United States
Environmental Protection
Agency

Office of Air Quality
Planning and Standards
Research Triangle Park, NC 27711

EPA-454/R-93-002
(Revises EPA-450/4-91-007)
May 1993

Air

EPA

GUIDANCE ON THE APPLICATION OF REFINED DISPERSION MODELS FOR HAZARDOUS/TOXIC AIR RELEASES

Office of Air Quality
Clean Air
OAQPS
Planning and Standards

EPA-454/R-93-002

Guidance on the Application of Refined Dispersion Models for Hazardous/Toxic Air Releases

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Chicago, IL 60604-3590

U.S. Environmental Protection Agency
Office of Air Quality Planning and Standards
Technical Support Division
Research Triangle Park, NC 27711

May 1993

This report has been reviewed by the Office of Air Quality Planning and Standards, U.S. Environmental Protection Agency, and has been approved for publication. Any mention of trade names and commercial products is not intended to constitute endorsement or recommendation for use.

EPA-454/R-93-002

ACKNOWLEDGEMENTS

This report was prepared by Radian Corporation for the United States Environmental Protection Agency under contract number 68-D0-0125 with Mr. Jawad S. Touma as the Work Assignment Manager. He is on assignment to the U.S. EPA from the National Oceanic and Atmospheric Administration, U.S. Department of Commerce. Providing assistance were Messrs. Jim Yohn and Doug Blewitt, Amoco Corporation (SLAB and HGSYSTEM model application and interpretation), Drs. Jerry Galt and Roy Overstreet, National Oceanic and Atmospheric Administration (ALOHA model application and interpretation), Dr. David Yeh, South Coast Air Quality Management District (general review), and Dr David Guinnup, EPA (general review).

PREFACE

This document supersedes "Guidance on the Application of Refined Dispersion Models for Air Toxic Releases," EPA-450/4-91-007.

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SECTION 1

INTRODUCTION

The "Guideline on Air Quality Models (Revised)"[1] provides guidance on the use of air quality modeling techniques for a variety of pollutants. Although many of the models in the guideline have been used in simulating releases of hazardous air pollutants, it has been recognized that there is a need to provide models that specifically address impacts of hazardous air pollutants.

To meet this need, EPA published "Workbook of Screening Techniques for Assessing Impacts of Toxic Air Pollutants(Revised)"[2] and developed the TSCREEN model[3]. The workbook provides a logical approach to the selection and use of appropriate screening techniques for estimating emission rates and ambient concentrations resulting from eighteen different types of release scenarios. TSCREEN, a model for screening toxic air pollutant concentrations, is an IBM-personal computer model that implements the methods described in the workbook. EPA co-sponsored the development of the DEGADIS refined dense gas model[4] and conducted a statistical model evaluation study of several dense gas models using three experimental programs[5]. In 1990, EPA provided general guidance considerations on determining input and applying several dense gas models that are in the public domain[6]. EPA has recently published a guidance document that illustrates the possible range of different kinds of accidental releases of hazardous air pollutants that might take place at Superfund sites and demonstrates how atmospheric dispersion models, including dense gas models, should be applied[7].

Title III of the Clean Air Act Amendments (CAAA) of 1990 lists many chemicals as hazardous air pollutants and requires establishing regulations to prevent the accidental release and to minimize the consequence of any such

releases. With the large number of potential release scenarios that are associated with these chemicals, there is a need for a systematic approach for applying mathematical models to estimate impact from these potential release scenarios. Because many chemicals may form dense gas clouds upon release, and refined mathematical models that can simulate these releases are complex, particular attention is paid to models can address these types of releases.

This document provides general guidance on characterizing hazardous air pollutant releases and shows how to apply appropriate dispersion models. It supersedes the document "Guidance on the Application of Refined Dispersion Models for Air Toxic Releases"[6] published in 1991. Specifically, this document:

- Helps determine likely or reasonable storage conditions for specific chemicals for which a release might occur;
- Helps determine release classes (e.g., liquid or gaseous phase) of a hazardous release;
- Defines the steps to be taken when determining if a release should be considered a dense gas release (and thus require the use of a model capable of such a simulation);
- Defines the methods used to determine the input variables used by commonly-used refined models in the public domain;
- Points out the implications and effects of various choices for input information;
- Shows, by example, the calculation of the input variables used by the models;
- Describes the outputs available from the models; and
- Discusses how to determine the input that gives the "worst-case" impact conditions.

