.9910	34.173	.0000	30.96
172.2	315.4	1.9910	33.024	.0000	26.87
174.4	319.8	1.9910	31.930	.0000	21.87
176.7	324.3	1.9910	30.887	.0000	15.12
178.6	328.2	1.9910	29.892	.0000	.0000

ALOHA

Test Problem Evaluations

Introduction

The ALOHA computer code was used to evaluate the following sample problems, as described in Section 6.2 of this report (taken from Hanna and Strimaitis (1989)):

Problem 1(a):	Pressurized Liquid Release of Anhydrous Ammonia (Tank orifice release)
Problem 1(b):	Pressurized Liquid Release of Anhydrous Ammonia (Pipe release)
Problem 2:	High-Pressure Gas Release of Carbon Monoxide
Problem 3:	Pressurized Liquid Release of Chlorine
Problem 4:	Liquid Spill of Acetone

The following section gives an overall discussion of using the ALOHA code to solve the sample problems, along with separate discussions pertaining to the specifics of the individual problems.

General Information:

In order to evaluate the problem using ALOHA, parameters in addition to those given in Hanna and Strimaitis (1989) had to be specified. A list of those parameters required in all of the sample problems and their assumed values are given below:

time: 1200 hours

date: July 4, 1995

geographic location: Aiken, SC

percentage cloud cover: 0% for F-stability, 100% for D-stability

Three sets of wind speed and stability class are given in the sample problems (2 m/s, F-stability; 2 m/s, D-stability; and 5 m/s, D-stability), along with two ground roughness length scales (3 cm and 0.3 cm). These parameters will only impact the source term generation rate in cases where evaporation occurs from a liquid pool; however, ALOHA always requires them as part of its input. Default values of 2 m/s, D-stability, and 3 were used in the sample problems without pool evaporation.

The ALOHA output consists of an input echo, and the following source term output data:

- a maximum source term release rate,
- a maximum average sustained source term release rate,
- the total amount released,
- a note specifying if the release was two-phase, and
- a graph of release rate vs. time.

Data relating to the dispersion of the source term is also given in the output listing.

The following shortcomings of the output should be noted: (1) the time at which the maximum release rate occurs is not specified; (2) the maximum average sustained release rate is the average release rate over the period during which the first 20% of the total source term inventory is released; (3) the graph of release rate vs. time depicts nothing more than the average release rates over the periods of time during which 1/5 of the total source term inventory is released; (4) no information is given as to the aerosol fraction for two-phase releases; and (5) the release is limited to one hour in duration.

Problem 1(a): Pressurized Liquid Release of Anhydrous Ammonia (nozzle failure)

This problem considers a pressurized liquid release of anhydrous ammonia (at saturated conditions; 25 C and 8.9 bar) via a 1.5 inch tank orifice.

ALOHA required the size of the tank from which the release occurs as an input, therefore it was assumed that the tank was spherical with a 5.25 meter diameter. Also, it had to be specified at what location the release occurred and whether the release occurred from a short pipe/valve or directly from the tank; at the bottom and short pipe/valve were assumed, respectively.

ALOHA predicts this release to be two-phase; in Hanna and Strimaitis this release is modeled as a liquid release.

Problem 1(a)

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA

Building Air Exchanges Per Hour: 0.51 (Unsheltered single storied)

Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: AMMONIA, ANHYDROUS

Molecular Weight: 17.03 kg/kmol

TLV-TWA: 25.00 ppm IDLH: 500.00 ppm

Footprint Level of Concern: 500 ppm

Boiling Point: -33.43° C

Vapor Pressure at Ambient Temperature: greater than 1 atm

Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 2 meters/sec from N No Inversion Height

Stability Class: D Air Temperature: 25° C

Relative Humidity: 80% Ground Roughness: 3 centimeters

Cloud Cover: 10 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in spherical tank selected

Tank Diameter: 5.25 meters

Tank Volume: 75.8 cubic meters

Internal Temperature: 25° C

Chemical Mass in Tank: 40000 kilograms

Tank is 88% full

Circular Opening Diameter: 1.5 inches

Opening is 0 meters from tank bottom

Release Duration: ALOHA limited the duration to 1 hour

Max Computed Release Rate: 475 kilograms/min

Max Average Sustained Release Rate: 207 kilograms/min

(averaged over a minute or more)

Total Amount Released: 9,604 kilograms

Note: The release was a two phase flow.

Figure C-1: Release Rate of Ammonia from nozzle over time

Problem 1(b): Pressurized Liquid Release of Anhydrous Ammonia (pipe release)

This problem considers a pressurized liquid release of anhydrous ammonia (at saturated conditions; 25 C and 8.9 bar) via a 1.5 inch, 150 inch pipe.

ALOHA will not model a pipe release with an L/D of less than 200; therefore the pipe length was assumed to be 25 feet (300 inches). Also, it had to be specified whether the pipe was rough or smooth; it was assumed that the pipe was rough.

ALOHA predicts this release to be gas-phase; in Hanna and Strimaitis this release is modeled as a two-phase release.

Problem 1(b)

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA
Building Air Exchanges Per Hour: 0.51 (Unsheltered single storied)
Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: AMMONIA, ANHYDROUS
Molecular Weight: 17.03 kg/kmol
TLV-TWA: 25.00 ppm IDLH: 500.00 ppm
Footprint Level of Concern: 500 ppm
Boiling Point: -33.43° C
Vapor Pressure at Ambient Temperature: greater than 1 atm
Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 2 meters/sec from N No Inversion Height
Stability Class: D Air Temperature: 25° C
Relative Humidity: 80% Ground Roughness: 3 centimeters
Cloud Cover: 10 tenths

SOURCE STRENGTH INFORMATION:

Pipe Diameter: 1.5 inches Pipe Length: 25 feet
Pipe Temperature: 25° C Pipe Press: 8.78 atmospheres
Pipe Roughness: rough Hole Area: 1.77 sq in
Unbroken end of the pipe is connected to an infinite source
Release Duration: ALOHA limited the duration to 1 hour
Max Computed Release Rate: 40.4 kilograms/min
Max Average Sustained Release Rate: 40.4 kilograms/min
(averaged over a minute or more)
Total Amount Released: 2,426 kilograms

Figure C-2: Release Rate of Ammonia from pipe over time

Problem 2: High Pressure Gas Release of Carbon Monoxide

This problem considers a pressurized gas release of carbon monoxide via a 0.3 inch safety valve.

ALOHA requires that relative humidity be specified in the input; a value of 50% was assumed. ALOHA required the size of the tank from which the release occurs as an input, therefore it was assumed that the tank was spherical with a 5.25 meter diameter. ALOHA will not model a pipe release with an L/D of less than 200; therefore the pipe length was assumed to be 25 feet (300 inches). Also, it had to be specified whether the pipe was rough or smooth; it was assumed that the pipe was rough. Finally, ALOHA will not accept the initial tank pressure of 2230 psig (the code returns an error message for pressures above 1000 psig). The problem was evaluated using a reduced initial tank pressure of 999.9 psig.

Problem 2

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA

Building Air Exchanges Per Hour: 0.46 (Unsheltered single storied)

Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: CARBON MONOXIDE

Molecular Weight: 28.01 kg/kmol

TLV-TWA: 25.00 ppm IDLH: 1500.00 ppm

Footprint Level of Concern: 1500 ppm

Boiling Point: -191.45° C

Vapor Pressure at Ambient Temperature: greater than 1 atm

Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 2 meters/sec from N No Inversion Height

Stability Class: D Air Temperature: 21° C

Relative Humidity: 50% Ground Roughness: Open country

Cloud Cover: 10 tenths

SOURCE STRENGTH INFORMATION:

Gas leak from short pipe or valve in spherical tank selected

Tank Diameter: 5.25 meters

Tank Volume: 75.8 cubic meters

Internal Temperature: 21° C

Internal Press: 999.9 lbs/sq in

Chemical Mass in Tank: 6,129 kilograms

Circular Opening Diameter: .3 inches

Release Duration: ALOHA limited the duration to 1 hour

Max Computed Release Rate: 26.9 kilograms/min

Max Average Sustained Release Rate: 23.9 kilograms/min
(averaged over a minute or more)

Total Amount Released: 1,374 kilograms

Figure C-3: Release Rate of Carbon Monoxide over time

Problem 3: Pressurized Liquid Release of Chlorine

This considers a pressurized liquid release of chlorine (at saturated conditions; 30 C and 1 atm) via a 0.3 inch valve.

ALOHA required the size of the tank from which the release occurs as an input, therefore it was assumed that the tank was a horizontal cylinder, 2 meters long with a 0.75 meter diameter. Also, it had to be specified at what location the release occurred and whether the release occurred from a short pipe/valve or directly from the tank; at the bottom and short pipe/valve were assumed, respectively.

ALOHA predicts this release to be two-phase; in Hanna and Strimaitis this release is modeled as a liquid release.

Problem 3

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA

Building Air Exchanges Per Hour: 0.55 (Unsheltered single storied)

Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: CHLORINE Molecular Weight: 70.90 kg/kmol

TLV-TWA: 0.50 ppm IDLH: 30.00 ppm

Footprint Level of Concern: 30 ppm

Boiling Point: -34.03° C

Vapor Pressure at Ambient Temperature: greater than 1 atm

Ambient Saturation Concentration: 1,000,000 ppm or 100.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 2 meters/sec from N No Inversion Height

Stability Class: D Air Temperature: 30° C

Relative Humidity: 80% Ground Roughness: 3 centimeters

Cloud Cover: 10 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in horizontal cylindrical tank selected

Tank Diameter: .75 meters Tank Length: 2 meters

Tank Volume: 0.88 cubic meters

Internal Temperature: 30° C

Chemical Mass in Tank: 1 tons

Tank is 74% full

Circular Opening Diameter: .3 inches

Opening is 0 meters from tank bottom

Release Duration: ALOHA limited the duration to 1 hour

Max Computed Release Rate: 31.8 kilograms/min

Max Average Sustained Release Rate: 17.1 kilograms/min

(averaged over a minute or more)

Total Amount Released: 421 kilograms

Note: The release was a two phase flow.

Figure C-4: Release Rate of Chlorine over time

Problem 4: Liquid Release of Acetone

This problem considers a liquid release of acetone via a 2 inch nozzle. The tank is within a 72-foot diameter diked area.

ALOHA required the location at which the release occurred and whether the release occurred from a short pipe/valve or directly from the tank as an input; at the bottom and short pipe/valve were assumed, respectively.

Although in the sample problem the tank footprint is not available as evaporative area, no credit was taken in the evaluations for this reduction in area.

Problem 4 (1 of 6)

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA

Building Air Exchanges Per Hour: 0.56 (Unsheltered single storied)

Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: ACETONE Molecular Weight: 58.08 kg/kmol

TLV-TWA: 750.00 ppm IDLH: 20000.00 ppm

Footprint Level of Concern: 20000 ppm

Boiling Point: 56.29° C

Vapor Pressure at Ambient Temperature: 0.37 atm

Ambient Saturation Concentration: 379,933 ppm or 38.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 2 meters/sec from N No Inversion Height

Stability Class: F Air Temperature: 30° C

Relative Humidity: 50% Ground Roughness: .3 centimeters

Cloud Cover: 0 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in vertical cylindrical tank selected

Tank Diameter: 25 feet Tank Length: 25 feet

Tank Volume: 91,800 gallons

Internal Temperature: 30° C

Chemical Mass in Tank: 270,963 kilograms

Tank is 100% full

Circular Opening Diameter: 2 inches

Opening is 0 feet from tank bottom

Soil Type: Concrete

Ground Temp: equal to ambient

Max Puddle Diameter: 72 feet

Release Duration: ALOHA limited the duration to 1 hour

Max Computed Release Rate: 109 kilograms/min

Max Average Sustained Release Rate: 86.9 kilograms/min

(averaged over a minute or more)

Total Amount Released: 4,496 kilograms

Figure C-5: Release Rate of Acetone over time (F stability, 2 m/s, 0.3 cm roughness)

Problem 4 (2 of 6)

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA

Building Air Exchanges Per Hour: 0.56 (Unsheltered single storied)

Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: ACETONE Molecular Weight: 58.08 kg/kmol

TLV-TWA: 750.00 ppm IDLH: 20000.00 ppm

Footprint Level of Concern: 20000 ppm

Boiling Point: 56.29° C

Vapor Pressure at Ambient Temperature: 0.37 atm

Ambient Saturation Concentration: 379,933 ppm or 38.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 2 meters/sec from N No Inversion Height

Stability Class: F Air Temperature: 30° C

Relative Humidity: 50% Ground Roughness: 3 centimeters

Cloud Cover: 0 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in vertical cylindrical tank selected

Tank Diameter: 25 feet Tank Length: 25 feet

Tank Volume: 91,800 gallons

Internal Temperature: 30° C

Chemical Mass in Tank: 270,963 kilograms

Tank is 100% full

Circular Opening Diameter: 2 inches

Opening is 0 feet from tank bottom

Soil Type: Concrete

Ground Temp: equal to ambient

Max Puddle Diameter: 72 feet

Release Duration: ALOHA limited the duration to 1 hour

Max Computed Release Rate: 109 kilograms/min

Max Average Sustained Release Rate: 86.9 kilograms/min
(averaged over a minute or more)

Total Amount Released: 4,496 kilograms

Figure C-6: Release Rate of Acetone over time (F stability, 2 m/s, 3 cm roughness)

Problem 4 (3 of 6)

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA

Building Air Exchanges Per Hour: 0.55 (Unsheltered single storied)

Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: ACETONE Molecular Weight: 58.08 kg/kmol

TLV-TWA: 750.00 ppm IDLH: 20000.00 ppm

Footprint Level of Concern: 20000 ppm

Boiling Point: 56.29° C

Vapor Pressure at Ambient Temperature: 0.37 atm

Ambient Saturation Concentration: 379,933 ppm or 38.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 2 meters/sec from N No Inversion Height

Stability Class: D Air Temperature: 30° C

Relative Humidity: 50% Ground Roughness: .3 centimeters

Cloud Cover: 10 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in vertical cylindrical tank selected

Tank Diameter: 25 feet Tank Length: 25 feet

Tank Volume: 91,800 gallons

Internal Temperature: 30° C

Chemical Mass in Tank: 270,963 kilograms

Tank is 100% full

Circular Opening Diameter: 2 inches

Opening is 0 feet from tank bottom

Soil Type: Concrete

Ground Temp: equal to ambient

Max Puddle Diameter: 72 feet

Release Duration: ALOHA limited the duration to 1 hour

Max Computed Release Rate: 93.4 kilograms/min

Max Average Sustained Release Rate: 71.6 kilograms/min

(averaged over a minute or more)

Total Amount Released: 3,507 kilograms

Figure C-7: Release Rate of Acetone over time (D stability, 2 m/s, 0.3 cm roughness)

Problem 4 (4 of 6)

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA

Building Air Exchanges Per Hour: 0.55 (Unsheltered single storied)

Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: ACETONE Molecular Weight: 58.08 kg/kmol

TLV-TWA: 750.00 ppm IDLH: 20000.00 ppm

Footprint Level of Concern: 20000 ppm

Boiling Point: 56.29° C

Vapor Pressure at Ambient Temperature: 0.37 atm

Ambient Saturation Concentration: 379,933 ppm or 38.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 2 meters/sec from N No Inversion Height

Stability Class: D Air Temperature: 30° C

Relative Humidity: 50% Ground Roughness: 3 centimeters

Cloud Cover: 10 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in vertical cylindrical tank selected

Tank Diameter: 25 feet Tank Length: 25 feet

Tank Volume: 91,800 gallons

Internal Temperature: 30° C

Chemical Mass in Tank: 270,963 kilograms

Tank is 100% full

Circular Opening Diameter: 2 inches

Opening is 0 feet from tank bottom

Soil Type: Concrete

Ground Temp: equal to ambient

Max Puddle Diameter: 72 feet

Release Duration: ALOHA limited the duration to 1 hour

Max Computed Release Rate: 93.4 kilograms/min

Max Average Sustained Release Rate: 71.6 kilograms/min

(averaged over a minute or more)

Total Amount Released: 3,507 kilograms

Figure C-8: Release Rate of Acetone over time (D stability, 2 m/s, 3 cm roughness)

Problem 4 (5 of 6)

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA
Building Air Exchanges Per Hour: 1.16 (Unsheltered single storied)
Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: ACETONE Molecular Weight: 58.08 kg/kmol
TLV-TWA: 750.00 ppm IDLH: 20000.00 ppm
Footprint Level of Concern: 20000 ppm
Boiling Point: 56.29° C
Vapor Pressure at Ambient Temperature: 0.37 atm
Ambient Saturation Concentration: 379,933 ppm or 38.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 5 meters/sec from N No Inversion Height
Stability Class: D Air Temperature: 30° C
Relative Humidity: 50% Ground Roughness: .3 centimeters
Cloud Cover: 10 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in vertical cylindrical tank selected
Tank Diameter: 25 feet Tank Length: 25 feet
Tank Volume: 91,800 gallons
Internal Temperature: 30° C
Chemical Mass in Tank: 270,963 kilograms
Tank is 100% full
Circular Opening Diameter: 2 inches
Opening is 0 feet from tank bottom
Soil Type: Concrete
Ground Temp: equal to ambient
Max Puddle Diameter: 72 feet
Release Duration: ALOHA limited the duration to 1 hour
Max Computed Release Rate: 207 kilograms/min
Max Average Sustained Release Rate: 149 kilograms/min
(averaged over a minute or more)
Total Amount Released: 8,577 kilograms

Figure C-9: Release Rate of Acetone over time (D stability, 2 m/s, 0.3 cm roughness)

Problem 4 (6 of 6)

SITE DATA INFORMATION:

Location: AIKEN, SOUTH CAROLINA

Building Air Exchanges Per Hour: 1.16 (Unsheltered single storied)

Date and Time: Fixed at July 4, 1995 1200 hours

CHEMICAL INFORMATION:

Chemical Name: ACETONE Molecular Weight: 58.08 kg/kmol

TLV-TWA: 750.00 ppm IDLH: 20000.00 ppm

Footprint Level of Concern: 20000 ppm

Boiling Point: 56.29° C

Vapor Pressure at Ambient Temperature: 0.37 atm

Ambient Saturation Concentration: 379,933 ppm or 38.0%

ATMOSPHERIC INFORMATION: (MANUAL INPUT OF DATA)

Wind: 5 meters/sec from N No Inversion Height

Stability Class: D Air Temperature: 30° C

Relative Humidity: 50% Ground Roughness: 3 centimeters

Cloud Cover: 10 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in vertical cylindrical tank selected

Tank Diameter: 25 feet Tank Length: 25 feet

Tank Volume: 91,800 gallons

Internal Temperature: 30° C

Chemical Mass in Tank: 270,963 kilograms

Tank is 100% full

Circular Opening Diameter: 2 inches

Opening is 0 feet from tank bottom

Soil Type: Concrete

Ground Temp: equal to ambient

Max Puddle Diameter: 72 feet

Release Duration: ALOHA limited the duration to 1 hour

Max Computed Release Rate: 207 kilograms/min

Max Average Sustained Release Rate: 149 kilograms/min

(averaged over a minute or more)

Total Amount Released: 8,577 kilograms

Figure C-10: Release Rate of Acetone over time (D stability, 5 m/s, 3 cm roughness)

CASRAM

Test Problem Evaluations

Introduction

CASRAM was used to evaluate test problems 1(a) and 4, as described in Section 6.2 of this report (taken from Hanna and Strimaitis (1989)). The associated input and output are provided here. Where appropriate, limitations, or exceptional features of the code are brought to the reader's attention.

Problem 1(a): Pressurized Liquid Release of Anhydrous Ammonia (nozzle failure)

This scenario describes the ground level release of anhydrous ammonia from a nozzle failure. The 1.5 in. ID nozzle is very near the tank. This case illustrates the extremes of all liquid emissions (from the nozzle). Figure C-11 illustrates this scenario.

Calculations of the maximum anhydrous ammonia emission rate are desired.

Figure C-11: Anhydrous ammonia rupture. Nozzle failure, the inner diameter of the opening is 1.5 in.

Given Spill Conditions:

1.	Properties of Anhydrous Ammonia (NH ₃):	<u>Given</u>	<u>CASRAM</u>
	Molecular weight	M _g =17.03	kg/kg-mol
	Density of liquid	ρ _l =608.76	602.1 kg/m ³ @298K/8.9 bars
		^a	681.4 kg/m ³ @240K/8.9 bars
	Density of gas	ρ _g =6.2	kg/m ³ @298K/8.9 bars
	Vapor pressure	P _{g1} = ^a	9.95 kPa@298K
		P _{g2} = ^a	1.026 kPa@298K
	Latent heat of vaporization	H _{v2} =1,170	1,167 kJ/kg@298K
		^a	1,369 kJ/kg@240K
	Specific heat of liquid	C _{pl} =4.49	9.999 kJ/kg K
	Specific heat of vapor	C _{pv} = ^a	2.087/2.009 kJ/kg K@298/240K
	Normal boiling point	T _b =240.0	239.7 K
2.	Tank Data:		
	Mass of tank	M _t =4.0x10 ⁴	same kg
	Temperature	T _t =25(298)	25(298) °C(K)
	Pressure	p _t =8.9	9.95 bars (saturation)
	Rupture diameter	D _n =1.5	1.5 in (3.81x10 ⁻² m)
3.	Site Conditions/Ambient		
	Meteorology:		
	Temperature	T _a =25	same °C(K)
	Pressure	P _a =1.013x10 ⁵	same pa
	Relative humidity	RH=80	same %
	Specific heat at constant pressure	C _p =1004	same J/kg K
	Atmospheric Density	ρ _a =1.184	same kg/m ³ @atm/298K
	Stability Class D	u=2.0	same m/s
	Stability Class D	u=5.0	same m/s at release height
	Stability Class F	u=2.0	same m/s
	Surface roughness	z ₀ =0.03	same cm

^aParameter not provided in sample problem.