Section 2 introduces the term "release class" and defines the eight release classes used in this document. General release scenarios which may occur, and lead to the release classes, are tabulated. A method is described

for the determination of likely or reasonable storage conditions for specific chemicals.

Section 3 describes the models used in this document, which include:

- ADAM;
- ALOHA;
- DEGADIS;
- HGSYSTEM; and
- SLAB.

Section 4 provides a method to determine a release class from observable parameters. This section also describes the methods to calculate model input parameters and how to determine if a release should be considered a dense release.

Section 5 gives examples of how inputs are calculated for each of the release classes using the methods described in Section 4. Section 6 documents which of the inputs calculated in Section 5 are used by each model and some of the implications and effects of various choices for input. Section 7 describes how to determine specific output parameters from the models. Section 8 discusses how to determine input that yields the "worst case" impact. Appendix A discusses the relationship between some of the SI units (Le Système International d'Unités). This document gives all calculation results in SI units. Appendix B contains data associated with the chemicals considered in this project.

The information contained in this document, especially sections 6, 7, and 8, was obtained directly from the developers of the models or, when those individuals were not available, from others who are intimately familiar with that model. Specifically, the model consultants performed the following:

- Selection of final model input;
- Running the model;

- Providing direction on how to interpret the output; and
- Reviewing and contributing to the section of the report on determining input for modeling the "worst case" impacts.

SECTION 2

SCENARIO AND CHEMICAL SELECTION

This section describes the chemicals, release classes, and release scenarios addressed by the models in this study. Section 2.1 describes the chemical selection criteria. Section 2.2 introduces and defines the chemical "release classes" under which the model input guidance is categorized in Sections 4 and 5. Section 2.3 summarizes the example "release scenarios" which were chosen for analysis. Section 2.4 provides guidance on how to use model input to make an initial release class determination.

2.1 SELECTION OF CHEMICALS FOR RELEASE MODELING

The following chemicals were chosen for the modeling study:

- Ammonia (NH_3), anhydrous and aqueous;
- Chlorine (Cl_2);
- Hydrogen Fluoride (HF), anhydrous and aqueous;
- Hydrogen Chloride (HCl), anhydrous and aqueous;
- Ethylene Oxide (CH_2CH_2O); and
- Sulfur Dioxide (SO_2).

These chemicals were selected because each one meets the criteria established for the modeling study: 1) they are all commonly used chemicals that may form dense gas clouds when released; and 2) they all present acute toxicity or flammability hazards and are, therefore, of particular interest to regulatory agencies. In addition, the six chemicals together represent all of the five basic release classes (identified and described in the following section) when released under certain conditions.

2.2 DESCRIPTION OF CHEMICAL RELEASE CLASSES

The release class defines the physical state of the chemical as it leaves containment and the manner in which it enters the atmosphere to form a vapor cloud. Depending on the physical properties (vapor pressure or boiling point) and pre-release storage conditions, hazardous chemicals can be emitted from a container as a liquid, a vapor, or both (a two-phase release). Released liquids may form a vapor cloud through volatilization. A liquid can be volatilized either completely or partially as it is released, forming a vapor cloud or a vapor and droplet mixture. Conversely, vapors may partially or completely condense to form liquid droplets when released. The degree of condensation, if it occurs, will again depend on the pre-release conditions and physical properties of the material. Condensed vapor may fall to the ground to form a pool which, in turn, volatilizes to the atmosphere.

For purposes of defining dense gas model input, hazardous material releases have been separated into eight general categories of release classes. A separate set of calculations and considerations for defining model input is required for each release class. The methods and procedures for determining the release class and establishing necessary model input are defined in Section 4.0. The release class categories are listed and described in Sections 2.2.1 through 2.2.8. Section 2.2.9 discusses additional release class considerations, and includes an example of a hazardous material release that falls into multiple release classes.