Assumptions used in construction of CASRAM source model scenario:

- (1) Initially, 40,000 kg of saturated anhydrous ammonia is contained in a sealed tank at 298 K. Using the DIPPR 9 equation of state for ammonia, the tank pressure is calculated to be 9.95 bars, which is in substantial conflict with the tank pressure stated in the problem.
- (2) The discharge coefficient for the rupture is 0.6. This is characteristic for a circular hole with sharp edges.
- (3) The tank is initially full of liquid with no vapor. Additionally, the tank is cylindrical with a height of twice its diameter.

This release was modeled using the pressurized release sub-model of CASRAM. This model has recently been added to CASRAM to treat cases where: (1) adequate statistical data are unavailable, or (2) critical release scenario data are available (e.g., size, location, and geometry of hole). The pressurized release sub-model solves the time dependent, one dimensional mass and energy conservation equations. Within this framework, the flash fraction is simply the ratio of the mass of the vapor to the total mass of the two phase mixture when exiting the tank. For this problem, we assumed that 10% of the remaining liquid is entrained along with the flashed liquid. After flashing and entrainment, the remaining liquid forms a pool on the ground surface, which evaporates over time. Within the pressurized release sub-model, the pool evaporation rate is calculated using a simple thermal resistance relation between the pool and the environment. In future work, pool evaporation within the pressurized release sub-model will be determined with the more general and robust pool evaporation model in CASRAM.

The ammonia emission rate into the atmosphere as a function of time is provided in Figure C-y. Initially, the emission rate is due solely to flashing and entrainment into the flashed liquid. However, the emission rate quickly climbs as pool evaporation becomes important. After about 2000 seconds, the release rate from the tank decreases to near zero. Subsequent emissions into the atmosphere are due only to pool evaporation. Due to the large initial tank pressure, the emission characteristics were not found to vary greatly with tank geometry or initial liquid fraction.

It is important to note that the solution methodology would be considerably different if we treated this problem in the statistical model of CASRAM. The statistical approach is used for cases where critical input parameters such as hole size, hole location, tank temperature and ambient meteorological conditions are not known a priori. Here, CASRAM would perform many trials to obtain a distribution of consequences. For each of these trials, a release fraction would be randomly selected from a prescribed

distribution. (Release fraction distributions are currently available only for transportation accidents.) Each modeled release is assumed to occur instantaneously. Flash and entrainment fractions are determined using ammonia properties along with ambient and storage temperatures. Emissions from liquids not flashed or entrained are determined from the CASRAM pool evaporation model. The downwind concentration for a given averaging time (typically corresponding to the averaging time of a toxicological value) is then determined using a plume dispersion model modified to account for initial puff releases of flashed and entrained aerosol material.

Table C-1: Average anhydrous ammonia emission rates as a function of meteorology and spill duration

Emission rates Q (kg/s) from flashing, aerosol entrainment, and pool evaporation			
t = 30 min CASRAM	t = 30 min. Hand Calc	t = 1 s CASRAM	t = 50 min CASRAM
19 ¹	4.79 ²	6.9	3.0

¹instantaneous emission rate @ t = 30 min.; $Q_{\min} = 6.93 \text{ kg/s}$ @ t = 1 sec, $Q_{\max} = 21.3 \text{ kg/s}$ @ t = 10 - 20 min

²average emission rate, calculation does not include contribution from pool evaporation or aerosol entrainment (from Hanna and Strimaitis, 1989).

Figure C-12: Ammonia emission rate from a cylindrical tank initially containing 40,000 kg of saturated anhydrous ammonia at 298 K. Ammonia is released through a 1.5 in. circular, sharp-edged orifice at the lowest point in the tank. Emission to the atmosphere occurs through flashing, aerosol entrainment, and pool evaporation. After the release ends, emission to the atmosphere is due only to evaporation from the ammonia pool.

Problem 4: Acetone Spilled within a Diked Area

A spill of liquid acetone from a 2 in. nozzle connection near the base of a cylindrical tank of height 25 ft and diameter 25 ft occurs over a 30 min. period into a concrete diked area of height 3 ft and diameter 72 ft. Figure C-3 contains a schematic drawing of this case. The chemical is stored at ambient pressure and temperature (303 K).

The emission rate of acetone to the atmosphere from this spill is desired for estimating maximum downwind concentrations. The evaporation rate from the diked area is calculated using the CASRAM model.

Figure C-13: Acetone spill - the spilled liquid is contained within the diked area.

Given Spill Conditions:

Acetone is a slowly evaporating chemical that will spill as a liquid from the tank, with no flashing.

1.	Properties of Acetone:	<u>Given</u>	<u>CASRAM</u>	
	Molecular weight	$M_g=58.1$	58.08	kg/kg-mol
	Density of liquid	$\rho_l=791.0$	786.0	kg/m ³ @303K
	Density of gas	$\rho_g=2.34$	n/a	kg/m ³ @303K
	Vapor pressure	$P_{g1}=a$	17.1	kPa@285K
		$P_{g2}=a$	37.4	kPa@303K
	Latent heat of vaporization	$H_{v2}=a$	533.0	kJ/kg@303K
	Binary Diffusion Coef.	$D_b=a$	1.09x10 ⁻⁵	m ² /s
2.	Tank Data:			
	Tank diameter	$D_t=7.62$	same	in
	Tank height	$H=7.62$	same	in
	Nozzle diameter	$D_n=0.051$	same	in
	Liquid stored at ambient P and T			
3.	Site Conditions/Ambient Meteorology:			
	Temperature	$T_a=303$	same	K
	Pressure	$P_a=1.013 \times 10^5$	same	Pa
	Relative humidity	$RH=50$	same	%
	Stability Class D	$u=2.0$	same	m/s
	Stability Class D	$u==5.0$	same	m/s at release height
	Stability Class F	$u==2.0$	same	m/s
	Spill duration	$t_s=30$	same	min

Assumptions used in construction of CASRAM source model scenario:

- (1) Acetone fills only diked area, and does so instantaneously.
- (2) Wind speed is measured at 10 m.
- (3) The roughness length of 0.10 m, typical for suburban area.

^aParameter not provided in sample problem.

- (4) Initial ground temperature is the same as air temperature and with no surface heat flux associated with an initial vertical ground temperature gradient ($dT_g/dz_g = 0$ before spill).

The example problem lists atmospheric properties in terms of stability class. This information is converted into the necessary heat and momentum flux parameters required for the CASRAM source model. Acetone properties are determined from the DIPPR data base.

Table C-2 provides a summary of CASRAM average release rate estimates along with the estimates provided in the sample problem from the SPILLS model and from hand calculations. Average CASRAM estimated evaporation rates are also give for 15 and 60 minutes release duration. Note that within the CASRAM model, emission rates are dependent upon roughness lengths, all else being equal (stability, wind speed at 10 m, and spill scenario). For example, in the D stability cases, lowering z_0 to 0.01 m will decrease emission rates by about 25%. Increasing z_0 to 0.3 m will increase the emission rates by roughly 25%.

Table C-2: Average acetone pool evaporation rates as a function of meteorology and spill duration

Meteorology	Average emission rates Q (g/s) from pool				
	$t_s = 30$ min CASRAM	$t_s = 30$ min SPILLS	$t_s = 30$ min Hand Calc.	$t_s = 60$ min CASRAM	$t_s = 15$ min CASRAM
D stability, 2 m/s wind speed	975.1 ³	840.0	960.0	861.0	1,117.0
D stability, 5 m/s wind speed	1,666.0 ⁴	1,880.0	2,100.0	1,499.0	1,881.0
F stability, 2 m/s wind speed	685.4 ⁵	(d)	(d)	597.6	783.8

³ $Q_{min} = 796.9$ g/s; $Q_{max} = 1,667.0$ g/s

⁴ $Q_{min} = 1,395.0$ g/s; $Q_{max} = 2,980.0$ g/s

⁵ $Q_{min} = 551.5$ g/s; $Q_{max} = 1,149.0$ g/s

^d Calculated or computed value not provided in the test problem results.

Sample CASRAM OUTPUT

Time dependent pool evaporation release rate data for the acetone spill. The data are for D stability with $u = 5$ m/s.

Time (sec)	Q (kg/s)	Time (sec)	Q (kg/s)	Time (sec)	Q (kg/s)
1.	4.4319	39.	2.7551	111.	2.2534
2.	3.8732	40.	2.7423	114.	2.2413
3.	3.8795	41.	2.7299	117.	2.2295
4.	3.7628	42.	2.7177	120.	2.2182
5.	3.6929	43.	2.7059	123.	2.2071
6.	3.6236	44.	2.6943	126.	2.1964
7.	3.5636	45.	2.6830	129.	2.1860
8.	3.5091	46.	2.6719	132.	2.1759
9.	3.4595	47.	2.6611	135.	2.1661
10.	3.4139	48.	2.6506	138.	2.1566
11.	3.3717	49.	2.6403	141.	2.1473
12.	3.3325	50.	2.6302	144.	2.1382
13.	3.2959	51.	2.6203	147.	2.1294
14.	3.2614	52.	2.6106	150.	2.1208
15.	3.2290	53.	2.6022	153.	2.1124
16.	3.1984	54.	2.5919	156.	2.1043
17.	3.1693	55.	2.5827	159.	2.0963
18.	3.1417	56.	2.5738	162.	2.0885
19.	3.1153	57.	2.5651	165.	2.0809
20.	3.0902	58.	2.5565	168.	2.0734
21.	3.0662	59.	2.5480	171.	2.0661
22.	3.0432	60.	2.5398	174.	2.0590
23.	3.0211	63.	2.5316	177.	2.0521
24.	2.9999	66.	2.5045	180.	2.0452
25.	2.9795	69.	2.4821	184.	2.0386
26.	2.9598	72.	2.4065	190.	2.0268
27.	2.9409	75.	2.4401	195.	2.0162
28.	2.9226	78.	2.4207	200.	2.0060
29.	2.9049	81.	2.4022	205.	1.9961
30.	2.8878	84.	2.3845	210.	1.9866
31.	2.8712	87.	2.3675	215.	1.9773
32.	2.8552	90.	2.3513	220.	1.9684
33.	2.8396	93.	2.3357	225.	1.9597
34.	2.8245	96.	2.3207	230.	1.9512
35.	2.8098	99.	2.3063	235.	1.9431
36.	2.7956	102.	2.2923	240.	1.9351
37.	2.7817	105.	2.2789	245.	1.9274
38.	2.7682	108.	2.2659	250.	1.9198

Time (sec)	Q (kg/s)	Time (sec)	Q (kg/s)
255.	1.9125	1080.	1.4972
260.	1.9053	1125.	1.4880
265.	1.8984	1170.	1.4794
270.	1.8916	121.5	1.4713
275.	1.8849	1260.	1.4636
280.	1.8784	1305.	1.4564
285.	1.8721	1350.	1.4494
290.	1.8659	1395.	1.4429
295.	1.8599	1440.	1.4366
300.	1.8540	1485.	1.4306
320.	1.8482	1530.	1.4248
340.	1.8215	1575.	1.4193
360.	1.7999	1620.	1.4141
380.	1.7815	1665.	1.4090
400.	1.7641	1710.	1.4041
420.	1.7480	1755.	1.3995
440.	1.7330	1800.	1.3950
460.	1.7190	1890.	1.3906
480.	1.7058	1980.	1.3807
500.	1.6934	2070.	1.3724
520.	1.6817	2160.	1.3656
540.	1.6706	2250.	1.3587
560.	1.6600	2340.	1.3524
580.	1.6500	2430.	1.3464
600.	1.4605	2520.	1.3408
620.	1.6314	2610.	1.3354
640.	1.6227	2700.	1.3303
660.	1.6144	2790.	1.3255
680.	1.6064	2880.	1.3208
700.	1.5988	2970.	1.3165
720.	1.5914	3060.	1.3122
740.	1.5843	3150.	1.3082
760.	1.5775	3240.	1.3044
780.	1.5710	3330.	1.3006
800.	1.5647	3420.	1.2971
820.	1.5586	3510.	1.2937
840.	1.5527	3600.	1.2904
860.	1.5470		
880.	1.5415		
900.	1.5361		
945.	1.5309		
990.	1.5178		
1025.	1.5067		

HGSystem

Test Problem Evaluations

Introduction

The HGSystem computer program for the simulation of chemical source-term and toxic air pollutant concentrations was used to evaluate the following scenarios, as described in Section 6.2 of this report (taken from Hanna and Strimaitis (1989)):

Problem 1(a):	Pressurized Liquid Release of Anhydrous Ammonia (Tank orifice release)
Problem 1(b):	Pressurized Liquid Release of Anhydrous Ammonia (Pipe release)
Problem 2:	High-Pressure Gas Release of Carbon Monoxide
Problem 3:	Pressurized Liquid Release of Chlorine
Problem 4:	Liquid Spill of Acetone

Each release scenario has been analyzed by the computer model with the associated input and output presented. Where appropriate, limitations or concerns encountered when applying the model to these scenarios as well as any exceptional capabilities encountered in the process are brought to the reader's attention.

The results of each scenario test case begins with a series of text boxes containing input data for the analysis. Shaded information in each of these blocks indicate intermediate source-term values calculated by the program. Final source-term estimates are summarized in the shaded text columns immediately following the input text boxes and preceding the results of the dispersion analysis.

Problem 1(a): Pressurized Liquid Release of Anhydrous Ammonia (nozzle failure)

HGSystem computes the time-dependent mass outflow rate from a reservoir based on the initial mass inventory, system pressure, vessel size (volume) and ambient conditions. The vessel volume was based on the volume occupied by 40 tonnes of liquid anhydrous ammonia at saturation pressure. Note that the true saturation pressure at the given ambient temperature of 298 K is approximately 9.9 atmospheres and not $p_s=8.78$ atmospheres given in the handbook. This is important to observe since otherwise the vessel is continuously venting and the outflow will be pure vapor (as also predicted by HGSystem). The total surface area exposed to solar flux was assumed to be equal to the surface area of a sphere with the required volume capacity. The calculations were terminated when the total inventory remaining inside the reservoir was less than 0.1 kg. The physical/chemical property data was generated by the HGSystem database utility DATAPROP.

Input

```

* ===== SPILL standard input file =====

TITLE Pressurized Liquid Release of Anhydrous Ammonia

RESERVOIR      * RESERVOIR DATA
  TRES      = 24.85 * Storage/reservoir temperature (C).
  PRES      = 9.9   * Reservoir (absolute) pressure (atm).
                *   If -1.0, SPILL uses the mixture saturation
                *   pressure assuming all compounds are in liquid
                *   state.
                *   User MUST specify SPECIES keyword to use this
                *   option.
  VRES      = 65.7 * Reservoir volume (m3).
  MRES      = 40.0 * Reservoir mass contents (tonnes).

* ----- DATAPROP/AEROPLUME link file nh3 .APL -----
* AEROPLUME input data from program DATAPROP
*
* For each compound in pollutant (excluding water) data in SPECIES keyword are:
* - line 1: name of species, mole fraction in pollutant, aerosol class
* - line 2: specific heats of vapour and liquid (J/mole/C)
*           heat of vaporisation (J/mole)
*           critical temperature (K), critical pressure (atm)
* - line 3: vapour-pressure function fitting parameters (-)
*           molecular mass (g/mole), liquid density (kg/m**3)
* -----

TITLE DATAPROP standard input file (no HF)
*
GASDATA      * -----> [pollutant = dry pollutant (aerosol), water]
  WATERPOL= .0000 * - water in pollutant (mole fraction)
  CPGAS     = 35.52 * J/MOLE/C specific heat of dry pollutant
  MMGAS     = 17.03 * KG/KMOLE molecular mass of dry pollutant
  HEATGR    = 21.59 * ..... heat group (used for HEGADAS link only)
  SPECIES   = AMMONIA , 1.00000 , 4
              35.5177 , 78.9089 , 21936.9 , 405.400 , 111.848
              -7.16190 , 1.12460 , -2.15890 , -2.15070 , 17.0310
              646.964

PIPE          * PIPE EXIT-PLANE (CHOKE-FRONT) CONDITIONS
  DEXIT      = 0.0381 * (Effective) release orifice diameter (m).

AMBIENT CONDITIONS * ATMOSPHERIC AMBIENT CONDITIONS
  AIRPRESS   = 1.00   * Atmosphere pressure at release height (atm).
* Following parameters are used for calculation of heat transfer
* between ambient atmosphere and reservoir
  TATM       = 24.85  * Atmosphere temperature (degC)
  QSOLAR     = 200.0  * Solar heat flux (directly from the sun) (W/m2)
  EMISS      = 0.8    * Emissivity of reservoir surface (-)
  AREA       = 78.74  * Surface area over which heat flux occurs (m2)
                * Setting AREA to 0.0 set heat transfer to 0.0

TERMINAT      * RESERVOIR RELEASE TERMINATION CRITERIA
                * SPILL ignores criteria set to -1.0
  TLST       = -1.0   * Last required elapsed time after release start (s)
  MLST       = 0.0001 * Last required reservoir mass content (tonnes)
  LLST       = -1.0   * Last required reservoir liquid molefraction (%)
  PLST       = -1.0   * Last required reservoir pressure (atm)
  RLST       = -1.0   * Last required reservoir mixture density (kg/m3)

```

Results

Output from SPILL				Version 1.1		Title: DATAPROP standard input file (no HF)				Date: 25/08/95 Time: 12:31:43			
Reservoir conditions					Atmosphere reference conditions					Release orifice properties			
res. init. temperature:		24.85 degC			ambient atmospheric pressure:		1.00 atm		release orifice diameter:				
3.81 cm													
res. init. pressure:		9.90 atm			ambient atm. temperature:		24.85 degC		vapour discharge				
coefficient: 1.00													
reservoir volume (fixed):		65.70 m3			emissivity factor of tank:		.80 (-)		liquid discharge				
coefficient: .61													
res. init. mass content:		1.57 ton			heat transfer area:		78.74 m2		empty				
empty					solar heat flux:		200.00 W/m2		empty				
empty					empty				empty				
empty					empty				empty				
TIME	MRES	DMDT	PRES	TRES	RRES	HRES	LRES	MMRES	RHOLIQ	QATM	PHASE	DMDTAV	
.0	1.6	5.3	9.90	24.85	23.9	-828.3	71.91	17.04	647.0	.200	two phase	5.3	
1.0	1.6	5.3	9.90	24.85	23.8	-827.2	71.81	17.04	647.0	.200	two phase	5.3	
2.0	1.6	5.3	9.90	24.84	23.8	-826.0	71.72	17.04	647.0	.200	two phase	5.3	
3.0	1.6	5.3	9.90	24.84	23.7	-824.8	71.62	17.04	647.0	.200	two phase	5.3	
4.0	1.5	5.3	9.90	24.84	23.6	-823.6	71.52	17.04	647.0	.200	two phase	5.3	
5.0	1.5	5.3	9.90	24.84	23.5	-822.4	71.42	17.04	647.0	.200	two phase	5.3	
6.0	1.5	5.3	9.89	24.83	23.4	-821.2	71.32	17.04	647.0	.200	two phase	5.3	
7.0	1.5	5.3	9.89	24.83	23.3	-819.9	71.22	17.04	647.0	.200	two phase	5.3	
8.0	1.5	5.3	9.89	24.83	23.3	-818.7	71.12	17.04	647.0	.200	two phase	5.3	
9.0	1.5	5.3	9.89	24.82	23.2	-817.5	71.02	17.04	647.0	.200	two phase	5.3	
10.0	1.5	5.3	9.89	24.82	23.1	-816.2	70.91	17.04	647.0	.200	two phase	5.3	
20.0	1.5	5.3	9.88	24.79	22.3	-803.2	69.84	17.04	647.0	.200	two phase	5.3	
30.0	1.4	5.3	9.89	24.83	21.6	-789.1	68.80	17.04	647.0	.200	two phase	5.3	
40.0	1.4	5.3	9.86	24.73	20.7	-774.2	67.46	17.04	647.0	.201	two phase	5.3	
50.0	1.3	5.3	9.86	24.70	19.9	-757.9	66.12	17.05	647.0	.201	two phase	5.3	
60.0	1.3	5.3	9.85	24.67	19.1	-740.3	64.67	17.05	647.0	.201	two phase	5.3	
70.0	1.2	5.3	9.84	24.64	18.3	-721.1	63.10	17.05	647.0	.201	two phase	5.3	
80.0	1.1	5.3	9.83	24.61	17.5	-700.2	61.38	17.05	647.0	.201	two phase	5.3	
90.0	1.1	5.3	9.82	24.58	16.7	-677.2	59.50	17.05	647.0	.202	two phase	5.3	
100.0	1.0	5.3	9.81	24.55	15.9	-652.0	57.43	17.05	647.0	.202	two phase	5.3	
120.0	.9	5.3	9.79	24.49	14.3	-593.0	52.60	17.05	647.0	.202	two phase	5.3	
140.0	.8	5.3	9.77	24.42	12.7	-519.2	46.56	17.05	647.0	.203	two phase	5.3	
160.0	.7	5.2	9.75	24.35	11.1	-424.1	38.79	17.06	647.0	.203	two phase	5.3	
180.0	.6	5.2	9.73	24.28	9.5	-297.1	28.40	17.06	647.0	.204	two phase	5.3	
200.0	.5	5.2	9.71	24.21	7.9	-119.0	13.84	17.07	647.0	.204	two phase	5.3	
250.0	.4	1.6	7.90	11.26	5.8	23.4	.00	17.07	.0	.324	vapour	4.8	
300.0	.3	1.3	6.05	-3.94	4.7	-8.2	.00	17.07	.0	.460	vapour	4.2	
350.0	.2	1.0	4.69	-16.05	3.8	-33.4	.00	17.07	.0	.571	vapour	3.8	
400.0	.2	.8	3.70	-25.05	3.1	-52.1	.00	17.07	.0	.652	vapour	3.4	
450.0	.2	.7	2.95	-30.93	2.5	-64.3	.00	17.07	.0	.705	vapour	3.1	
500.0	.1	.5	2.39	-33.76	2.1	-70.2	.00	17.07	.0	.729	vapour	2.9	
600.0	.1	.3	1.63	-30.74	1.4	-63.9	.00	17.07	.0	.693	vapour	2.5	
700.0	.1	.2	1.20	-16.80	1.0	-34.9	.00	17.07	.0	.554	vapour	2.2	
800.0	.1	.1	1.03	5.37	.8	11.2	.00	17.07	.0	.346	vapour	1.9	
848.8	.0	.0	1.01	16.04	.7	33.4	.00	17.07	.0	.270	vapour	1.8	
Interpretation:													
TIME:	elapsed time since release start (s)							MRES:	reservoir total mass content (tonnes)				
DMDT:	release mass flow rate (kg/s)							PRES:	reservoir absolute pressure (atm)				
TRES:	reservoir temperature (degC)							RRES:	reservoir mixture density (kg/m3)				
HRES:	reservoir total enthalpy (kJ/kg)							LRES:	reservoir molefraction liquid (%)				
MMRES:	reservoir average molar mass (kg/kmole)							RHOLIQ:	reservoir liquid density (kg/m3)				
QATM:	heat flux from ambient to reservoir (kW/m2)							PHASE:	reservoir fluid state (vapour/two-phase)				
DMDTAV:	average release rate since release start (kg/s)												

Figure C-14:

Anhydrous Ammonia Mass Release Rate

Figure C-15:

Anhydrous Ammonia Reservoir Pressure

Figure C-16:

Anhydrous Ammonia Reservoir Temperature

Figure C-17:

Anhydrous Ammonia Vessel Mixture Density

Figure C-18:

Anhydrous Ammonia Vessel Liquid Mole Fraction

Problem 1(b): Pressurized Liquid Release of Anhydrous Ammonia (pipe release)

HGSystem is not suitable for cases where there is pipework between the reservoir and the discharge orifice.

Problem 2: High Pressure Gas Release of Carbon Monoxide

HGSystem computes the time-dependent mass outflow rate from a reservoir based on the initial mass inventory, system pressure, vessel size (volume) and ambient conditions. In order to proceed with the calculations, an initial mass inventory and vessel volume needed to be specified. Several different mass inventories were assumed (see graphs below) and the associated volume in each case was based on the volume occupied by pure saturated liquid under the given system pressure. The input quantities which were varied between each run are shaded in the input text box description below. The total surface area exposed to solar flux was assumed to be equal to the surface area of a sphere with the required volume capacity. The calculations were terminated when the total inventory remaining inside the reservoir was less than 0.1 kg. The physical/chemical property data was generated by the HGSystem database utility DATAPROP.

Input

```

* ===== SPILL standard input file =====

TITLE High-Pressure Gas Release of Carbon Monoxide

RESERVOIR          * RESERVOIR DATA
  TRES   = 20.85    * Storage/reservoir temperature (C).
  PRES   = 152.0    * Reservoir (absolute) pressure (atm).
                  *   If -1.0, SPILL uses the mixture saturation
                  *   pressure assuming all compounds are in liquid
                  *   state.
                  *   User MUST specify SPECIES keyword to use this
                  *   option.
  VRES   = 0.567    * Reservoir volume (m3).
  MRES   = 10.0     * Reservoir mass contents (tonnes).

GASDATA            * -----> [pollutant = dry pollutant (aerosol), water]
  WATERPOL= .0000   * -      water in pollutant (mole fraction)
  CPGAS   = 29.07   * J/MOLE/C specific heat of dry pollutant
  MMGAS   = 28.01   * KG/KMOLE molecular mass of dry pollutant
  HEATGR  = 19.99   * ..... heat group (used for HEGADAS link only)
  SPECIES = CO      *   , 1.00000   , 9
                  *   29.0697   , 62.6929   , 4650.78   , 132.920   , 34.5324
                  *   -6.15590   , 1.23480   , -1.58060   , -1.33330   , 28.0110
                  *   660.839

PIPE               * PIPE EXIT-PLANE (CHOKE-FRONT) CONDITIONS
  DEXIT   = 0.0127 * (Effective) release orifice diameter (m).

AMBIENT CONDITIONS * ATMOSPHERIC AMBIENT CONDITIONS
  AIRPRESS = 1.00  * Atmosphere pressure at release height (atm).
* Following parameters are used for calculation of heat transfer
* between ambient atmosphere and reservoir
  TATM    = 20.85  * Atmosphere temperature (degC)
  QSOLAR  = 200.0  * Solar heat flux (directly from the sun) (W/m2)
  EMISS   = 0.8    * Emissivity of reservoir surface (-)
  AREA    = 3.31   * Surface area over which heat flux occurs (m2)
                  * Setting AREA to 0.0 set heat transfer to 0.0

TERMINAT           * RESERVOIR RELEASE TERMINATION CRITERIA
                  *   SPILL ignores criteria set to -1.0
  TLST    = -1.0   * Last required elapsed time after release start (s)
  MLST    = 0.0001 * Last required reservoir mass content (tonnes)
  LLST    = -1.0   * Last required reservoir liquid molefraction (%)
  PLST    = -1.0   * Last required reservoir pressure (atm)
  RLST    = -1.0   * Last required reservoir mixture density (kg/m3)

```

Results

Output from SPILL				Version 1.1		Title: High-Pressure Gas Release of Carbon Monoxide				Date: 24/08/95 Time: 15:16:20			
Reservoir conditions					Atmosphere reference conditions					Release orifice properties			
res. init. temperature:		20.85 degC			ambient atmospheric pressure:		1.00 atm		release orifice diameter:				
1.27 cm													
res. init. pressure:		152.00 atm			ambient atm. temperature:		20.85 degC		vapour discharge				
coefficient: 1.00					emissivity factor of tank:		.80 (-)		liquid discharge				
reservoir volume (fixed):		.57 m3			heat transfer area:		3.31 m2		empty				
coefficient: .61					solar heat flux:		200.00 W/m2		empty				
res. init. mass content:		.10 ton			empty				empty				
empty					empty				empty				
empty					empty				empty				
empty					empty				empty				
TIME	MRES	DMDT	PRES	TRES	RRES	HRES	LRES	MMRES	RHOLIQ	QATM	PHASE	DMDTAV	
.0	.1	4.5	151.90	20.80	176.4	21.6	.00	28.01	.0	.200	vapour	4.5	
1.0	.1	4.3	142.75	15.63	168.7	16.2	.00	28.01	.0	.240	vapour	4.4	
2.0	.1	4.1	134.13	10.56	161.4	11.0	.00	28.01	.0	.282	vapour	4.3	
3.0	.1	3.8	126.11	5.61	154.4	5.8	.00	28.01	.0	.325	vapour	4.2	
4.0	.1	3.7	118.63	.80	147.8	.8	.00	28.01	.0	.368	vapour	4.1	
5.0	.1	3.5	111.66	-3.88	141.6	-4.0	.00	28.01	.0	.410	vapour	4.0	
6.0	.1	3.3	105.15	-8.44	135.6	-8.8	.00	28.01	.0	.451	vapour	3.9	
7.0	.1	3.1	99.07	-12.89	129.9	-13.4	.00	28.01	.0	.492	vapour	3.8	
8.0	.1	3.0	93.39	-17.21	124.6	-17.9	.00	28.01	.0	.531	vapour	3.7	
9.0	.1	2.8	88.08	-21.43	119.5	-22.2	.00	28.01	.0	.570	vapour	3.6	
10.0	.1	2.7	83.12	-25.54	114.6	-26.5	.00	28.01	.0	.608	vapour	3.5	
20.0	.0	1.7	48.09	-60.62	77.2	-62.9	.00	28.01	.0	.939	vapour	2.8	
30.0	.0	1.1	28.78	-88.82	53.3	-92.2	.00	28.01	.0	1.194	vapour	2.3	
40.0	.0	.7	17.95	-110.59	37.7	-114.8	.00	28.01	.0	1.390	vapour	2.0	
50.0	.0	.5	11.62	-127.12	27.2	-131.9	.00	28.01	.0	1.540	vapour	1.7	
60.0	.0	.3	7.81	-139.14	19.9	-144.4	.00	28.01	.0	1.649	vapour	1.5	
70.0	.0	.2	5.45	-146.96	14.7	-152.5	.00	28.01	.0	1.719	vapour	1.3	
80.0	.0	.2	3.94	-150.73	11.0	-156.4	.00	28.01	.0	1.753	vapour	1.2	
90.0	.0	.1	2.95	-150.40	8.2	-156.1	.00	28.01	.0	1.748	vapour	1.1	
100.0	.0	.1	2.28	-145.81	6.1	-151.3	.00	28.01	.0	1.704	vapour	1.0	
120.0	.0	.1	1.48	-122.99	3.4	-127.6	.00	28.01	.0	1.478	vapour	.8	
140.0	.0	.0	1.11	-79.28	2.0	-82.3	.00	28.01	.0	1.082	vapour	.7	
160.0	.0	.0	1.02	-26.32	1.4	-27.3	.00	28.01	.0	.599	vapour	.6	
166.7	.0	.0	1.01	-11.85	1.3	-12.3	.00	28.01	.0	.481	vapour	.6	

Interpretation:

TIME:	elapsed time since release start (s)	MRES:	reservoir total mass content (tonnes)
DMDT:	release mass flow rate (kg/s)	PRES:	reservoir absolute pressure (atm)
TRES:	reservoir temperature (degC)	RRES:	reservoir mixture density (kg/m3)
HRES:	reservoir total enthalpy (kJ/kg)	LRES:	reservoir molefraction liquid (%)
MMRES:	reservoir average molar mass (kg/kmole)	RHOLIQ:	reservoir liquid density (kg/m3)
QATM:	heat flux from ambient to reservoir (kW/m2)	PHASE:	reservoir fluid state (vapour/two-phase)
DMDTAV:	average release rate since release start (kg/s)		

Figure C-19:

Carbon Monoxide Release Rate at Various Initial Inventories

Figure C-20:

CO Reservoir Pressure at Various Initial Inventories

Figure C-21:

CO Reservoir Temperature at Various Initial Inventories

Problem 3: Pressurized Liquid Release of Chlorine

HGSystem computes the time-dependent mass outflow rate from a reservoir based on the initial mass inventory, system pressure, vessel size (volume) and ambient conditions. The vessel volume was based on the volume occupied by 1 ton of liquid anhydrous chlorine at saturation pressure. Note that the true saturation pressure at the given ambient temperature of 303 K is approximately 9.5 atmospheres and not $p_s=7$ atmospheres given in the handbook. This is important to observe since otherwise the vessel is continuously venting and the outflow will be pure vapor (as also predicted by HGSystem). The total surface area exposed to solar flux was assumed to be equal to the surface area of a sphere with the required volume capacity. The calculations were terminated when the total inventory remaining inside the reservoir was less than 0.1 kg. The physical/chemical property data was generated by the HGSystem database utility DATAPROP. Two of the coefficients generated for Wagner function describing the temperature dependence of the saturated vapor pressure required sign corrections.

Input

```

* ===== SPILL standard input file =====

TITLE Pressurized Liquid Release of Chlorine

RESERVOIR      * RESERVOIR DATA
  TRES   = 29.85 * Storage/reservoir temperature (C).
  PRES   = 9.506 * Reservoir (absolute) pressure (atm).
              * If -1.0, SPILL uses the mixture saturation
              * pressure assuming all compounds are in liquid
              * state.
              * User MUST specify SPECIES keyword to use this
              * option.
  VRES   = 0.638 * Reservoir volume (m3).
  MRES   = 0.908 * Reservoir mass contents (tonnes).

* ----- DATAPROP/AEROPLUME link file CL2 .APL -----
*
* AEROPLUME input data from program DATAPROP
*
* For each compound in pollutant (excluding water) data in SPECIES keyword are:
* - line 1: name of species, mole fraction in pollutant, aerosol class
* - line 2: specific heats of vapour and liquid (J/mole/C)
*           heat of vaporisation (J/mole)
*           critical temperature (K), critical pressure (atm)
* - line 3: vapour-pressure function fitting parameters (-)
*           molecular mass (g/mole), liquid density (kg/m**3)
* -----

TITLE DATAPROP standard input file (no HF)
*
GASDATA      * -----> [pollutant = dry pollutant (aerosol), water]
  WATERPOL= .0000 * - water in pollutant (mole fraction)
  CPGAS   = 33.74 * J/MOLE/C specific heat of dry pollutant
  MMGAS   = 70.91 * KG/KMOLE molecular mass of dry pollutant
  HEATGR  = 15.69 * ..... heat group (used for HEGADAS link only)
  SPECIES = CHLORINE , 1.00000 , 2
            33.7374 , 64.7764 , 19365.5 , 416.950 , 76.9011
            -5.76580 , 2.153100E-02, 1.318500E-02, -4.10970 , 70.9060
            1491.03

PIPE          * PIPE EXIT-PLANE (CHOKE-FRONT) CONDITIONS
  DEXIT      = 0.0076 * (Effective) release orifice diameter (m).

AMBIENT CONDITIONS * ATMOSPHERIC AMBIENT CONDITIONS
  AIRPRESS = 1.00 * Atmosphere pressure at release height (atm).
* Following parameters are used for calculation of heat transfer
* between ambient atmosphere and reservoir
  TATM     = 29.85 * Atmosphere temperature (degC)
  QSOLAR   = 200.0 * Solar heat flux (directly from the sun) (W/m2)
  EMISS    = 0.8   * Emissivity of reservoir surface (-)
  AREA     = 3.58  * Surface area over which heat flux occurs (m2)
              * Setting AREA to 0.0 set heat transfer to 0.0

TERMINAT      * RESERVOIR RELEASE TERMINATION CRITERIA
              * SPILL ignores criteria set to -1.0
  TLST     = -1.0 * Last required elapsed time after release start (s)
  MLST     = 0.0001 * Last required reservoir mass content (tonnes)
  LLST     = -1.0 * Last required reservoir liquid molefraction (%)
  PLST     = -1.0 * Last required reservoir pressure (atm)
  RLST     = -1.0 * Last required reservoir mixture density (kg/m3)

```

Results

Output from SPILL		Version 1.1		Title: DATAPROP standard input file (no HF)					Date: 25/08/95 Time: 14:02:32				
Reservoir conditions					Atmosphere reference conditions					Release orifice properties			
res. init. temperature:		29.85 degC			ambient atmospheric pressure:		1.00 atm		release orifice diameter:				
.76 cm													
res. init. pressure:		9.51 atm			ambient atm. temperature:		29.85 degC		vapour discharge				
coefficient: 1.00					emissivity factor of tank:		.80 (-)		liquid discharge				
reservoir volume (fixed):		.64 m3											
coefficient: .61													
res. init. mass content:		.55 ton			heat transfer area:		3.58 m2		empty				
empty					solar heat flux:		200.00 W/m2		empty				
empty					empty				empty				
empty					empty				empty				
TIME	MRES	DMDT	PRES	TRES	RRES	HRES	LRES	MMRES	RHOLIQ	QATM	PHASE	DMDTAV	
.0	.5	.4	9.51	29.85	855.2	-242.4	98.63	70.86	1491.0	.200	two phase	.4	
1.0	.5	.4	9.50	29.85	854.6	-242.4	98.62	70.86	1491.0	.200	two phase	.4	
2.0	.5	.4	9.50	29.85	853.9	-242.4	98.62	70.86	1491.0	.200	two phase	.4	
3.0	.5	.4	9.50	29.84	853.3	-242.4	98.62	70.86	1491.0	.200	two phase	.4	
4.0	.5	.4	9.50	29.84	852.7	-242.4	98.62	70.86	1491.0	.200	two phase	.4	
5.0	.5	.4	9.50	29.84	852.1	-242.4	98.61	70.86	1491.0	.200	two phase	.4	
6.0	.5	.4	9.50	29.84	851.4	-242.4	98.61	70.86	1491.0	.200	two phase	.4	
7.0	.5	.4	9.50	29.84	850.9	-242.4	98.61	70.86	1491.0	.200	two phase	.4	
8.0	.5	.4	9.50	29.83	850.2	-242.4	98.61	70.86	1491.0	.200	two phase	.4	
9.0	.5	.4	9.50	29.83	849.6	-242.4	98.61	70.86	1491.0	.200	two phase	.4	
10.0	.5	.4	9.49	29.83	849.0	-242.4	98.60	70.86	1491.0	.200	two phase	.4	
20.0	.5	.4	9.48	29.81	842.7	-242.3	98.58	70.86	1491.0	.200	two phase	.4	
30.0	.5	.4	9.47	29.79	836.5	-242.3	98.56	70.86	1491.0	.200	two phase	.4	
40.0	.5	.4	9.46	29.76	830.3	-242.3	98.54	70.86	1491.0	.201	two phase	.4	
50.0	.5	.4	9.45	29.74	824.2	-242.2	98.51	70.86	1491.0	.201	two phase	.4	
60.0	.5	.4	9.44	29.72	818.0	-242.2	98.49	70.86	1491.0	.201	two phase	.4	
70.0	.5	.4	9.43	29.70	811.8	-242.1	98.46	70.86	1491.0	.201	two phase	.4	
80.0	.5	.4	9.42	29.68	805.6	-242.1	98.44	70.86	1491.0	.201	two phase	.4	
90.0	.5	.4	9.41	29.66	799.5	-242.1	98.42	70.86	1491.0	.201	two phase	.4	
100.0	.5	.4	9.40	29.64	793.3	-242.0	98.39	70.86	1491.0	.201	two phase	.4	
120.0	.5	.4	9.37	29.59	781.0	-241.9	98.34	70.86	1491.0	.202	two phase	.4	
140.0	.5	.4	9.35	29.55	768.8	-241.8	98.29	70.86	1491.0	.202	two phase	.4	
160.0	.5	.4	9.33	29.51	756.5	-241.7	98.24	70.86	1491.0	.202	two phase	.4	
180.0	.5	.4	9.31	29.46	744.3	-241.6	98.18	70.86	1491.0	.203	two phase	.4	
200.0	.5	.4	9.29	29.42	732.1	-241.5	98.12	70.86	1491.0	.203	two phase	.4	
250.0	.4	.4	9.25	29.31	701.8	-241.2	97.97	70.85	1491.0	.204	two phase	.4	
300.0	.4	.4	9.20	29.19	671.5	-240.9	97.81	70.85	1491.0	.204	two phase	.4	
350.0	.4	.4	9.15	29.07	641.5	-240.6	97.64	70.85	1491.0	.205	two phase	.4	
400.0	.4	.4	9.11	28.96	611.5	-240.2	97.45	70.85	1491.0	.206	two phase	.4	
450.0	.4	.4	9.06	28.83	581.7	-239.8	97.24	70.84	1491.0	.207	two phase	.4	
500.0	.4	.4	9.02	28.71	552.0	-239.3	97.01	70.84	1491.0	.208	two phase	.4	
600.0	.3	.4	8.94	28.45	492.8	-238.2	96.47	70.83	1491.0	.210	two phase	.4	
700.0	.3	.4	8.85	28.17	434.3	-236.7	95.79	70.82	1491.0	.212	two phase	.4	
800.0	.2	.4	8.76	27.88	376.3	-234.7	94.93	70.81	1491.0	.214	two phase	.4	
900.0	.2	.4	8.67	27.56	318.8	-232.0	93.76	70.79	1491.0	.217	two phase	.4	
1000.0	.2	.4	8.58	27.22	261.8	-228.1	92.11	70.77	1491.0	.220	two phase	.4	
1100.0	.1	.4	8.48	26.85	205.3	-222.0	89.60	70.73	1491.0	.223	two phase	.4	
1200.0	.1	.4	8.38	26.43	149.4	-211.2	85.26	70.66	1491.0	.226	two phase	.4	
1300.0	.1	.4	8.26	25.93	94.1	-187.6	75.99	70.52	1491.0	.230	two phase	.4	
1400.0	.0	.3	8.13	25.33	39.4	-98.8	41.78	69.97	1491.0	.235	two phase	.4	
1500.0	.0	.1	3.98	-4.03	12.5	-1.9	.00	69.37	.0	.513	vapour	.4	
1600.0	.0	.0	1.76	9.74	5.3	4.7	.00	69.37	.0	.364	vapour	.3	
1700.0	.0	.0	1.01	42.01	2.7	20.3	.00	69.37	.0	.079	vapour	.3	
1714.9	.0	.0	1.00	45.49	2.7	22.0	.00	69.37	.0	.055	vapour	.3	