Vapor release rates may be limited due to the "choked" flow phenomenon which develops when containment pressures are relatively high. Choked flow refers to the velocity limit at which a material may be released and depends on the containment pressure and the physical properties of the material. Since the release velocity is limited under choked flow conditions, the volumetric flow rate through a given hole size is also limited, and is independent of containment pressure. However, the mass emission rate will vary with containment pressure above the choked flow limit, since the material's density varies with pressure.

2.2.1 Two-phase Gas Release (Choked)

A two-phase gas release is a release of a gas that partially condenses to form two phases (gas and liquid). Conversely, a two-phase liquid release begins as a liquid and partially vaporizes to form two phases. In terms of post-release characteristics, two-phase releases are similar regardless of whether the material is initially a gas or liquid. However, the distinction between two-phase gas and liquid releases is important, since the model input calculations (primarily to determine the emission rate) are different for the two cases.

A two-phase gas release is a release of a material that is normally a gas under ambient conditions. The material may be stored either as a compressed gas or as a liquified gas; however, a two-phase gas release (as opposed to a two-phase liquid release) from liquified gas storage must come from the vapor space within the storage container. A two-phase gas release occurs due to cooling of the gas when it expands as the material's pressure drops upon release. The resulting adiabatic expansion subcools some or all of the material (subcooling refers to cooling to a temperature below a material's boiling point). Thus, a liquid phase is formed immediately after the release.

Figure 2-1 illustrates the two-phase gas release class. As the figure shows, there are several possible fates for the liquid formed in the gas. The liquid may "rain out" from the vapor/liquid release and form a liquid pool which will evaporate. The condensed liquid may also form an "aerosol", or finely dispersed mist, which is transported downwind in the vapor cloud where it ultimately vaporizes. The formation of a liquid pool, aerosol, or combination of the two is dependent upon the material and its release characteristics.

In a two-phase choked gas release, containment pressures are sufficiently high as to cause both condensation upon depressurization and attainment of choked flow conditions. At containment pressures above the

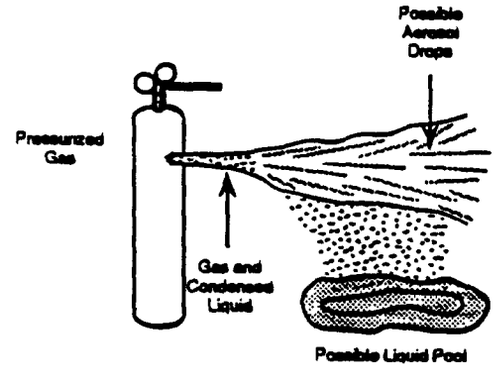


Figure 2-1. Two-phase Gas Release

choked flow threshold, the release velocity (and, therefore, the volumetric release rate through a given hole size) is independent of containment pressure. However, the mass emission rate will vary with containment pressure above the choked flow limit since the material's density varies with pressure.

2.2.2 Two-phase Gas Release (Unchoked)

The conditions defining a two-phase unchoked gas release are similar to those that define a two-phase choked gas release. In a two-phase unchoked gas release, containment pressures are sufficiently high to cause condensation upon depressurization, but not so high as to result in choked flow conditions.

Model input calculations, particularly those for determining the emission rate, are different for choked and unchoked gas release conditions. At pressures below the choked limitation, the release velocity (and therefore, the volumetric release rate through a given hole size) is a function of the containment pressure. At pressures above the choked flow limitation, the release velocity through a given hole size is independent of containment pressure.

2.2.3 Two-phase Pressurized Liquid Release

A two-phase liquid release is a release of a liquid that partially vaporizes to form two phases (liquid and gas). A "two phase pressurized liquid" release is a release of a liquid phase material that is a gas at ambient conditions. The material is held in the liquid phase via pressure in the containment vessel. Upon release, the liquid pressure immediately drops to ambient pressure, resulting in sudden vaporization of some or all of the liquid. This phenomenon is termed "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., the a ambient boiling temperature and the heat of vaporization of the material).

Figure 2-2 illustrates a two-phase liquid release under conditions where flashing occurs. As in the case with two-phase gas releases, the liquid portion of the release may either 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 (described in the following section) since the release energy tends to be relatively high for pressurized releases.