Interpretation:	
TIME:	elapsed time since release start (s)
DMDT:	release mass flow rate (kg/s)
TRES:	reservoir temperature (degC)
HRES:	reservoir total enthalpy (kJ/kg)
MMRES:	reservoir average molar mass (kg/kmole)
QATM:	heat flux from ambient to reservoir (kW/m2)
DMDTAV:	average release rate since release start (kg/s)
MRES:	reservoir total mass content (tonnes)
PRES:	reservoir absolute pressure (atm)
RRES:	reservoir mixture density (kg/m3)
LRES:	reservoir molefraction liquid (%)
RHOLIQ:	reservoir liquid density (kg/m3)
PHASE:	reservoir fluid state (vapour/two-phase)

Figure C-22:

Chlorine Mass Release Rate

Figure C-23:

Chlorine Reservoir Pressure

Figure C-24:

Chlorine Reservoir Temperature

Figure C-25:
Chlorine Vessel Mixture Density

Figure C-26:

Chlorine Vessel Liquid Mole Fraction

Problem 4: Liquid Release of Acetone

HGSystem computes the time-dependent mass outflow rate from a cylindrical tank with axis in the vertical direction. This application of HGSystem used the LPOOL model which includes the LSM90 modules for the time-dependent pool evaporation simulation. The 2-inch nozzle was assumed to be elevated 1-foot above the bottom of the tank and no consideration was given for frictional losses inside the pipe (i.e. the nozzle was modeled as a simple orifice). The vessel volume was based on the volume occupied by 40 tonnes of liquid anhydrous ammonia at saturation pressure. Note that the true saturation pressure at the given ambient temperature of 298 K is approximately 9.9 atmospheres and not $p_s=8.78$ atmospheres given in the handbook. This is important to observe since otherwise the vessel is continuously venting and the outflow will be pure vapor (as also predicted by HGSystem). The total surface area exposed to solar flux was assumed to be equal to the surface area of a sphere with the required volume capacity. The calculations were terminated when all inventory at a fluid level above the elevation of the nozzle was evacuated from the tank. The HGSystem database utility DATAPROP does not currently have the capability of generating the necessary physical/chemical data for acetone. The data was therefore manually entered as was based on tabulated values or well-established correlations. In particular, the viscosity was estimated using the Chapman-Enskog equation:

where η is the viscosity ($\text{g}/\text{cm}\cdot\text{s}$), M denotes the molecular weight (g/mole), R represents the ideal gas constant, T is the pool vapor film temperature (K), F is the hard-sphere diameter (angstroms), and W_v signifies the collision integral evaluated using the Leonard-Jones potential function (see Reid, Prausnitz, and Poling, 1986, *The Properties of Gases & Liquids*, 4th edition for details).

Computer runs were performed for a 2 m/s and 5 m/s wind speed. The input quantities which were varied between each run are shaded in the input text box description below.

Input

```

* ===== LPOOL standard input data file SKELETON.LPI =====
*
* To be used with LPOOL version 1.1 and later (using LSM90 model)
*
* -----
TITLE   Liquid Pool of Acetone

CONTROL
  MAXTIM   = 7200      * CONTROL PARAMETERS
  MINFILM   = 10       * Maximum simulation time (s)
  * DTLINK   = 10      * Minimum pool film thickness (mm!)
                        * Time step for pool data in link file (s)
                        *
GROUND
  GRCOMP    = 3        * GROUND AND DIKE SPECIFICATION
                        * Ground surface composition (1-7), default is 3.
                        *   1: Wet sand           2: Dry sand
                        *   3: Concrete          4: Insulated concrete
                        *   5: Steel            6: Insulated plastic
                        *   7: Water (has to be used for release on water)
  GRTEMP    = 29.85    * Ground surface temperature (deg C)
  DIKEPRES  = 1        * Dike presence indicator (0 or 1)
                        *   0: No dike           1: With dike
  DIKECOMP  = 3        * Dike composition (0-6), default is 0 (no dike).
                        *   1-6 as for ground surface composition.
  DIKEHEIGHT = 0.914   * Dike height (m)
  DIKERADIUS = 10.97   * Dike radius (m)
                        * DIKERADIUS must exceed RRADIUS.
                        *
SPILL
  SPTYPE    = 1        * SPILL RATE DATA
                        * Type of spill rate specification (0 or 1 or 2)
                        *   0: user-specified using SPILDATA parameter
                        *   1: Choked two-phase flow, calculated by LPOOL
                        *   2: Bernoulli liquid, calculated by LPOOL
  CD        = 0.6      * Discharge coefficient (-)
  * DURATION = 10000    * Spill duration (s)
                        * Use only if spill stops before liquid is
                        * exhausted, otherwise set larger than MAXTIM.
                        * LPOOL calculates the 'normal' spill duration.
                        * Not used if SPTYPE = 0.
                        * Will be set to MAXTIM+100 if not user-specified
  SPILDATA  = 0.0,0.0  * User-specified spill rate, duration (m3/s, s)
  SPILDATA  = 0.0,0.0  * User-specified spill rate, duration (m3/s, s)
  SPILDATA  = 0.0,0.0  * User-specified spill rate, duration (m3/s, s)
  SPILDATA  = 0.0,0.0  * User-specified spill rate, duration (m3/s, s)
  SPILDATA  = 0.0,0.0  * User-specified spill rate, duration (m3/s, s)
                        * Up to 5 spill rate/duration pairs.
                        *
RESERVOIR
  TRES      = 29.85    * RESERVOIR (TANK) DATA
                        * Shape is assumed to be a vertical cylinder.
  PRES      = 1.37     * Reservoir temperature (deg C).
                        * Reservoir pressure (atm).
                        * Set to PATM for vented reservoir.
  RRADIUS   = 3.81     * Reservoir radius (m)
  RFLHEIGHT = 7.62     * Initial fluid level (height) in reservoir (m).
  DEXIT     = 0.051    * Equivalent diameter of reservoir orifice (m).
  ZEXIT     = 0.3048   * Elevation (height) of orifice (m).
                        * RFLHEIGHT and ZEXIT with respect to ground level.
                        * N.B. RFLHEIGHT must be larger than ZEXIT!
                        *
AMBIENT
  TATM      = 29.85    * AMBIENT ATMOSPHERE DATA
                        * Ambient temperature (deg C)
  PATM      = 1.0      * Ambient pressure (atm)
  UATM      = 2.0      * Wind speed (m/s) at 10 m height.
                        * For air/pool heat transfer.
  RHPERC    = 50.0     * Relative ambient humidity (%).
                        * For aerosol calculation and HEGADAS-T link file
  CLCOVER   = 0.0      * Fraction of sky covered by clouds (-)
  SPSTART   = 12.0     * Spill starting time (24 hour clock)
  SUNRISE   = 6.0      * Sun rise (24 hour clock)

```

SUNSET	=	18.0	* Sun set (24 hour clock)
			* These three numbers should be DECIMAL using
			* a 24 hour clock.
			* Example: 7:30 am is 7.5
			* 7:15 pm is 19.25
			*
FLASH			* FLASH DATA
FLASHFRAC	=	0.0	* User-specified flash fraction (-).
AEROSFRAC	=	0.0	* User-specified aerosol fraction (-).
			*
GASDATA			* RESERVOIR FLUID DATA
WATERPOL	=	0.0	* Water mole fraction in fluid (-)
CPGAS	=	22.35	* Specific heat of fluid without water (J/mole/K)
			* Only used by HEGADAS, not by LPOOL itself!
MMGAS	=	58.08	* Molecular mass of dry pollutant (kg/kmole)
			* Only used by HEGADAS, not by LPOOL itself!
HEATGR	=	34.88	* Heat group (.....)
			* Only used by HEGADAS, not by LPOOL itself!
SPECIES	=	ACETONE , 1.0000 , 8	
		75.38 , 126.9, 2.9679E+04, 508 , 46.38	
		-7.45514 , 1.202, -2.43926 , -3.35590 , 58.08 , 791.0	
		329.3 , 7.62E-06	
			* For every compound in the reservoir fluid
			* (except water) a SPECIES keyword must be
			* specified. Sum of mole fractions must be 1.0
			* (incl. water)
			* Use of DATAPROP to generate this data is strongly
			* recommended.

Results

LIQUID SPILLS MODEL

Aug 25 1995 17:07:34

<<<< HGSYSTEM VERSION (LPOOL) >>>>

Computer Model : LSM90

Case Description: Liquid Pool of Acetone

Engineer : -

Output File Name: ACETONE .LPT

Time	Total Vapor Rate	Flash Rate	Aerosol Rate	Evap. Rate	Cumulat Mass Out	Mass in Pool	Pool Area	Pool Temp
HH:MM:SS	(Kg/s)	(Kg/s)	(Kg/s)	(Kg/s)	(Kg)	(Kg)	(M2)	(K)
-----	-----	-----	-----	-----	-----	-----	-----	-----
00:00:00	.000	.000	.000	.000	.0	.0	.0	303.0
00:00:01	.004	.000	.000	.004	15.0	15.0	1.5	303.0
00:00:02	.014	.000	.000	.014	29.9	29.9	3.8	302.9
00:00:03	.025	.000	.000	.025	44.9	44.8	5.7	302.9
00:00:04	.034	.000	.000	.034	59.8	59.8	7.6	302.8
00:00:05	.043	.000	.000	.043	74.8	74.7	9.4	302.8
00:00:06	.052	.000	.000	.052	89.8	89.6	11.3	302.7
00:00:07	.060	.000	.000	.060	104.7	104.5	13.2	302.7
00:00:08	.069	.000	.000	.069	119.7	119.4	15.1	302.6
00:00:09	.077	.000	.000	.077	134.7	134.3	17.0	302.6
00:00:10	.086	.000	.000	.086	149.6	149.1	18.9	302.6
00:00:15	.110	.000	.000	.110	224.4	223.4	28.2	302.4
00:00:20	.150	.000	.000	.150	299.2	297.4	37.6	302.2
00:00:25	.189	.000	.000	.189	374.0	371.3	46.9	302.1
00:00:30	.227	.000	.000	.227	448.8	444.9	56.2	301.9
00:00:35	.264	.000	.000	.264	523.5	518.4	65.5	301.8
00:00:40	.300	.000	.000	.300	598.3	591.6	74.8	301.6
00:00:45	.335	.000	.000	.335	673.1	664.7	84.1	301.5
00:00:50	.370	.000	.000	.370	747.8	737.6	93.3	301.4
00:00:55	.404	.000	.000	.404	822.6	810.3	102.5	301.3
00:01:00	.437	.000	.000	.437	897.3	882.9	111.7	301.1
00:01:15	.504	.000	.000	.504	1121.5	1099.5	139.0	300.8
00:01:30	.600	.000	.000	.600	1345.6	1314.6	166.2	300.5
00:01:45	.691	.000	.000	.691	1569.7	1528.4	193.3	300.3
00:02:00	.780	.000	.000	.780	1793.7	1740.7	220.3	300.0
00:02:15	.866	.000	.000	.866	2017.6	1951.6	246.8	299.8
00:02:30	.951	.000	.000	.951	2241.5	2161.3	273.8	299.6
00:02:45	1.031	.000	.000	1.031	2465.4	2369.6	300.1	299.4
00:03:00	1.111	.000	.000	1.111	2689.2	2576.8	326.2	299.2
00:04:00	1.138	.000	.000	1.138	3583.7	3403.1	332.5	298.6
00:05:00	1.116	.000	.000	1.116	4477.4	4229.8	332.5	298.3

LIQUID SPILLS MODEL

Aug 25 1995 17:07:34

<<<< HGSYSTEM VERSION (LPOOL) >>>>

Computer Model : LSM90

Case Description: Liquid Pool of Acetone

Engineer : -

Output File Name: ACETONE .LPT

Time HH:MM:SS	Total Vapor Rate (Kg/s)	Flash Rate (Kg/s)	Aerosol Rate (Kg/s)	Evap. Rate (Kg/s)	Cumulat Mass Out (Kg)	Mass in Pool (Kg)	Pool Area (M2)	Pool Temp (K)
00:06:00	1.102	.000	.000	1.102	5370.2	5056.4	332.5	298.0
00:07:00	1.093	.000	.000	1.093	6262.1	5882.7	332.5	297.9
00:08:00	1.087	.000	.000	1.087	7153.0	6708.4	332.5	297.8
00:09:00	1.082	.000	.000	1.082	8043.1	7533.6	332.5	297.7
00:10:00	1.078	.000	.000	1.078	8932.3	8358.0	332.5	297.6
00:11:00	1.075	.000	.000	1.075	9820.5	9181.8	332.5	297.5
00:12:00	1.073	.000	.000	1.073	10707.8	10004.8	332.5	297.5
00:13:00	1.070	.000	.000	1.070	11594.3	10827.0	332.5	297.5
00:14:00	1.068	.000	.000	1.068	12479.8	11648.4	332.5	297.4
00:15:00	1.067	.000	.000	1.067	13364.5	12469.1	332.5	297.4
00:16:00	1.065	.000	.000	1.065	14248.2	13288.9	332.5	297.3
00:17:00	1.063	.000	.000	1.063	15131.0	14107.9	332.5	297.3
00:18:00	1.062	.000	.000	1.062	16012.9	14926.1	332.5	297.3
00:19:00	1.061	.000	.000	1.061	16893.9	15743.4	332.5	297.3
00:20:00	1.060	.000	.000	1.060	17774.0	16559.9	332.5	297.2
00:21:00	1.059	.000	.000	1.059	18653.2	17375.6	332.5	297.2
00:22:00	1.058	.000	.000	1.058	19531.5	18190.4	332.5	297.2
00:23:00	1.057	.000	.000	1.057	20408.8	19004.3	332.5	297.2
00:24:00	1.056	.000	.000	1.056	21285.3	19817.5	332.5	297.2
00:25:00	1.055	.000	.000	1.055	22160.9	20629.7	332.5	297.1
00:26:00	1.055	.000	.000	1.055	23035.7	21441.2	332.5	297.1
00:27:00	1.054	.000	.000	1.054	23909.5	22251.8	332.5	297.1
00:28:00	1.053	.000	.000	1.053	24782.4	23061.5	332.5	297.1
00:29:00	1.052	.000	.000	1.052	25654.4	23870.3	332.5	297.1
00:30:00	1.052	.000	.000	1.052	26525.5	24678.3	332.5	297.1
00:35:00	1.050	.000	.000	1.050	30867.3	28705.2	332.5	297.0
00:40:00	1.047	.000	.000	1.047	35186.5	32710.2	332.5	297.0
00:45:00	1.045	.000	.000	1.045	39483.2	36693.4	332.5	296.9
00:50:00	1.043	.000	.000	1.043	43757.3	40654.7	332.5	296.9
00:55:00	1.041	.000	.000	1.041	48008.6	44593.8	332.5	296.8
01:00:00	1.039	.000	.000	1.039	52237.2	48510.9	332.5	296.8

LIQUID SPILLS MODEL

Aug 25 1995 17:07:34

<<<< HGSYSTEM VERSION (LPOOL) >>>>

Computer Model : LSM90

Case Description: Liquid Pool of Acetone

Engineer : -

Output File Name: ACETONE .LPT

Time	Total Vapor Rate HH:MM:SS (Kg/s)	Flash Rate (Kg/s)	Aerosol Rate (Kg/s)	Evap. Rate (Kg/s)	Cumulat Mass Out (Kg)	Mass in Pool (Kg)	Pool Area (M2)	Pool Temp (K)
-----	-----	-----	-----	-----	-----	-----	-----	-----
01:30:00	1.032	.000	.000	1.032	77137.7	71553.9	332.5	296.5
02:00:00	1.020	.000	.000	1.020	101223.6	93803.2	332.5	296.2

Figure C-27:

Acetone Pool Evaporation Rate

Figure C-28:

Acetone Pool Temperature

Figure C-29:

Acetone Pool Area

Figure C-30:

Acetone Pool Mass Inventory

TScreen

Test Problem Evaluations

Introduction

The TScreen computer program for screening toxic air pollutant concentrations was used to evaluate the following scenarios, as described in Section 6.2 of this report (taken from Hanna and Strimaitis (1989)):

Problem 1(a):	Pressurized Liquid Release of Anhydrous Ammonia (Tank orifice release)
Problem 1(b):	Pressurized Liquid Release of Anhydrous Ammonia (Pipe release)
Problem 2:	High-Pressure Gas Release of Carbon Monoxide
Problem 3:	Pressurized Liquid Release of Chlorine
Problem 4:	Liquid Spill of Acetone

Each release scenario has been analyzed by the computer model with the associated input and output presented. Where appropriate, limitations or concerns encountered when applying the model to these scenarios as well as any exceptional capabilities encountered in the process are brought to the reader's attention.

The results of each scenario test case begins with a series of text boxes containing input data for the analysis. Shaded information in each of these blocks indicate intermediate source-term values calculated by the program. Final source-term estimates are summarized in the shaded text columns immediately following the input text boxes and preceding the results of the dispersion analysis.

Problem1(a): Pressurized Liquid Release of Anhydrous Ammonia (nozzle failure)

Results

```
File      Initial Form of Release  Chemical Database  Quit
  Initial Form of Release
  Particulate Matter Release Type
  Gaseous Release Type
  Liquid Release Type
  Su      Liquid Release Type      Workbook Scenario
  Surface Impoundments (Lagoons)      - 3.1
  2-Phase Saturated Liquid from Pressurized Storage - 3.2,3.3
  2-Phase Release Duration      ressured Storage - 3.4,3.5
  High Vol Continuous      - 3.6,3.7
  Low Vol Instantaneous      - 3.8,3.9

<F1>Help      <--><-->Scroll Vertical Menus      <--><-->Scroll Horizontal Menu
<Enter>/Letter=Select Menu Item      <F9>Exit Current Menu      <Esc>Exit All Menus
```

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Pressurized Liquid Release of Anhydrous Ammonia (Tank)
SOURCE OF LEAK

Area (Ao) of Hole or Opening -> 11.4 cm²
Enter P for Pipe - T for Tank -> T

DISCHARGE TEMPERATURE

Discharge Temperature (T2) -> 239.72 °K

Ambient Pressure (Pa)	-> 101325	Pa
Boiling Point Temperature (Tb)	-> 239.72	°K
Latent Heat of Vaporization (Lvap)	-> 13.672E5	J/kg
Molecular Weight (Mw)	-> 17.030	kg/kmol

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 2 of 4

VAPOR FRACTION AFTER DEPRESSURIZATION

Vapor Fraction after Depressurization (X2) -> 0.191396

Liquid Heat Capacity (Cpl)	-> 4.49E+03	J/kg °K
Reservoir Temperature (Tl)	-> 298	°K

EMISSION RATE

Emission Rate (Qm) -> 21195.48 g/s

Reservoir Pressure (Pl)	-> 8.9E+05	Pa
Liquid Heat Capacity at Tl (Cpl)	-> 4.49E+03	J/kg °K
Contaminant Liquid Density (fl)	-> 608.76	kg/cubic m

Vapor Heat Capacity (Cp)	-> 2093.19	J/kg °K
--------------------------	------------	---------

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 3 of 4

DISCHARGE DENSITY

Discharge Density (ρ_2) -> 4.496581 kg/cubic m

DENSITY OF AIR

Density of Air (ρ_{air}) -> 1.20209 kg/cubic m

Ambient Temperature (T_a) -> 293 °K

Buoyancy is Negative

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2
SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET

Does the release result in a vertically
directed jet (Y/N) -> N

TIME

Release Duration (T_d) -> 31.45325 min

Total Amount of Material Released (Q) -> 40000 kg

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS

Relative Humidity (R_h) -> 80 %

Desired Averaging Time for the Calculation
of Concentrations -> 10 min

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE

Enter the distance from the nearest edge of
the source to the plant fenceline -> 100 m

RECEPTOR LOCATIONS

Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

<F2> Edit <F9> Previous Screen <F10> Run Model <Esc> Abort

10-03-95
08:19:01

*** B&M MODEL RUN ***

Pressurized Liquid Release of Anhydrous Ammonia (Tank)

INPUTS:

AMBIENT PRESSURE (ATM) = 1.000
AMBIENT TEMP (K) = 293.0
AVERAGING TIME (MIN) = 10.00
BOILING PT TEMP (K) = 239.7
DURATION (S) = 1887.
EMISSION RATE (KG/S) = 21.20
EXIT TEMP (K) = 239.7
GAS HEAT CAPACITY (J/KG K) = 2093.
LATENT HEAT (J/KG) = .1367E+07
MASS (KG) = .4000E+05
MOL. WEIGHT (G/G-MOLE) = 17.03
RELATIVE HUMIDITY (%) = 80.00
VAPOR FRACTION = .1914

*** SUMMARY OF B&M MODEL RESULTS ***

MAX CONC (UG/M**3)	MAX CONC (PPM)	DIST TO MAX (M)	WIND SPEED (M/S)
.7762E+07	.1096E+05	100.	1.

** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

*** B&M DISTANCES ***

DIST (M)	CONC (UG/M**3)	CONC (PPM)	WIND SPEED (M/S)
100.	.7762E+07	.1096E+05	1.
200.	.7762E+07	.1096E+05	1.
300.	.7762E+07	.1096E+05	1.
400.	.7762E+07	.1096E+05	1.
500.	.7762E+07	.1096E+05	1.
600.	.6491E+07	9164.	1.
700.	.6491E+07	9164.	1.
800.	.5366E+07	7575.	2.
900.	.4356E+07	6149.	2.
1000.	.3615E+07	5103.	2.
1100.	.2979E+07	4205.	2.
1200.	.2399E+07	3387.	2.
1300.	.1966E+07	2775.	2.
1400.	.1635E+07	2308.	2.
1500.	.1377E+07	1944.	2.
1600.	.1029E+07	1453.	5.
1700.	.9340E+06	1319.	5.
1900.	.7826E+06	1105.	5.
2100.	.6765E+06	955.0	5.
2300.	.5926E+06	836.6	5.
2500.	.5249E+06	741.0	5.
2700.	.4702E+06	663.7	3.
2900.	.4238E+06	598.3	4.
3100.	.3760E+06	530.8	4.
3300.	.3187E+06	449.8	4.
3600.	.2531E+06	357.3	4.
3900.	.2048E+06	289.1	4.
4200.	.1857E+06	262.1	1.
4500.	.1717E+06	242.3	1.
5000.	.1523E+06	215.0	1.

CALCULATED VALUES:

DENSITY OF DEPRESSURIZED CONTAMINANT (KG/M**3) = 1.408
DENSITY OF AMBIENT AIR (KG/M**3) = 1.197
MOLE FRACTION = .9164E-01
MIN DIST INST (M) = .6291E+05
MAX DIST CNST (M) = .1510E+05

***** NOTES & DEFINITIONS *****

- (a) "inst" refers to an instantaneous release (Section 3.6 of B-M Workbook)
(b) "cnst" refers to a continuous release (Section 3.6 of B-M Workbook)
(c) "MIN DIST INST" is the minimum distance downwind at which the release

may be treated as instantaneous
(d) "MAX DIST CNST" is the maximum distance downwind at which the release
may be treated as continuous

*** END OF B&M OUTPUT ***

Problem 1(b): Pressurized Liquid Release of Anhydrous Ammonia (pipe release)

Results

File	Initial Form of Release	Chemical Database	Quit
	Initial Form of Release		
	Particulate Matter Release Type		
	Gaseous Release Type		
	Liquid Release Type		
	Surface Impoundments (Lagoons)	Workbook Scenario	
	2-Phase Saturated Liquid from Pressurized Storage	- 3.1	
	2-Phase Release Duration	- 3.2,3.3	
	High Vol Continuous	- 3.4,3.5	
	Low Vol Instantaneous	- 3.6,3.7	
		- 3.8,3.9	

<F1>Help <=>/<=>Scroll Vertical Menus <->/<->Scroll Horizontal Menu
<Enter>/Letter=Select Menu Item <F9>Exit Current Menu <Esc>Exit All Menus

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Pressurized Liquid Release of Anhydrous Ammonia (Pipe)
SOURCE OF LEAK

Area (Ao) of Hole or Opening -> 14.52 cm²
Enter P for Pipe - T for Tank -> P

Pipe Diameter (Dp) -> 3.81E-02 m
Pipe Length (Lp) -> 3.81 m

DISCHARGE TEMPERATURE

Discharge Temperature (T2) -> 239.72 °K

Ambient Pressure (Pa) -> 101325 Pa
Boiling Point Temperature (Tb) -> 239.72 °K
Latent Heat of Vaporization (Lvap) -> 13.672E5 J/kg
Molecular Weight (Mw) -> 17.030 kg/kmol

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 2 of 4

VAPOR FRACTION AFTER DEPRESSURIZATION

Vapor Fraction after Depressurization (X2) -> 0.191396

Liquid Heat Capacity (Cpl) -> 4.49E+03 J/kg °K
Reservoir Temperature (T1) -> 298 °K

EMISSION RATE

Emission Rate (Qm) -> 8300.146 g/s

Reservoir Pressure (P1) -> 8.9E+05 Pa
Liquid Heat Capacity at T1 (Cpl) -> 4.49E+03 J/kg °K
Contaminant Liquid Density (f1) -> 608.76 kg/cubic m

Vapor Heat Capacity (Cp) -> 2093.19 J/kg °K

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 3 of 4

DISCHARGE DENSITY

Discharge Density (ρ_2) -> 4.496581 kg/cubic m

DENSITY OF AIR

Density of Air (ρ_{air}) -> 1.20209 kg/cubic m

Ambient Temperature (Ta) -> 293 °K

Buoyancy is Negative

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET

Does the release result in a vertically
directed jet (Y/N) -> N

TIME

Release Duration (Td) -> 80.31987 min

Total Amount of Material Released (Q) -> 40000 kg

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS

Relative Humidity (Rh) -> 80 %

Desired Averaging Time for the Calculation
of Concentrations -> 10 min

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE

Enter the distance from the nearest edge of
the source to the plant fenceline -> 100 m

RECEPTOR LOCATIONS

Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

<F2> Edit <F9> Previous Screen <F10> Run Model <Esc> Abort

08-15-95
16:01:02

*** B&M MODEL RUN ***

Pressurized Liquid Release of Anhydrous Ammonia (Pipe)

INPUTS:

AMBIENT PRESSURE (ATM) = 1.000
AMBIENT TEMP (K) = 293.0
AVERAGING TIME (MIN) = 10.00
BOILING PT TEMP (K) = 239.7
DURATION (S) = 4819.
EMISSION RATE (KG/S) = 8.300
EXIT TEMP (K) = 239.7
GAS HEAT CAPACITY (J/KG K) = 2093.
LATENT HEAT (J/KG) = .1367E+07
MASS (KG) = .4000E+05
MOL. WEIGHT (G/G-MOLE) = 17.03
RELATIVE HUMIDITY (%) = 80.00
VAPOR FRACTION = .1914

*** SUMMARY OF B&M MODEL RESULTS ***

MAX CONC (UG/M**3)	MAX CONC (PPM)	DIST TO MAX (M)	WIND SPEED (M/S)
.7762E+07	.1096E+05	100.	1.

** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

*** B&M DISTANCES ***

DIST (M)	CONC (UG/M**3)	CONC (PPM)	WIND SPEED (M/S)
100.	.7762E+07	.1096E+05	1.
200.	.7762E+07	.1096E+05	1.
300.	.7762E+07	.1096E+05	1.
400.	.6491E+07	9164.	1.
500.	.6491E+07	9164.	1.
600.	.6491E+07	9164.	1.
700.	.5475E+07	7729.	1.
800.	.4322E+07	6102.	1.
900.	.3509E+07	4953.	1.
1000.	.2786E+07	3933.	1.
1100.	.2198E+07	3103.	1.
1200.	.1770E+07	2499.	1.
1300.	.1451E+07	2048.	1.
1400.	.1232E+07	1740.	1.
1500.	.1091E+07	1540.	1.
1600.	.9728E+06	1373.	1.
1700.	.8738E+06	1234.	1.
1900.	.7176E+06	1013.	1.
2100.	.3998E+06	564.4	1.
2300.	.3591E+06	507.0	1.
2500.	.3328E+06	469.8	1.
2700.	.3068E+06	433.1	1.
2900.	.2829E+06	399.3	1.
3100.	.2622E+06	370.2	1.
3300.	.2408E+06	339.9	1.
3600.	.2025E+06	285.9	1.
3900.	.1727E+06	243.8	1.
4200.	.1490E+06	210.4	1.
4500.	.1299E+06	183.4	1.
5000.	.9935E+05	140.3	1.

CALCULATED VALUES:

DENSITY OF DEPRESSURIZED CONTAMINANT (KG/M**3) = 1.408
DENSITY OF AMBIENT AIR (KG/M**3) = 1.197
MOLE FRACTION = .9164E-01
MIN DIST INST (M) = .1606E+06
MAX DIST CNST (M) = .3855E+05

***** NOTES & DEFINITIONS *****

- (a) "inst" refers to an instantaneous release (Section 3.6 of B-M Workbook)
(b) "cnst" refers to a continuous release (Section 3.6 of B-M Workbook)
(c) "MIN DIST INST" is the minimum distance downwind at which the release

may be treated as instantaneous
(d) "MAX DIST CNST" is the maximum distance downwind at which the release
may be treated as continuous

*** END OF B&M OUTPUT ***

Problem 2: High-Pressurize Gas Release of Carbon Monoxide

Results

File	Initial Form of Release	Chemical Database	Quit
	Initial Form of Release		
	Particulate Matter Release Type		
	Gaseous Release Type		
Li		Gaseous Release Type	Workbook Scenario
Su			
	Flared Stack Emissions		- 2.1
	Stacks, Vents, Conventional Point Sources		- 2.2
	Leaks from Reservoir		- 2.3, 2.4
	Leaks from a Pipe Attached to Reservoir		- 2.5, 2.6
	Multiple Fugitive Sources		- 2.7
	Land Tr Release Duration		- 2.8
	Municip Continuous		- 2.9
	Pestici Instantaneous	s	- 2.10
	Dischar	ngs	- 2.11

<F1>Help <-->Scroll Vertical Menus <-->Scroll Horizontal Menu
<Enter>/Letter=Select Menu Item <F9>Exit Current Menu <Esc>Exit All Menus

Continuous Leaks from Reservoir - Scenario 2.3

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
High Pressure Gas Release of Carbon Monoxide

SOURCE OF LEAK

Area (Ao) of Hole or Opening -> 1.27 cm²
Enter P for Pipe - T for tank -> T

FLOW CHARACTERISTIC

Critical Pressure (P*) -> 8145863 Pa

Gas Heat Capacity (Cp) -> 1046.7	J/kg °K
Reservoir Pressure (P1) -> 1.54E+7	Pa
Molecular Weight (Mw) -> 28.0	kg/kmol

Flow Characteristic -> Choked

Ambient Pressure (Pa) -> 101325	Pa
---------------------------------	----

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Leaks from Reservoir - Scenario 2.3

SOURCE PARAMETERS - Page 2 of 4

TEMPERATURES

Gas Temperature (T*) at Critical Pressure -> 245.4064 °K

Reservoir Temperature (T1) -> 294	°K
-----------------------------------	----

Critical Temperature (Tc) -> 133 °K

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Leaks from Reservoir - Scenario 2.3

SOURCE PARAMETERS - Page 3 of 4

EMISSION RATE

Emission Rate (Qm) -> 3396.102 g/s

Density at Reservoir Conditions (f1) -> 176.41 kg/cubic m

DISCHARGE CHARACTERISTICS

Discharge Temperature (T2) -> 252.6954 °K

Discharge Density (f2) -> 1.350415 kg/cubic m

Density of Air (fair) -> 1.198001 kg/cubic m

Ambient Temperature (Ta) -> 294 °K

Buoyancy is Negative

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Leaks from Reservoir - Scenario 2.3

SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET

Does the release result in a vertically
directed jet (Y/N) -> N

TIME

Release Duration (Td) -> 4.907587 min

Total Amount of Material Released (Q) -> 1000 kg

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Leaks from Reservoir - Scenario 2.3

Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS

Relative Humidity (Rh) -> 80 %

Desired Averaging Time for the Calculation
of Concentrations -> 10 min

Pollutant Boiling Point Temperature (Tb) -> 81.7 °K

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE

Enter the distance from the nearest edge of
the source to the plant fenceline -> 100 m

RECEPTOR LOCATIONS

Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

<F2> Edit <F9> Previous Screen <F10> Run Model <Esc> Abort

08-15-95
17:13:57

*** B&M MODEL RUN ***

High Pressure Gas Release of Carbon Monoxide

INPUTS:

AMBIENT PRESSURE (ATM) = 1.000
AMBIENT TEMP (K) = 294.0
AVERAGING TIME (MIN) = 10.00
BOILING PT TEMP (K) = 81.70
DURATION (S) = 294.5
EMISSION RATE (KG/S) = 3.396
EXIT TEMP (K) = 252.7
MASS (KG) = 1000.
MOL. WEIGHT (G/G-MOLE) = 28.00
RELATIVE HUMIDITY (%) = 80.00
VAPOR FRACTION = 1.000

*** SUMMARY OF B&M MODEL RESULTS ***

MAX CONC (UG/M**3)	MAX CONC (PPM)	DIST TO MAX (M)	WIND SPEED (M/S)
.1083E+09	.9334E+05	100.	1.

** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

*** B&M DISTANCES ***

DIST (M)	CONC (UG/M**3)	CONC (PPM)	WIND SPEED (M/S)
100.	.1083E+09	.9334E+05	1.
200.	.2679E+08	.2308E+05	2.
300.	.1142E+08	9838.	2.
400.	.7581E+07	6531.	2.
500.	.4626E+07	3986.	2.
600.	.2842E+07	2449.	2.
700.	.2093E+07	1803.	1.
800.	.1776E+07	1530.	1.
900.	.1537E+07	1324.	1.
1000.	.1775E+07	1529.	2.
1100.	.1399E+07	1205.	2.
1200.	.2159E+07	1860.	1.
1300.	.1768E+07	1523.	1.
1400.	.1469E+07	1265.	1.
1500.	.1236E+07	1065.	1.
1600.	.1052E+07	906.2	1.
1700.	.9039E+06	778.7	1.
1900.	.6845E+06	589.7	1.
2100.	.5465E+06	470.9	4.
2300.	.4354E+06	375.1	4.
2500.	.3535E+06	304.5	4.
2700.	.2916E+06	251.2	4.
2900.	.2439E+06	210.1	4.
3100.	.2064E+06	177.8	4.
3300.	.1766E+06	152.1	4.
3600.	.1420E+06	122.4	4.
3900.	.1163E+06	100.2	4.
4200.	.9662E+05	83.24	4.
4500.	.8131E+05	70.05	4.
5000.	.6248E+05	53.83	4.

CALCULATED VALUES:

DENSITY OF DEPRESSURIZED CONTAMINANT (KG/M**3) = 1.351
DENSITY OF AMBIENT AIR (KG/M**3) = 1.192
MOLE FRACTION = 1.000
MIN DIST INST (M) = 9815.
MAX DIST CNST (M) = 2356.

***** NOTES & DEFINITIONS *****

- (a) "inst" refers to an instantaneous release (Section 3.6 of B-M Workbook)
(b) "cnst" refers to a continuous release (Section 3.6 of B-M Workbook)
(c) "MIN DIST INST" is the minimum distance downwind at which the release may be treated as instantaneous
(d) "MAX DIST CNST" is the maximum distance downwind at which the release

may be treated as continuous

*** END OF B&M OUTPUT ***

Problem 3: Pressurized Liquid Release of Chlorine

Results

```
File      Initial Form of Release  Chemical Database  Quit
          Initial Form of Release
          Particulate Matter Release Type
          Gaseous Release Type
          Liquid Release Type
          Su      Liquid Release Type
                Surface Impoundments (Lagoons)      Workbook Scenario
                2-Phase Saturated Liquid from Pressurized Storage - 3.1
                2-Phase      Release Duration      ressured Storage - 3.2,3.3
                High Vol Continuous                  - 3.4,3.5
                Low Vol Instantaneous                 - 3.6,3.7
                - 3.8,3.9

<F1>Help      <>/<>Scroll Vertical Menus      <->/<->Scroll Horizontal Menu
<Enter>/Letter=Select Menu Item      <F9>Exit Current Menu      <Esc>Exit All Menus
```

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:

Pressurized Release of Liquid Chlorine

SOURCE OF LEAK

Area (Ao) of Hole or Opening -> 0.456 cm²
Enter P for Pipe - T for Tank -> T

DISCHARGE TEMPERATURE

Discharge Temperature (T2) -> 239 °K

Ambient Pressure (Pa) -> 101325 Pa
Boiling Point Temperature (Tb) -> 239 °K
Latent Heat of Vaporization (Lvap) -> 2.88E+05 J/kg
Molecular Weight (Mw) -> 71.0 kg/kmol

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 2 of 4

VAPOR FRACTION AFTER DEPRESSURIZATION

Vapor Fraction after Depressurization (X2) -> 0.206667

Liquid Heat Capacity (Cpl) -> 930 J/kg °K
Reservoir Temperature (T1) -> 303 °K

EMISSION RATE

Emission Rate (Qm) -> 1149.677 g/s

Reservoir Pressure (P1) -> 7.11E+05 Pa
Liquid Heat Capacity at T1 (Cpl) -> 930 J/kg °K
Contaminant Liquid Density (f1) -> 1423 kg/cubic m

Vapor Heat Capacity (Cp) -> 480 J/kg °K

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 3 of 4

DISCHARGE DENSITY

Discharge Density (ρ_2) -> 17.34902 kg/cubic m

DENSITY OF AIR

Density of Air (ρ_{air}) -> 1.162417 kg/cubic m

Ambient Temperature (T_a) -> 303 °K

Buoyancy is Negative

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET

Does the release result in a vertically
directed jet (Y/N) -> N

TIME

Release Duration (T_d) -> 13.16312 min

Total Amount of Material Released (Q) -> 908 kg

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS

Relative Humidity (R_h) -> 80 %

Desired Averaging Time for the Calculation
of Concentrations -> 10 min

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE

Enter the distance from the nearest edge of
the source to the plant fenceline -> 100 m

RECEPTOR LOCATIONS

Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

<F2> Edit <F9> Previous Screen <F10> Run Model <Esc> Abort

07-11-95
15:01:23

*** B&M MODEL RUN ***

Pressurized Release of Liquid Chlorine

INPUTS:

AMBIENT PRESSURE (ATM) = 1.000
AMBIENT TEMP (K) = 303.0
AVERAGING TIME (MIN) = 10.00
BOILING PT TEMP (K) = 239.0
DURATION (S) = 789.8
EMISSION RATE (KG/S) = 1.150
EXIT TEMP (K) = 239.0
GAS HEAT CAPACITY (J/KG K) = 480.0
LATENT HEAT (J/KG) = .2880E+06
MASS (KG) = 908.0
MOL. WEIGHT (G/G-MOLE) = 71.00
RELATIVE HUMIDITY (%) = 80.00
VAPOR FRACTION = .2067

*** SUMMARY OF B&M MODEL RESULTS ***

MAX CONC (UG/M**3)	MAX CONC (PPM)	DIST TO MAX (M)	WIND SPEED (M/S)
.2758E+08	9658.	100.	2.

** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

*** B&M DISTANCES ***

DIST (M)	CONC (UG/M**3)	CONC (PPM)	WIND SPEED (M/S)
100.	.2758E+08	9658.	2.
200.	.7707E+07	2699.	2.
300.	.3922E+07	1373.	2.
400.	.2546E+07	891.6	2.
500.	.1841E+07	644.5	2.
600.	.1219E+07	426.8	2.
700.	.8119E+06	284.3	2.
800.	.5236E+06	183.3	1.
900.	.4220E+06	147.8	1.
1000.	.3480E+06	121.9	1.
1100.	.2770E+06	96.98	1.
1200.	.2228E+06	78.02	1.
1300.	.1824E+06	63.87	1.
1400.	.1516E+06	53.07	1.
1500.	.1276E+06	44.66	1.
1600.	.1085E+06	38.01	1.
1700.	.9406E+05	32.94	2.
1900.	.7530E+05	26.37	2.
2100.	.6164E+05	21.58	2.
2300.	.5139E+05	17.99	2.
2500.	.4349E+05	15.23	2.
2700.	.6979E+05	24.44	2.
2900.	.5837E+05	20.44	2.
3100.	.4941E+05	17.30	2.
3300.	.4226E+05	14.80	2.
3600.	.3400E+05	11.90	2.
3900.	.2783E+05	9.746	2.
4200.	.3839E+05	13.44	3.
4500.	.3231E+05	11.31	3.
5000.	.2483E+05	8.693	3.

CALCULATED VALUES:

DENSITY OF DEPRESSURIZED CONTAMINANT (KG/M**3) = 1.715
DENSITY OF AMBIENT AIR (KG/M**3) = 1.150
MOLE FRACTION = .1185
MIN DIST INST (M) = .2633E+05
MAX DIST CNST (M) = 6318.

***** NOTES & DEFINITIONS *****

- (a) "inst" refers to an instantaneous release (Section 3.6 of B-M Workbook)
(b) "cnst" refers to a continuous release (Section 3.6 of B-M Workbook)
(c) "MIN DIST INST" is the minimum distance downwind at which the release

may be treated as instantaneous
(d) "MAX DIST CNST" is the maximum distance downwind at which the release
may be treated as continuous

*** END OF B&M OUTPUT ***

Problem 4: Liquid Spill of Acetone - 2 m/s Wind

Results

File	Initial Form of Release	Chemical Database	Quit
	Initial Form of Release		
	Particulate Matter Release Type		
	Gaseous Release Type		
	Liquid Release Type		
	Surface Impoundments (Lagoons)	Workbook Scenario	
	2-Phase Saturated Liquid from Pressurized Storage	- 3.1	
	2-Phase Subcooled Liquid from Pressurized Storage	- 3.2,3.3	
	High Volatility Liquid Leaks	- 3.4,3.5	
	Low Volatility Liquid Leaks	- 3.6,3.7	
	Release Duration	- 3.8,3.9	
	Continuous		
	Instantaneous		

<F1>Help </></>Scroll Vertical Menus <->/<->Scroll Horizontal Menu
 <Enter>/Letter=Select Menu Item <F9>Exit Current Menu <Esc>Exit All Menus

Continuous Low Volatility Liquid Leaks - 3.8

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
 Liquid Spill of Acetone: Evaporation at 2 m/s Wind Speed

SOURCE OF LEAK

Area (Ao) of Hole or Opening -> 20.43 cm²
 Enter P for Pipe - T for Tank -> T

TEMPERATURE

Discharge Temperature (T2) -> 303 °K

Storage Temperature (T1) -> 303 °K
 Ambient Temperature (Ta) -> 303 °K

PUDDLE AREA

Is Maximum Puddle Area (Ap) Known (Y/N) -> Y
 Maximum Puddle Area (Ap) -> 70.12 m²

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Low Volatility Liquid Leaks - 3.8

SOURCE PARAMETERS - Page 2 of 4

PRESSURE

Liquid Pressure (P*) -> 155643 Pa

Ambient Pressure (Pa) -> 101325 Pa
 Reservoir Pressure (Pl) -> 101325 Pa
 Contaminant Liquid Density (ρl) -> 791 kg/cubic m
 Distance between Hole or Opening and Top of the Liquid Level (Hl) -> 7 m

VAPOR PRESSURE

Vapor Pressure (Pv) -> 39543.44 Pa

Molecular Weight (Mw) -> 58.08 kg/kmol
 Latent Heat of Vaporization (Lvap) -> 5.11E+05 J/kg
 Boiling Point Temperature (Tb) -> 329.3 °K

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Low Volatility Liquid Leaks - 3.8

SOURCE PARAMETERS - Page 3 of 4

EMISSION RATE

Emission Rate (Qm) -> 355.811 g/s

Wind Speed (Ur) -> 2 m/s

AREA

Area -> 70.12 m²

DISCHARGE DENSITY

Discharge Density (f2) -> 2.336095 kg/cubic m

DENSITY OF AIR

Density of Air (fair) -> 1.162417 kg/cubic m

Buoyancy is Negative

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Low Volatility Liquid Leaks - 3.8

SOURCE PARAMETERS - Page 4 of 4

TIME

Release Duration (Td) -> 11804.02 min

Total Amount of Material Released (Q) -> 2.52E+05 kg

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Low Volatility Liquid Leaks - 3.8

Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS

Relative Humidity (Rh) -> 80 %

Desired Averaging Time for the Calculation
of Concentrations -> 10 min

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE

Enter the distance from the nearest edge of
the source to the plant fenceline -> 100 m

RECEPTOR LOCATIONS

Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

<F2> Edit <F9> Previous Screen <F10> Run Model <Esc> Abort

08-15-95
16:31:24

*** B&M MODEL RUN ***

Liquid Spill of Acetone: Evaporation at 2 m/s Wind Speed

INPUTS:

AMBIENT PRESSURE (ATM) = 1.000
AMBIENT TEMP (K) = 303.0
AVERAGING TIME (MIN) = 10.00
BOILING PT TEMP (K) = 329.3
DURATION (S) = .7082E+06
EMISSION RATE (KG/S) = .3558
EXIT TEMP (K) = 303.0
MASS (KG) = .2520E+06
MOL. WEIGHT (G/G-MOLE) = 58.08
RELATIVE HUMIDITY (%) = 80.00
VAPOR FRACTION = 1.000

*** SUMMARY OF B&M MODEL RESULTS ***

MAX CONC (UG/M**3)	MAX CONC (PPM)	DIST TO MAX (M)	WIND SPEED (M/S)
.1304E+08	5581.	100.	1.

** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

*** B&M DISTANCES ***

DIST (M)	CONC (UG/M**3)	CONC (PPM)	WIND SPEED (M/S)
100.	.1304E+08	5581.	1.
200.	.2623E+07	1123.	1.
300.	.1166E+07	499.0	1.
400.	.6557E+06	280.7	1.
500.	.4196E+06	179.6	1.
600.	.2914E+06	124.7	1.
700.	.2141E+06	91.65	1.
800.	.1639E+06	70.17	1.
900.	.1295E+06	55.44	1.
1000.	.1049E+06	44.91	1.
1100.	.8670E+05	37.11	1.
1200.	.7285E+05	31.18	1.
1300.	.6208E+05	26.57	1.
1400.	.5352E+05	22.91	1.
1500.	.4663E+05	19.96	1.
1600.	.4098E+05	17.54	1.
1700.	.3630E+05	15.54	1.
1900.	.2906E+05	12.44	1.
2100.	.2379E+05	10.18	1.
2300.	.1983E+05	8.489	1.
2500.	.1679E+05	7.185	1.
2700.	.1439E+05	6.160	1.
2900.	.1247E+05	5.340	1.
3100.	.1092E+05	4.673	1.
3300.	9633.	4.124	1.
3600.	8095.	3.465	1.
3900.	6897.	2.952	1.
4200.	5947.	2.546	1.
4500.	5181.	2.218	1.
5000.	4196.	1.796	1.

CALCULATED VALUES:

DENSITY OF DEPRESSURIZED CONTAMINANT (KG/M**3) = 2.336
DENSITY OF AMBIENT AIR (KG/M**3) = 1.150
MOLE FRACTION = 1.000
MIN DIST INST (M) = .2361E+08
MAX DIST CNST (M) = .5666E+07

***** NOTES & DEFINITIONS *****

- (a) "inst" refers to an instantaneous release (Section 3.6 of B-M Workbook)
- (b) "cnst" refers to a continuous release (Section 3.6 of B-M Workbook)
- (c) "MIN DIST INST" is the minimum distance downwind at which the release may be treated as instantaneous
- (d) "MAX DIST CNST" is the maximum distance downwind at which the release

may be treated as continuous

```
*****  
***      END OF B&M OUTPUT      ***  
*****
```

Problem 4: Liquid Spill of Acetone - 5 m/s Wind

Results

File	Initial Form of Release	Chemical Database	Quit
	Initial Form of Release		
	Particulate Matter Release Type		
	Gaseous Release Type		
	Liquid Release Type		
	Surface Impoundments (Lagoons)	Workbook Scenario	
	2-Phase Saturated Liquid from Pressurized Storage	- 3.1	
	2-Phase Subcooled Liquid from Pressurized Storage	- 3.2,3.3	
	High Volatility Liquid Leaks	- 3.4,3.5	
	Low Volatility Liquid Leaks	- 3.6,3.7	
	Release Duration	- 3.8,3.9	
	Continuous		
	Instantaneous		

<F1>Help </></>Scroll Vertical Menus <->/<->Scroll Horizontal Menu
<Enter>/Letter=Select Menu Item <F9>Exit Current Menu <Esc>Exit All Menus

Continuous Low Volatility Liquid Leaks - 3.8

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Liquid Spill of Acetone: Evaporation at 5 m/s Wind Speed

SOURCE OF LEAK

Area (Ao) of Hole or Opening -> 20.43 cm²
Enter P for Pipe - T for Tank -> T

TEMPERATURE

Discharge Temperature (T2) -> 303 °K

Storage Temperature (T1) -> 303 °K
Ambient Temperature (Ta) -> 303 °K

PUDDLE AREA

Is Maximum Puddle Area (Ap) Known (Y/N) -> Y
Maximum Puddle Area (Ap) -> 70.12 m²

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Continuous Low Volatility Liquid Leaks - 3.8

SOURCE PARAMETERS - Page 2 of 4

PRESSURE

Liquid Pressure (P*) -> 155643 Pa

Ambient Pressure (Pa) -> 101325 Pa
Reservoir Pressure (P1) -> 101325 Pa

Contaminant Liquid Density (f1) -> 791 kg/cubic m
Distance between Hole or Opening
and Top of the Liquid Level (H1) -> 7 m

VAPOR PRESSURE

Vapor Pressure (Pv) -> 39543.44 Pa

Molecular Weight (Mw) -> 58.08 kg/kmol
Latent Heat of Vaporization (Lvap) -> 5.11E+05 J/kg
Boiling Point Temperature (Tb) -> 329.3 °K

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

SOURCE PARAMETERS - Page 3 of 4

EMISSION RATE

Emission Rate (Qm) -> 707.4151 g/s

Wind Speed (Ur) -> 5 m/s

AREA

Area -> 70.12 m²

DISCHARGE DENSITY

Discharge Density (f2) -> 2.336095 kg/cubic m

DENSITY OF AIR

Density of Air (fair) -> 1.162417 kg/cubic m

Buoyancy is Negative

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

SOURCE PARAMETERS - Page 4 of 4

TIME

Release Duration (Td) -> 5937.108 min

Total Amount of Material Released (Q) -> 2.52E+05 kg

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS

Relative Humidity (Rh) -> 80 %

Desired Averaging Time for the Calculation
of Concentrations -> 10 min

<F2> Edit <F9> Previous Screen <F10> Next Screen <Esc> Abort

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE

Enter the distance from the nearest edge of
the source to the plant fenceline -> 100 m

RECEPTOR LOCATIONS

Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

<F2> Edit <F9> Previous Screen <F10> Run Model <Esc> Abort

08-15-95
16:32:24

*** B&M MODEL RUN ***

Liquid Spill of Acetone: Evaporation at 5 m/s Wind Speed

INPUTS:

AMBIENT PRESSURE (ATM) = 1.000
AMBIENT TEMP (K) = 303.0
AVERAGING TIME (MIN) = 10.00
BOILING PT TEMP (K) = 329.3
DURATION (S) = .3562E+06
EMISSION RATE (KG/S) = .7074
EXIT TEMP (K) = 303.0
MASS (KG) = .2520E+06
MOL. WEIGHT (G/G-MOLE) = 58.08
RELATIVE HUMIDITY (%) = 80.00
VAPOR FRACTION = 1.000

*** SUMMARY OF B&M MODEL RESULTS ***

MAX CONC (UG/M**3)	MAX CONC (PPM)	DIST TO MAX (M)	WIND SPEED (M/S)
.1926E+08	8243.	100.	2.

** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

*** B&M DISTANCES ***

DIST (M)	CONC (UG/M**3)	CONC (PPM)	WIND SPEED (M/S)
100.	.1926E+08	8243.	2.
200.	.4684E+07	2005.	1.
300.	.2020E+07	864.6	1.
400.	.1136E+07	486.4	1.
500.	.7272E+06	311.3	1.
600.	.5050E+06	216.2	1.
700.	.3710E+06	158.8	1.
800.	.2841E+06	121.6	1.
900.	.2244E+06	96.07	1.
1000.	.1818E+06	77.82	1.
1100.	.1502E+06	64.31	1.
1200.	.1262E+06	54.04	1.
1300.	.1076E+06	46.05	1.
1400.	.9275E+05	39.70	1.
1500.	.8080E+05	34.58	1.
1600.	.7101E+05	30.40	1.
1700.	.6290E+05	26.93	1.
1900.	.5036E+05	21.56	1.
2100.	.4122E+05	17.65	1.
2300.	.3437E+05	14.71	1.
2500.	.2909E+05	12.45	1.
2700.	.2494E+05	10.67	1.
2900.	.2162E+05	9.253	1.
3100.	.1892E+05	8.097	1.
3300.	.1669E+05	7.146	1.
3600.	.1403E+05	6.004	1.
3900.	.1195E+05	5.116	1.
4200.	.1031E+05	4.411	1.
4500.	8977.	3.843	1.
5000.	7272.	3.113	1.

CALCULATED VALUES:

DENSITY OF DEPRESSURIZED CONTAMINANT (KG/M**3) = 2.336
DENSITY OF AMBIENT AIR (KG/M**3) = 1.150
MOLE FRACTION = 1.000
MIN DIST INST (M) = .1187E+08
MAX DIST CNST (M) = .2850E+07

***** NOTES & DEFINITIONS *****

- (a) "inst" refers to an instantaneous release (Section 3.6 of B-M Workbook)
- (b) "cnst" refers to a continuous release (Section 3.6 of B-M Workbook)
- (c) "MIN DIST INST" is the minimum distance downwind at which the release may be treated as instantaneous
- (d) "MAX DIST CNST" is the maximum distance downwind at which the release

may be treated as continuous

*** END OF B&M OUTPUT ***

Appendix D: Resuspension Methodologies

ESTIMATION OF SURFACE-ORIGINATED AIRBORNE RADIONUCLIDE CONCENTRATIONS--RESUSPENSION

The purpose of this document is to present a rationale for estimation of concentrations of airborne radionuclides from resuspended particles. A discussion of airborne particle size is also included, so that estimations of inhalation exposure can be made based on the expected lung deposition.

METHOD 1, ESTIMATION OF C BY "MODIFIED MASS LOADING "

The primary objective is to estimate the concentration of airborne radionuclide

$$C = E_f S M \quad (1)$$

where E_f is the enhancement factor defined as the ratio of airborne particle activity (Bq/g) to total surface activity (Bq/g), S is the total surface activity of loose material (e.g. soil), and M is the total suspended particulate concentration (g/m³) of loose material or soil, also known as the "mass loading". At many contaminated-soil sites such factors as M and S are monitored routinely, however, it is implicitly assumed that the particles in M have their origin in the soil where S is measured. There are many cases where this is obviously not true, and good judgment must be passed that the airborne M is truly representative of the contaminated soil.

Estimates of the factors E_f and M in Eq (1) can be made from experimental values, but S must be measured locally. The following rule of thumb may be applied for soil. Where there are no measurements of the enhancement factor,

$$E_f = 0.7 \quad \text{in the case of } \textit{undisturbed surface soil} \quad (2a)$$

$$E_f = 4 \quad \text{in the case where } \textit{soil is recently disturbed} \quad (2b)$$

$$E_f = 0.01 \quad \text{in the vicinity of a } \textit{site of nuclear detonation} \quad (2c)$$

These values of enhancement factor were taken from observations of radionuclide resuspension under different environmental conditions by Shinn (1992). The undisturbed soil value is a median value from observations at sites at Bikini Island, Nevada, South Carolina, and California, and the range of values was 0.21 to 1.04. The value for recently disturbed soil is the median of observations during activities such as soil thawing, bulldozer

blading, vacuum cleanup, wildfire, and raked-off surface, that had a range from 2.2 to 6.5 reported by Shinn (1992). Values of the enhancement factor calculated from radioactivity in suspended dust during the agricultural tractor operations near Chernobyl gave a median of 4.4 for medium to highly contaminated soil, and had a range of values from 2.8 to 8.4 in the observations by Loshchilov *et al* (1992). In the case of a nuclear detonation where some of the radioactive material is held in a substance known as "shot glass", values given by Shinn (*loc cit*) had a range 0.002 to 0.024.

When the total suspended particulate concentration, M , cannot be measured it may be estimated from the observations by Shah *et al* (1986), who found annual averages of 28 and 75 mg/m³ for rural and urban locations respectively, for undisturbed conditions. During cleanup or disturbed soil conditions, however, one would expect that M values could increase dramatically. Loshchilov *et al* (1992) found that M values behind a tractor had a median of 15 mg/m³ and a range of 0.3 to 200 mg/m³. There is also an effect of seasonal climatology on values of M , for example, Shinn (1992) shows a range of 7 to 30 mg/m³ from Spring to Summer in rural Nevada.

While the effects of different particle-size distributions on the measured or estimated exposure concentration, C , are of concern, there is evidence that the effects are predictable. Outdoors there are usually three modes of size-component distributions, each approximately log-normal mass-distributions with particle diameter. Milford and Davidson (1985) studied size distributions of 11 crustal elements from suspended soil and found a median diameter of about 5 μ m. This is supported by observations from Shinn (1992) at many sites that had median suspended-soil aerodynamic diameters of 2 to 6 μ m. A coarse component is sometimes found also, with a median diameter of about 15 μ m, especially when the soil is disturbed or when very strong winds are present. This coarse component should be considered transient, however, because the gravitational settling velocities of the coarse particles are greater than the suspension velocities and their residence times in the atmosphere are short. In urban areas Milford and Davidson (1985), as well as many others, found a very fine size component with a median diameter of about 0.5 μ m. This component is almost universally not of crustal origin, but derives from combustion sources and is in a state of transformation by coagulation to larger particles. The fine size-component contributes very little to M , and in most cases would not carry locally-derived radioactivity. In the absence of measurements, one should assume all the suspended radioactivity is on soil particles having one mode of particle size with a median diameter in the range 2 to 6 μ m and log-normally distributed with geometric standard deviation of about 5. In the special case of disturbed soil, if measurements of size-distributions cannot be made, then PM₁₀ measurements are preferred. (PM₁₀ is the less than 10 μ m, fine-particle component of the particle-size distribution measured by M).

The soil-originated particles are broadly dispersed (geometric standard deviation greater than 4). In these cases, applying the lung deposition functions as did Milford and Davidson (1985), the retention fraction is predictable approximately as follows in Table 1.

Table 1. Inhalation Retention for Airborne Soil Particles, Broadly Dispersed.

	Median Diameter(mm)		
	0.5	1.0	5.0
Pulmonary (Low)	0.10	0.10	0.10
Pulmonary (High)	0.30	0.30	0.30
Tracheobronchial	0.10	0.10	0.15
Extrathoracic	0.10	0.15	0.35
Total (Low)	0.30	0.35	0.60
Total (High)	0.50	0.55	0.80

It can be seen that the larger median-diameter distribution effects mostly the extra-thoracic deposition, which should be kept in mind when calculating dose endpoints from estimated distributions.

Before considering the alternative methods of estimation of C, a statement should be made about the requirement for representative measurement of S. The loose material or soil which has been contaminated usually by a previous atmospheric deposition event, will have natural variability that cannot be characterized by a few samples. This natural variability is due to the complexity of the original deposition, surface effects where particles are deposited, and variability of the weathering process after initial deposition. Experience has shown that within a larger region of relatively homogeneous deposition, statistically stratified by extensive sampling, there will be spatial variability depending on the scale of the soil-surface sampled. That is, the area of the soil-surface sampled is the critical dimension. Since the air sampled for estimates of C contains particles whose trajectories came from many upwind locations, it is best to use a large area average of S, such as obtains from many soil samples or from an *in situ* gamma spectroscopy unit that has a large view of the soil surface.

METHOD 2, ESTIMATION OF C BY RESUSPENSION FACTOR

The second method of estimation of C is known as the *resuspension factor*:

$$C = S_f D \quad (3)$$

where S_f is the resuspension factor, and D is the total (original) soil deposition (Bq/m^2). By comparison with Eq 1, one sees that less information is available about factors that influence C, and in fact by rearranging Eq (3) one obtains the definition of the "resuspension factor", which is really an air concentration normalized to D and has units of inverse length (m^{-1}). The deposition, D, can be related to soil surface activity level, S, with some algebraic manipulation.

Experimental evidence abounds that the radioactivity distribution with depth in the soil shortly after a contaminating event will have an approximately exponential distribution with depth,

$$A = A_0 \exp(-\alpha z) \quad (4)$$

where α is known as the *inverse relaxation depth*, z is the depth below ground surface level, and A_0 is the extrapolated value of soil surface activity (Bq/g).

By definition, the deposition D is obtained by summing over all soil layers:

$$D = \rho \sum A_i \Delta z_i \quad (5)$$

where ρ is the soil bulk density. Thus, soil samples should obtain the vertical profile distribution of radioactivity A, in order to determine D, and to solve Eq (4) for the inverse relaxation depth. Obtaining many soil profiles may be prohibitive, so a curve-fitting least squares analysis of Eq (4) should be employed for best results.

We can express D in terms of the inverse relaxation depth:

$$D = \rho S h \quad (6)$$

and h is the *characteristic depth of deposition*,:

$$h \equiv (1/\alpha) \quad (7)$$

It should be noted that for soil relaxation depths commonly observed:

$$h \cong 5 \pm 1.5 \text{ cm} \quad (8)$$

That is, unless the soil is very sandy allowing deep penetration of radioactivity, the characteristic depth is conservative.

Estimates of deposition, D , can sometimes be made therefore by applying Eq (6), with knowledge of the surface-soil activity, S , a reasonable judgment of penetration of radioactivity so that h from Eq (7) applies, and using the soil bulk density:

$$\rho \cong 1.5 \text{ Mg/m}^3 \quad (9)$$

We can utilize the resuspension factor method of Eq (3) to estimate C , by applying available estimates of S_f . Where no measurements of this resuspension factor are available (here S_f has units of m^{-1}), and t is the time in days since the contaminating event, use the following estimates:

$$S_f = 10^{-6} / t \text{ for the first 1000 days} \quad (10a)$$

$$S_f = 10^{-9} \text{ m}^{-1} \text{ for longer times, out to many years.} \quad (10b)$$

The resuspension factors for the first two months were derived from the experiments by Garland (1982), those from two to 42 months from the observations following the Chernobyl event summarized by Garland and Pattenden (1991), and for long times, from the results of Anspaugh *et al* (1975). The equation (10a) is a problem however, if a dose is estimated by integration from $t = 0$; it is recommended that a constant S_f value be used for $t < 1$ day.

Anspaugh *et al* (1975) presented a method for estimating resuspension factors for all times, but the recent evidence from the Chernobyl accident shows a more rapid decline in resuspension factors with time in the short to intermediate times, than their formula predicts. Recent theoretical developments by Reeks *et al* (1988), argue that the turbulent resuspension phenomenon is analogous to molecular adhesion, and that the inverse time dependency (10a) arises in very short time after an initial exponential phase. In principle, then, the integral of S_f is bounded at very short times, but the empirical evidence is lacking for an estimate of an initial value. At long times, other natural phenomena result in a local equilibrium of air concentration with the deposition, D , leading to the constant in (10b). It should be noted, however, that disturbances can change this equilibrium, as discussed under Method 1, above.

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Appendix E: Listings of Important Chemicals

**TABLE 1 to §68.130 - LIST OF REGULATED TOXIC SUBSTANCES AND THRESHOLD
QUANTITIES FOR ACCIDENTAL RELEASE PREVENTION
[Alphabetical Order - 77 Substances]**

Chemical Name	CAS No	Threshold Quantity (lbs)	Basis for Listing
Acrolein [2-Propenal]	107-02-8	5,000	b
Acrylonitrile [2-Propenenitrile]	107-13-1	20,000	b
Acrylyl chloride [2-Propenoyl chloride]	814-68-6	5,000	b
Allyl alcohol [2-Propen-1-ol]	107-18-6	15,000	b
Allylamine [2-Propen-1-amine]	107-11-9	10,000	b
Ammonia (anhydrous)	7664-41-7	10,000	a, b
Ammonia (conc 20% or greater)	7664-41-7	20,000	a, b
Arsenous trichloride	7784-34-1	15,000	b
Arsine	7784-42-1	1,000	b
Boron trichloride [Borane, trichloro-]	10294-34-5	5,000	b
Boron trifluoride [Borane, trifluoro-]	7637-07-2	5,000	b
Boron trifluoride compound with methyl ether (1:1) [Boron, trifluoro[oxybis[metane]]-, T-4-	353-42-4	15,000	b
Bromine	7726-95-6	10,000	a, b
Carbon disulfide	75-15-0	20,000	b
Chlorine	7782-50-5	2,500	a, b
Chlorine dioxide [Chlorine oxide (ClO ₂)]	10049-04-4	1,000	c
Chloroform [Methane, trichloro-]	67-66-3	20,000	b
Chloromethyl ether [Methane, oxybis[chloro-]	542-88-1	1,000	b
Chloromethyl methyl ether [Methane, chloromethoxy-]	107-30-2	5,000	b
Crotonaldehyde [2-Butenal]	4170-30-3	20,000	b
Crotonaldehyde, (E)- [2-Butenal, (E)-]	123-73-9	20,000	b
Cyanogen chloride	506-77-4	10,000	c
Cyclohexylamine [Cyclohexanamine]	108-91-8	15,000	b
Diborane	19287-45-7	2,500	b
Dimethyldichlorosilane [Silane, dichlorodimethyl-]	75-78-5	5,000	b
1,1-Dimethylhydrazine [Hydrazine, 1,1-dimethyl-]	57-14-7	15,000	b
Epichlorohydrin [Oxirane, (chloromethyl)-]	106-89-8	20,000	b
Ethylenediamine [1,2-Ethanediamine]	107-15-3	20,000	b
Ethyleneimine [Aziridine]	151-56-4	10,000	b
Ethylene oxide [Oxirane]	75-21-8	10,000	a, b
Fluorine	7782-41-4	1,000	b
Formaldehyde (solution)	50-00-0	15,000	b

Furan	110-00-9	5,000	b
Hydrazine	302-01-2	15,000	b
Hydrochloric acid (conc 30% or greater)	7647-01-0	15,000	d
Hydrocyanic acid	74-90-8	2,500	a, b
Hydrogen chloride (anhydrous) [Hydrochloric acid]	7647-01-0	5,000	a
Hydrogen fluoride/Hydrofluoric acid (conc 50% or greater) [Hydrofluoric acid]	7664-39-3	1,000	a, b
Hydrogen selenide	7783-07-5	500	b
Hydrogen sulfide	7783-06-4	10,000	a, b
Iron, pentacarbonyl- [Iron carbonyl (Fe(CO) ₅), (TB-5-11)-]	13463-40-6	2,500	b
Isobutyronitrile [Propanenitrile, 2-methyl-]	78-82-0	20,000	b
Isopropyl chloroformate [Carbonochloridic acid, 1-methylethyl ester]	108-23-6	15,000	b
Methacrylonitrile [2-Propenenitrile, 2-methyl-]	126-98-7	10,000	b
Methyl chloride [Methane, chloro-]	74-87-3	10,000	a
Methyl chloroformate [Carbonochloridic acid, methylester]	79-22-1	5,000	b
Methyl hydrazine [Hydrazine, methyl-]	60-34-4	15,000	b
Methyl isocyanate [Methane, isocyanato-]	624-83-9	10,000	a, b
Methyl mercaptan [Methanethiol]	74-93-1	10,000	b
Methyl thiocyanate [Thiocyanic acid, methyl ester]	556-64-9	20,000	b
Methyltrichlorosilane [Silane, trichloromethyl-]	75-79-6	5,000	b
Nickel carbonyl	13463-39-3	1,000	b
Nitric acid (conc 80% or greater)	7697-37-2	15,000	b
Nitric oxide [Nitrogen oxide (NO)]	10102-43-9	10,000	b
Oleum (Fuming Sulfuric acid) [Sulfuric acid, mixture with sulfur trioxide] ¹	8014-95-7	10,000	e
Peracetic acid [Ethaneperoxoic acid]	79-21-0	10,000	b
Perchloromethylmercaptan [Methanesulfonyl chloride, trichloro-]	594-42-3	10,000	b
Phosgene [Carbonic dichloride]	75-44-5	500	a, b
Phosphine	7803-51-2	5,000	b
Phosphorus oxychloride [Phosphoryl chloride]	10025-87-3	5,000	b
Phosphorus trichloride [Phosphorous trichloride]	7719-12-2	15,000	b
Piperidine	110-89-4	15,000	b
Propionitrile [Propanenitrile]	107-12-0	10,000	b
Propyl chloroformate [Carbonochloridic acid, propylester]	109-61-5	15,000	b
Propyleneimine [Aziridine, 2-methyl-]	75-55-8	10,000	b

Propylene oxide [Oxirane, methyl-]	75-56-9	10,000	b
Sulfur dioxide (anhydrous)	7446-09-5	5,000	a, b
Sulfur tetrafluoride [Sulfur fluoride (SF ₄), (T-4)-]	7783-60-0	2,500	b
Sulfur trioxide	7446-11-9	10,000	a, b
Tetramethyllead [Plumbane, tetramethyl-]	75-74-1	10,000	b
Tetranitromethane [Methane, tetranitro-]	509-14-8	10,000	b
Titanium tetrachloride [Titanium chloride (TiCl ₄) (T-4)-]	7550-45-0	2,500	b
Toluene 2,4-diisocyanate [Benzene, 2,4-diisocyanato-1-methyl-] ¹	584-84-9	10,000	a
Toluene 2,6-diisocyanate [Benzene, 1,3-diisocyanato-2-methyl-] ¹	91-08-7	10,000	a
Toluene diisocyanate (unspecified isomer) [Benzene, 1,3-diisocyanatomethyl-] ¹	26471-62-5	10,000	a
Trimethylchlorosilane [Silane, chlorotrimethyl-]	75-77-4	10,000	b
Vinyl acetate monomer [Acetic acid ethenyl ester]	108-05-4	15,000	b

¹ The mixture exemption in §68.115(b)(1) does not apply to the substance.

Basis for Listing:

- ^a Mandated for listing by Congress.
- ^b On EHS list, vapor pressure 10 mmHg or greater.
- ^c Toxic gas.
- ^d Toxicity of hydrogen chloride, potential to release hydrogen chloride, and history of accidents.
- ^e Toxicity of sulfur trioxide and sulfuric acid, potential to release sulfur trioxide, and history of accidents.

TABLE 3 TO §68.130 - LIST OF REGULATED FLAMMABLE SUBSTANCES AND THRESHOLD

QUANTITIES FOR ACCIDENTAL RELEASE PREVENTION
[ALPHABETICAL ORDER - 63 SUBSTANCES]

Chemical Name	CAS No	Threshold Quantity (lbs)	Basis for Listing
Acetaldehyde	75-07-0	10,000	g
Acetylene [Ethyne]	74-86-2	10,000	f
Bromotrifluoroethylene [Ethene, bromotrifluoro-]	598-73-2	10,000	f
1,3-Butadiene	106-99-0	10,000	f
Butane	106-97-8	10,000	f
1-Butene	106-98-9	10,000	f
2-Butene	107-01-7	10,000	f
Butene	25167-67-3	10,000	f
2-Butene-cis	590-18-1	10,000	f
2-Butene-trans [2-Butene, (E)]	624-64-6	10,000	f
Carbon oxysulfide [Carbon oxide sulfide (COS)]	463-58-1	10,000	f
Chlorine monoxide [Chlorine oxide]	7791-21-1	10,000	f
2-Chloropropylene [1-Propene, 2-chloro-]	557-98-2	10,000	g
1-Chloropropylene [1-Propene, 1-chloro-]	590-21-6	10,000	g
Cyanogen [Ethanedinitrile]	460-19-5	10,000	f
Cyclopropane	75-19-4	10,000	f
Dichlorosilane [Silane, dichloro-]	4109-96-0	10,000	f
Difluoroethane [Ethane, 1,1-difluoro-]	75-37-6	10,000	f
Dimethylamine [Methanamine, N-methyl-]	124-40-3	10,000	f
2,2-Dimethylpropane [Propane, 2,2-dimethyl-]	463-82-1	10,000	f
Ethane	74-84-0	10,000	f
Ethyl acetylene [1-Butyne]	107-00-6	10,000	f
Ethylamine [Ethanamine]	75-04-7	10,000	f
Ethyl chloride [Ethane, chloro-]	75-00-3	10,000	f
Ethylene [Ethene]	74-85-1	10,000	f
Ethyl ether [Ethane, 1,1'-oxybis-]	60-29-7	10,000	g
Ethyl mercaptan [Ethanethiol]	75-08-1	10,000	g
Ethyl nitrite [Nitrous acid, ethyl ester]	109-95-5	10,000	f
Hydrogen	1333-74-0	10,000	f
Isobutane [Propane, 2-methyl]	75-28-5	10,000	f
Isopentane [Butane, 2-methyl-]	78-78-4	10,000	g
Isoprene [1,3-Butadiene, 2-methyl-]	78-79-5	10,000	g

Isopropylamine [2-Propanamine]	75-31-0	10,000	g
Isopropyl chloride [Propane, 2-chloro-]	75-29-6	10,000	g
Methane	74-82-8	10,000	f
Methylamine [Methanamine]	74-89-5	10,000	f
3-Methyl-1-butene	563-45-1	10,000	f
2-Methyl-1-butene	563-46-2	10,000	g
Methyl ether [Methane, oxybis-]	115-10-6	10,000	f
Methyl formate [Formic acid, methyl ester]	107-31-3	10,000	g
2-Methylpropene [1-Propene, 2-methyl-]	115-11-7	10,000	f
1,3-Pentadiene	504-60-9	10,000	f
Pentane	109-66-0	10,000	g
1-Pentene	109-67-1	10,000	g
2-Pentene, (E)-	646-04-8	10,000	g
2-Pentene, (Z)-	627-20-3	10,000	g
Propadiene [1,2-Propadiene]	463-49-0	10,000	f
Propane	74-98-6	10,000	f
Propylene [1-Propene]	115-07-1	10,000	f
Propyne [1-Propyne]	74-99-7	10,000	f
Silane	7803-62-5	10,000	f
Tetrafluoroethylene [Ethene, tetrafluoro-]	116-14-3	10,000	f
Tetramethylsilane [Silane, tetramethyl-]	75-76-3	10,000	g
Trichlorosilane [Silane, trichloro-]	10025-78-2	10,000	g
Trifluorochloroethylene [Ethene, chlorotrifluoro-]	79-38-9	10,000	f
Trimethylamine [Methanamine, N,N-dimethyl-]	75-50-3	10,000	f
Vinyl acetylene [1-Buten-3-yne]	689-97-4	10,000	f
Vinyl chloride [Ethene, chloro-]	75-01-4	10,000	a, f
Vinyl ethyl ether [Ethene, ethoxy-]	109-92-2	10,000	g
Vinyl fluoride [Ethene, fluoro-]	75-02-5	10,000	f
Vinylidene chloride [Ethene, 1,1-dichloro-]	75-35-4	10,000	g
Vinylidene fluoride [Ethene, 1,1-difluoro-]	75-38-7	10,000	f
Vinyl methyl ether [Ethene, methoxy-]	107-25-5	10,000	f

Basis for Listing:

- ^a Mandated for listing by Congress.
- ^f Flammable gas.
- ^g Volatile flammable liquid.

Appendix A to 1910.119 - List of Highly Hazardous Chemicals, Toxics and Reactives (Mandatory)

<u>Chemical Name</u>	<u>CAS No</u>	<u>Threshold Quantity (lbs)</u>
Acetaldehyde	75-07-0	2500
Acrolein (2-Propenal)	107-02-8	150
Acrylyl Chloride	814-68-6	250
Allyl Chloride	107-05-1	1000
Allylamine	107-11-9	1000
Alkylaluminums	Varies	5000
Ammonia, Anhydrous	7664-41-7	10000
Ammonia solutions (>44% ammonia by weight)	7664-41-7	15000
Ammonium Perchlorate	7790-98-9	7500
Ammonium Permanganate	7787-36-2	7500
Arsine (also called Arsenic Hydride)	7784-42-1	100
Bis(Chloromethyl) Ether	542-88-1	100
Boron Trichloride	10294-34-5	2500
Boron Trifluoride	7637-07-2	250
Bromine	7726-95-6	1500
Bromine Chloride	13863-41-7	1500
Bromine Pentafluoride	7789-30-2	2500
Bromine Trifluoride	7787-71-5	15000
3-Bromopropyne (also called Propargyl Bromide)	106-96-7	100
Butyl Hydroperoxide (Tertiary)	75-91-2	5000
Butyl Perbenzoate (Tertiary)	614-45-9	7500
Carbonyl Chloride (see Phosgene)	75-44-5	100
Carbonyl Fluoride	353-50-4	2500
Cellulose Nitrate (concentration >12.6% nitrogen)	9004-70-0	2500
Chlorine	7782-50-5	1500
Chlorine Dioxide	10049-04-4	1000
Chlorine Pentafluoride	13637-63-3	1000
Chlorine Trifluoride	7790-91-2	1000
Chlorodiethylaluminum (also called Diethyl aluminum Chloride)	96-10-6	5000

<u>Chemical Name</u>	<u>CAS No</u>	<u>Threshold Quantity (lbs)</u>
1-Chloro-2,4-Dinitrobenzene	97-00-7	5000
Chloromethyl Methyl Ether	107-30-2	500
Chloropicrin	76-06-2	500
Chloropicrin and Methyl Bromide mixture	None	1500
Chloropicrin and Methyl Chloride mixture	None	1500
Cumene Hydroperoxide	80-15-9	5000
Cyanogen	460-19-5	2500
Cyanogen Chloride	506-77-4	500
Cyanuric Fluoride	675-14-9	100
Diacetyl Peroxide (Concentration >70%)	110-22-5	5000
Diazomethane	334-88-3	500
Dibenzoyl Peroxide	94-36-0	7500
Diborane	19287-45-7	100
Dibutyl Peroxide (Tertiary)	110-05-4	5000
Dichloro Acetylene	7572-29-4	250
Dichlorosilane	4109-96-0	2500
Diethylzinc	557-20-0	10000
Diisopropyl Peroxydicarbonate	105-64-6	7500
Dilaluroyl Peroxide	105-74-8	7500
Dimethyldichlorosilane	75-78-5	1000
Dimethylhydrazine, 1,1-	57-14-7	1000
Dimethylamine, Anhydrous	124-40-3	2500
2,4-Dinitroaniline	97-02-9	5000
Ethyl Methyl Ketone Peroxide (also Methyl Ethyl Ketone Peroxide; concentration >60%)	1338-23-4	5000
Ethyl Nitrite	109-95-5	5000
Ethylamine	75-04-7	7500
Ethylene Fluorohydrin	371-62-0	100
Ethylene Oxide	75-21-8	5000
Ethyleneimine	151-56-4	1000
Fluorine	7782-41-4	1000
Formaldehyde (Formalin)	50-00-0	1000

<u>Chemical Name</u>	<u>CAS No</u>	<u>Threshold Quantity (lbs)</u>
Furan	110-00-9	500
Hexafluoroacetone	684-16-2	5000
Hydrochloric Acid, Anhydrous	7647-01-0	5000
Hydrofluoric Acid, Anhydrous	7664-39-3	1000
Hydrogen Bromide	10035-10-6	5000
Hydrogen Chloride	7647-01-0	5000
Hydrogen Cyanide, Anhydrous	74-90-8	1000
Hydrogen Fluoride	7664-39-3	1000
Hydrogen Peroxide (>52% by weight or greater)	7722-84-1	7500
Hydrogen Selenide	7783-07-5	150
Hydrogen Sulfide	7783-06-4	1500
Hydroxylamine	7803-49-8	2500
Iron, Pentacarbonyl	13463-40-6	250
Isopropylamine	75-31-0	5000
Ketene	463-51-4	100
Methacrylaldehyde	78-85-3	1000
Methacryloyl Chloride	920-46-7	150
Methacryloyloxyethyl Isocyanate	30674-80-7	100
Methyl Acrylonitrile	126-98-7	250
Methylamine, Anhydrous	74-89-5	1000
Methyl Bromide	74-83-9	2500
Methyl Chloride	74-87-3	15000
Methyl Chloroformate	79-22-1	500
Methyl Ethyl Ketone Peroxide (concentration >60%)	1338-23-4	5000
Methyl Fluoroacetate	453-18-9	100
Methyl Fluorosulfate	421-20-5	100
Methyl Hydrazine	60-34-4	100
Methyl Iodide	74-88-4	7500
Methyl Isocyanate	624-83-9	250
Methyl Mercaptan	74-93-1	5000
Methyl Vinyl Ketone	79-84-4	100
Methyltrichlorosilane	75-79-6	500
Nickel Carbonyl (Nickel Tetracarbonyl)	13463-39-3	150

<u>Chemical Name</u>	<u>CAS No</u>	<u>Threshold Quantity (lbs)</u>
Nitric Acid (94.5% by weight or greater)	7697-37-2	500
Nitric Oxide	10102-43-9	250
Nitroaniline (para Nitroaniline)	100-01-6	5000
Nitromethane	75-52-5	2500
Nitrogen Dioxide	10102-44-0	250
Nitrogen Oxides (NO; NO ₂ ; N ₂ O ₄ ; N ₂ O ₃)	10102-44-0	250
Nitrogen Tetroxide (also called Nitrogen Peroxide)	10544-72-6	250
Nitrogen Trifluoride	7783-54-2	5000
Nitrogen Trioxide	10544-73-7	250
Oleum (65% to 80% by weight; also called Fuming Sulfuric Acid)	8014-94-7	1000
Osmium Tetroxide	20816-12-0	100
Oxygen Difluoride (Fluoride Monoxide)	7783-41-7	100
Ozone	10028-15-6	100
Pentaborane	19624-22-7	100
Peracetic Acid (concentration >60% Acetic Acid; also called Peroxyacetic Acid)	79-21-0	1000
Perchloric Acid (concentration >60% by weight)	7601-90-3	5000
Perchloromethyl Mercaptan	594-42-3	150
Perchloryl Fluoride	7616-94-6	5000
Peroxyacetic Acid (concentration >60% Acetic Acid; also called Peracetic Acid)	79-21-0	1000
Phosgene (also called Carbonyl Chloride)	75-44-5	100
Phosphine (Hydrogen Phosphide)	7803-51-2	100
Phosphorus Oxychloride (also called Phosphoryl Chloride)	10025-87-3	1000
Phosphorus Trichloride	7719-12-2	1000

<u>Chemical Name</u>	<u>CAS No</u>	<u>Threshold Quantity (lbs)</u>
Phosphoryl Chloride (also called Phosphorus Oxychloride)	10025-87-3	1000
Propargyl Bromide	106-96-7	100
Propyl Nitrate	627-3-4	2500
Sarin	107-44-8	100
Selenium Hexafluoride	7783-79-1	1000
Stibine (Antimony Hydride)	7803-52-3	500
Sulfur Dioxide (liquid)	7446-09-5	1000
Sulfur Pentafluoride	5714-22-7	250
Sulfur Tetrafluoride	7783-60-0	250
Sulfur Trioxide (also called Sulfuric Anhydride)	7446-11-9	1000
Sulfuric Anhydride(also called Sulfur Trioxide)	7446-11-9	1000
Tellurium Hexafluoride	7783-80-4	250
Tetrafluoroethylene	116-14-3	5000
Tetrafluorohydrazine	10036-47-2	5000
Tetramethyl Lead	75-74-1	1000
Thionyl Chloride	7719-09-7	250
Trichloro (chloromethyl) Silane	1558-25-4	100
Trichloro (dichlorophenyl) Silane	27137-85-5	2500
Trichlorosilane	10025-78-2	5000
Trifluorochloroethylene	79-38-9	10000
Trimethoxysilane	2487-90-3	1500

DOE-EH List of Hazardous Chemicals and their Properties

Substance	CAS #	Acutely Toxic Concentration			Vapor Pressure		
		mg/m ³	ppm	Basis	mm Hg	Temp (°C)	Ref.
Beryllium	7440-41-7	10	27	IDLH	~0	727	K&A ¹
Dowanol EB (Butyl Cellosolve)	111-76-2		400	IDLH	0.6	20	MSDS
Perchloro- ethylene	127-18-4		500	IDLH	14	20	MSDS
PCBs (insul. fluid)	2051-60-7	5-10	~1	IDLH	0.005	38	MSDS
UF ₆		20		IDLH	111	25	K&A ¹

¹O. Kubaschewski and D.B. Alcock, "Metallurgical Thermochemistry", 1979.

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX DOE (1994b)

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
acetone	Colorless, volatile liquid; sweetish odor; miscible with water, alcohol, ether, chloroform, and most oils. Used in preparation of chemicals or as a solvent.	Flammable, dangerous fire risk. Acts as narcotic in high concentrations. Moderately toxic by ingestion and inhalation.
aluminum nitrate	White crystals that are soluble in cold water and decompose in hot water. Soluble in alcohol and acetone. Used in nucleonics and the manufacture of incandescent filaments; serves as an anticorrosion agent.	Strong oxidizing agent that cannot be stored near combustible materials.
arsine	Colorless gas, soluble in water, slightly soluble in alcohol, alkalis. Used in organic synthesis and as and as an agent for solid-state electronic components.	Highly poisonous by inhalation.
asbestos	Impure magnesium silicate occurring in fibrous form. Non-combustible. Fireproof fabrics can be found in brake lining, gaskets, roofing compositions, electrical and heat insulation, paint filler, and chemical filters. Reinforcing agent in rubber and plastics.	Highly toxic by inhalation of dust particles. An active carcinogen.
beryllium	Metallic element (atomic number 4). A hard, brittle, gray-white metal; soluble in acids (except nitric) and alkalis. Resistant to oxidation at ordinary temperatures. It is the lightest structural metal known; can be fabricated by rolling, forging, and machining. Joining is chiefly by shrink-fitting; brazing and welding are difficult. Highly permeable to x-rays. Structural material in space technology; moderator and reflector of neutrons in nuclear reactors; source of neutrons; special windows for x-ray tubes; in gyroscopes, computer parts, inertial guidance systems; additive in solid-propellant rocket fuels; beryllium-copper alloys.	A carcinogen. Very high toxicity, especially by inhalation of dust.
beryllium hydride	White solid. Reacts with water, dilute acids, and methanol to liberate hydrogen. Liberates hydrogen rapidly when heated to 220°C. Can be used in rocket fuels.	Fire risk when exposed to water, organic materials, and heat. Highly toxic.
carbon disulfide	Clear, colorless, or faintly yellow liquid with strong disagreeable odor. Soluble in alcohol, benzene, and ether; slightly soluble in water. Classed as an inorganic compound. Used as a solvent.	Highly flammable; dangerous fire and explosion risk; can be ignited by friction. A poison. Toxic by skin absorption.

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
carbon tetrachloride	A chlorinated hydrocarbon. Colorless liquid with sweetish distinctive color. Miscible with alcohol, ether, chloroform, benzene, solvent naphtha, and most of the fixed and volatile oils; insoluble in water. Noncombustible. Uses include refrigerants and propellants, metal degreasing, chlorinating organic compounds, production of semiconductors.	Highly toxic by ingestion, inhalation, and skin absorption. Narcotic. A suspect carcinogen that decomposes to phosgene at high temperatures.
carbonyl sulfide	Colorless gas with typical sulfide odor. Soluble in water and alcohol. Used in the synthesis of organic compounds.	Flammable; highly toxic; acts as narcotic in high concentrations.
chlorine	Nonmetallic halogen element (atomic number 17); a dense, greenish-yellow, diatomic gas. Noncombustible, but supports combustion; pungent irritating odor. Soluble in chlorides and alcohols. Extremely strong oxidizing agent. Slightly soluble in cold water. Used in manufacture of chemicals, water purification, flame-retardant compounds, and special batteries (with lithium or zinc).	Toxic as irritant and by inhalation. Moderate fire risk in contact with turpentine, ether, ammonia, hydrocarbons, hydrogen, powdered metals, and other reducing materials.
cyanogen	Colorless gas, pungent penetrating odor, burns with a purple-tinged flame. Soluble in water, alcohol, and ether. Uses include organic synthesis, welding and cutting metals, fumigant, and rocket propellant.	Flammable. Should be stored away from light and heat. A very toxic material.
ethyl ether	Colorless, volatile, mobile liquid; hygroscopic; aromatic odor; burning and sweet taste. Soluble in alcohol, chloroform, benzene, solvent naphtha, and oils; slightly soluble in water. Used in organic synthesis, as an industrial solvent, in analytical chemistry, or as in anesthetic or extractant.	Extremely flammable, severe fire and explosion hazard when exposed to heat or flame. Forms explosive peroxides. Central-nervous-system depressant via inhalation and skin absorption.
explosives	A chemical compound that detonates as a result of shock or heat.	Detonation or deflagration.
flammable materials	Any solid, liquid, vapor, or gas that will ignite easily and burn rapidly. Flammable solids are of several types: (1) dusts or fine powders; (2) solids that ignite spontaneously at low temperatures; (3) solids in which internal heat is built up by microbial or other degradation activity; (4) films, fibers, and fabrics of low-ignition-point materials. The most common flammable gases are hydrogen, carbon monoxide, acetylene, and other hydrocarbon gases.	Fire hazard. Flammable gases are extremely dangerous fire hazards and require precisely regulated storage conditions. Flammable liquids and solids are defined by a flash point (temperature at which a liquid or volatile solid gives off a vapor sufficient to form an ignitable mixture with the air near its surface).
heavy metals	A metal of atomic weight greater than sodium (e.g., aluminum, lead, cobalt).	Most heavy metals are toxic.

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
hexone	See methyl isobutyl ketone	Flammable; dangerous fire risk. Avoid ingestion and inhalation. Can be absorbed by skin.
hydrochloric acid	Hydrogen chloride in aqueous solution; colorless or slightly yellow, fuming, pungent liquid. Hydrochloric acid is a strong, highly corrosive acid. Soluble in water, alcohol, and benzene. Noncombustible. Uses include acidizing (activation) of petroleum wells, boiler scale removal, chemical intermediate, ore reduction, pickling and metal cleaning, industrial acidizing, general cleaning, alcohol denaturant, and laboratory reagent.	Highly toxic by ingestion and inhalation; strong irritant to eyes and skin.
hydrofluoric acid	Hydrogen fluoride in aqueous solution. Colorless, fuming, mobile liquid; will attack glass and any silicon-containing material. Used in aluminum production, fluorocarbons, pickling stainless steel, etching glass, acidizing oil wells, fluorides, processing uranium.	Toxic by ingestion and inhalation; highly corrosive to skin and mucous membranes.
hydrogen	Nonmetallic element (atomic number 1). A diatomic gas; very slightly soluble in water, alcohol, and ether. Noncorrosive. Uses include chemical production, reducing atmosphere to prevent oxidation, oxyhydrogen flame or high temperatures, atomic-hydrogen welding, instrument-carrying balloons, production of high-purity metals, cryogenic research.	Highly flammable and explosive. Dangerous when exposed to heat or flame. Classified as an asphyxiant.
hydrogen fluoride	Colorless, fuming gas or liquid; very soluble in water. Uses include catalyst in alkylation, isomerization, condensation, dehydration, and polymerization reactions; fluorinating agent in organic and inorganic reactions; production of fluorine and aluminum fluoride; additive in liquid rocket propellants; refining of uranium.	Nonflammable. Toxic by ingestion and inhalation, strong irritant to eyes, skin, and mucous membranes.
inorganics	Any chemical compound that does not contain the element carbon, with the exception of the oxides of carbon; compounds containing a carbonate group such as calcium carbonate, carbon disulfide, phosgene, carbonyl sulfide, and metallic carbonyl.	Inorganic compounds range from those that are almost wholly inert (sand, clay, limestone) to highly active and corrosive materials (hydrofluoric acid).
isobutane	A liquefied petroleum gas. Colorless gas with slight odor; stable, does not react with water; has no corrosive action on metals. Soluble in water, slightly soluble in alcohol, and soluble in ether. Uses include organic synthesis, refrigerant, fuel, aerosol propellant, and instrument calibration fluid.	Highly flammable. Dangerous fire and explosion risk.

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
lead	Metallic element (atomic number 82). Heavy, ductile, soft, gray solid. Soluble in dilute nitric acid; insoluble in water, but dissolves slowly in water containing a weak acid; resists corrosion; relatively impenetrable to radiation. Poor electrical conductor; good sound and vibration absorber. Noncombustible. Used in storage batteries, process equipment, radiation shielding, cable covering, sheet and pipe, solder and fusible alloys, type metal, vibration damping in heavy construction, and foil.	Toxic by ingestion or inhalation of dust or fumes. A cumulative poison.
lithium	Metallic element (atomic number 3). It is the lightest and least reactive of the alkali metals and the lightest solid element. Very soft silvery metal. Reacts exothermally with nitrogen in moist air at high temperatures. High electrical conductivity. Soluble in liquid ammonia. Used in production of tritium, scavenger and degasifier for stainless and mild steels in molten state, modular iron, soaps and greases; used as deoxidizer in copper and copper alloys. Catalyst and heat-transfer liquid. Component in storage batteries (with sulfur, selenium, tellurium, and chlorine), rocket propellants, silver solders, and nuclear reactor coolant.	Ignites in air near its melting point (179°C). Dangerous fire and explosion risk when exposed to water, acids, or oxidizing agents. Lithium in solution is toxic to the central nervous system.
lithium beryllium hydride	White crystalline mixed salt. Used for energy and nuclear studies.	Fire risk when exposed to water, organic materials, and heat. Highly toxic.
lithium carbonate	White powder; slightly soluble in water and insoluble in alcohol; soluble in dilute acid. Uses include ceramics and porcelain glazes; pharmaceuticals; catalyst; other lithium compounds; coating of arc-welding electrodes; nucleonics; luminescent paints, varnishes, and dyes; glass ceramics; aluminum production.	Strong irritant in water solution.
lithium chloride	White deliquescent crystals; very soluble in water, alcohols, ether, pyridine, and nitrobenzene. One of the most hygroscopic salts known. Uses include air conditioning, welding and soldering flux, dry batteries, heat-exchange media, salt baths, desiccant, production of lithium metals.	Low toxicity; should not be ingested.

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
lithium hydride	White, translucent, crystalline mass or powder. Decomposed by water, forming hydrogen and lithium hydroxide; insoluble in benzene and toluene; soluble in ether. Uses include desiccant, source of hydrogen, condensing agent in organic synthesis, preparation of lithium amide and double hydrides, nuclear shielding material.	Flammable, dangerous fire risk; ignites spontaneously in moist air. Toxic.
lithium hydroxide	Colorless crystals that are slightly soluble in alcohol; soluble in water; absorbs carbon dioxide and water from air. Uses include storage battery electrolyte, lubricating greases, and ceramics.	Strong irritant in water solutions.
mercury	Metallic element (atomic number 80). Silvery, extremely heavy liquid. Insoluble in hydrochloric acid; soluble in sulfuric acid upon boiling; readily soluble in nitric acid. Insoluble in water, alcohol, and ether. Uses include amalgams, catalysts, electrical apparatus, instruments (thermometers, barometers, etc.), mildew-proofing preparations, mercury vapor lamps, extractive metallurgy, arc lamps, coolant, and neutron absorber in nuclear power plants.	Metallic mercury is highly toxic by skin absorption and inhalation of fumes or vapors; absorbed by respiratory and intestinal tract. All inorganic compounds of mercury are highly toxic by ingestion, inhalation, and skin absorption. Most organic compounds of mercury are highly toxic. Spillage may be a toxic hazard because of droplet proliferation. Cleanup requires special care.
methane	Colorless, odorless, tasteless gas; lighter than air; practically inert toward sulfuric acid, nitric acid, alkalies, and salts; reacts with chlorine and bromine in light (explosive in direct sunlight). Soluble in alcohol and ether; slightly soluble in water. Used in the synthesis of chemicals; used as a fuel in the form of natural gas.	Severe fire explosion hazard; forms explosive mixtures with air. Methane is an asphyxiant gas.
methyl isobutyl ketone (hexone)	Colorless, stable liquid; pleasant odor. Slightly soluble in water; miscible with most organic solvents. Uses include solvent for paints, varnishes, nitrocellulose lacquers; manufacture of methyl amyl alcohol; extraction processes, including extraction of uranium from fission products; organic synthesis; denaturant for alcohol.	Flammable; dangerous fire risk. Avoid ingestion and inhalation. Can be absorbed by skin.

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
nitric acid	Transparent, colorless or yellowish, fuming, suffocating, hygroscopic, corrosive liquid. Will attack almost all metals. The yellow color is due to release of nitrogen dioxide on exposure to light. Strong oxidizing agent. Miscible with water; decomposes in alcohol. Uses include manufacture of ammonium nitrate for explosives, organic synthesis (dyes, drugs, explosives, cellulose nitrate, nitrate salts), metallurgy, photoengraving, etching steel, ore flotation, reagent, reprocessing spent nuclear fuel.	Dangerous fire risk in contact with organic materials. Highly toxic by inhalation. Corrosive to skin and mucous membranes.
nitric oxide	Colorless gas (readily reacts with oxygen at room temperature to form nitrogen dioxide, a reddish-brown gas), slightly soluble in water. Used as an intermediate in production of chemicals.	Supports combustion. Toxic by inhalation, strong irritant to skin and mucous membranes.
organic compounds	Any substance that contains the element carbon, except carbon oxides and various carbonates. Some 700,000 organic substances have been identified.	Organic compounds are typically combustible or flammable. Variety of hazards to living tissue depending on substances involved.
oxidizing materials	Any compound that spontaneously evolves oxygen either at room temperature or under slight heating. Includes such chemicals as peroxides, chlorates, perchlorates, nitrates, and permanganates.	Vigorous reactions at ambient temperatures when stored near or in contact with reducing materials such as cellulosic and other organic compounds. Storage areas should be well ventilated and kept as cool as possible.
phosgene	Liquid or easily liquefied gas; colorless or light yellow; odor varies from strong and stifling when concentrated to hay-like in dilute form; slightly soluble in water and slowly hydrolyzed by it; soluble in benzene and toluene. Used in organic synthesis, pesticides, and herbicides.	Very toxic via inhalation, strong irritant to eyes.
phosphine	Colorless gas, disagreeable, garlic-like odor. Soluble in alcohol, ether, and cuprous chloride solution; slightly soluble in cold water; insoluble in hot water. Uses include organic preparations, phosphonium halides, doping agent for n-type semiconductors, polymerization initiator, condensation catalyst.	Spontaneously flammable. Toxic by inhalation, strong irritant.
polychlorinated biphenyl (PCB)	One of several aromatic compounds containing two benzene nuclei with two or more substitute chlorine atoms. Colorless liquid. Chief use is in heat-exchange and insulating fluids in closed systems.	Highly toxic. Persistent ecological hazard. (Because of persistence, toxicity, and ecological damage via water pollution, the manufacture of PCBs was discontinued in the United States in 1976).

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
potassium dichromate	Bright, yellowish-red, transparent crystals; bitter, metallic taste. Soluble in water; insoluble in alcohol. Used as oxidizing agent (chemicals, dyes, intermediates) and analytical reagent. Also used for brass pickling compositions, electroplating, explosives, pyrotechnics, safety matches, textiles, dyeing and printing, glass, chrome glues and adhesives, process engraving and lithography, alloys, ceramic products, depolarizer in dry cell batteries.	Toxic by ingestion and inhalation. Dangerous fire risk in contact with organic materials. Strong oxidizing agent.
propylene	Colorless gas; soluble in alcohol and ether; slightly soluble in water. Used in chemical synthesis.	Highly flammable. Dangerous fire risk. An asphyxiant gas.
pyrophoric	Any liquid or solid that will ignite in air at about 130°F. Sodium and lithium hydride are spontaneously flammable in moist air because they react exothermically with water. Must be stored in an atmosphere of inert gas or under kerosene.	Dangerous fire risk near combustible materials.
sodium hydroxide (caustic soda)	White deliquescent solid; occurs chiefly in form of beads or pellets, or as 50% and 73% aqueous solutions. Absorbs water and carbon dioxide from the air. Soluble in water, alcohol, and glycerol. Uses include chemical manufacturing, regenerating ion exchange resins, organic fusions, laboratory reagent, etching, and electroplating.	Corrosive to tissue in presence of moisture. Strong irritant to tissue (eyes, skin, mucous membranes).
sodium hypochlorite	Strong oxidizing agent, usually stored and used in solution; disagreeable, sweetish odor and pale greenish color. Soluble in cold water; decomposed by hot water. Uses include water purification, intermediate, organic chemicals, medicine, fungicides, swimming pools, household bleach, laundering, and reagent.	Fire risk in contact with organic materials. Toxic by ingestion; strong irritant to tissue.
sodium- potassium alloy (NaK)	Soft, silvery solid or liquid; must be kept away from air and moisture. The liquid forms come under the class name potassium or sodium; metallic liquid alloy. Uses include heat exchange fluid, electric conductor, organic synthesis, and catalysis. Legal label name for NaK.	Ignites in air; explodes in presence of moisture, oxygen, halogens and acids. Store under kerosene.

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
solvents	A substance capable of dissolving another substance (solute) to form a uniformly dispersed mixture (solution). Water is the most common of all solvents. Aromatic hydrocarbons have higher solvent power than aliphatics (alcohols). Other organic solvent groups are esters, ethers, ketones, amines, and nitrated and chlorinated hydrocarbons. Uses include coatings (paints, varnishes, and lacquers), industrial cleaners, printing inks, extractive processes, and pharmaceuticals.	Many solvents are flammable and toxic to varying degrees. Contribute to air pollution and fire hazards.
sulfur dioxide	Colorless gas or liquid with sharp, pungent odor. Soluble in water, alcohol, and ether. An outstanding oxidizing and reducing agent. Noncombustible. Uses include chemicals (sulfuric acid, sulfites, hydrosulfites of potassium and sodium, thiosulfates, alum from shale, and recovery of volatile substances), ore and metal refining, intermediates, solvent extraction of lubricating oils, disinfecting, reducing agent, and antioxidant.	Toxic by inhalation. Strong irritant to eyes and mucous membranes, especially under pressure. Dangerous air contaminant and constituent of smog.
sulfuric acid	Strongly corrosive, dense, oily liquid; colorless to dark brown depending on purity. Miscible with water. Very reactive, dissolves most metals; concentrated acid oxidizes, dehydrates, or sulfonates most organic compounds, often causes charring. Uses include chemicals, dyes and pigments, etchant, alkylation catalyst, electroplating baths, industrial explosives, laboratory reagent, and nonferrous metallurgy.	Highly toxic. Strong irritant to tissue.
thorium	Metallic element (atomic number 90); a member of the actinide series. Soft metal with bright silvery luster when freshly cut; similar to lead in hardness when pure. Can be cold-rolled, extruded, or drawn and welded. Soluble in acids; insoluble in alkalies and water. Some alloys may ignite spontaneously; not flammable in massive form. Uses include nuclear fuel, sun lamps, photoelectric cells, target in x-ray tubes, and alloys.	Flammable and explosive in powder form. Dusts of thorium have very low ignition points and may ignite at room temperature. Radioactive decay isotopes are dangerous when ingested.
tributyl phosphate	Stable, colorless, odorless liquid. Miscible with most solvents and diluents. Soluble in water. Uses include heat-exchange; solvent extraction of metal ions from solution of reactor products; solvent for nitrocellulose, cellulose acetate; plasticizer; pigment-grinding assistant; antifoam agent; dielectric.	Combustible. Toxic by ingestion and inhalation. Irritant to skin.

SAMPLE LIST OF HAZARDOUS CHEMICALS WITHIN DOE COMPLEX

CHEMICAL OR TERM	CHARACTERISTICS AND USES	POTENTIAL HAZARDS
uranium hexafluoride	Colorless, volatile crystals; sublimes; soluble in liquid bromine, chlorine, symtetrachloroethane, carbon tetrachloride, and fluorocarbons. Reacts vigorously with water, alcohol, ether, and most metals. Vapor behaves as nearly perfect gas. Used in gaseous diffusion process for separating isotopes of uranium.	Highly corrosive. Radiation risk.

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