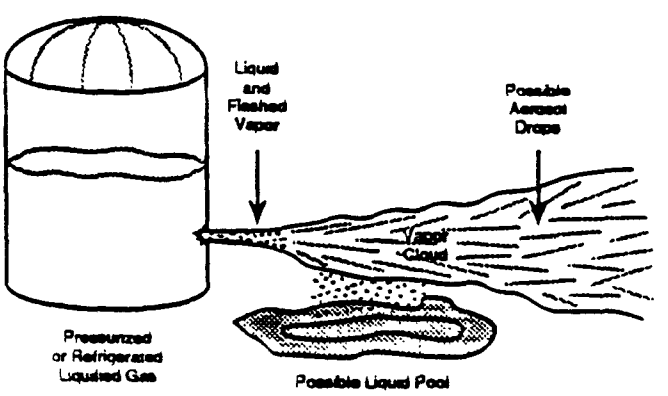


Figure 2-2. Two-phase Liquid Release

2.2.4 Two-phase Refrigerated Liquid Release

A two-phase refrigerated liquid release is a release from a containment vessel in which the material is held in the liquid phase via refrigeration. The material exists as a vapor at ambient temperature, but is stored at a temperature below its boiling point (i.e., it is stored as a subcooled liquid). If flashing occurs, the release is usually mildly flashing, since the release temperature is normally just above the material's boiling point. Therefore, the flashed fraction in a two-phase refrigerated liquid release is usually much less than that of a two-phase pressurized liquid release.

Regarding the determination of model input, the primary distinction between two-phase refrigerated liquid release and a two-phase pressurized liquid release involves the calculation of the emission rate, which is based on the difference between the containment pressure and the ambient pressure. Since refrigerated liquids are stored at ambient pressure, containment pressure is determined by the mass of liquid above the release location (i.e., the height of the liquid level). This force is typically much smaller than that of the pressurized case, and therefore usually results in a lower release rate.

The released material from a two-phase refrigerated liquid release may form an aerosol and/or a liquid pool. If a pool is formed, it will volatilize as it absorbs heat from the surroundings and the spill surface. As the pool evaporates it will cool and the evaporation rate should decrease. The tendency for aerosol formation from a refrigerated liquid may be minimal since the release energy is typically low.

2.2.5 Single-phase Gas Release (Choked)

A single-phase gas release is a release of a material that is a gas at ambient conditions and remains a gas throughout the release (i.e., no liquid phase develops). The material may be stored as either a compressed or a liquified gas. A single-phase gas release from liquified gas storage must come from the vapor space within the containment vessel.

Figure 2-3 illustrates a single-phase gas release. A gas release will not condense if its pressure is too low to result in "subcooling" the material during the release (i.e., to a temperature below its boiling point). Choked flow develops if release pressures are sufficiently high to reach the choking velocity limitation (refer to Section 2.2.1).

It should be noted that the development of choked velocities and the condensation of gas releases is highly dependent upon the physical properties of the released material. Section 2.2.2 described conditions where release pressures were such that condensation occurred but choked flow did not develop. For a single-phase, choked gas release, the situation is reversed. That is, the pressures are such that no condensation occurs but choked flow does. Since these phenomena are chemical-property dependent, one material may exhibit the "condensation but no choked flow" combination, whereas another may exhibit the "choked flow but no condensation" combination.

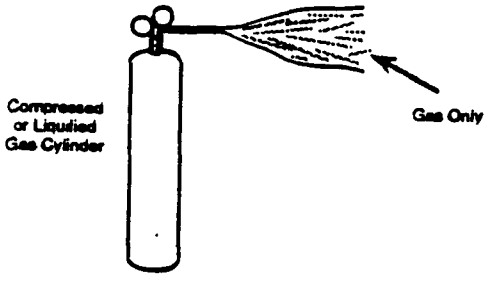


Figure 2-3. Single-phase Gas Release

2.2.6 Single-phase Gas Release (Unchoked)

Conditions resulting in a single-phase unchoked gas release are similar to those that result in single-phase choked gas releases. That is, containment pressures are below those that cause either condensation or choked-flow conditions during the release.

As discussed in Section 2.2.2, emission rate calculations for defining model input are different for choked and unchoked gas release conditions. At pressures below the choked limitation, the release velocity (and thus the

volumetric release rate through a given hole size) is a function of the containment pressure. For choked gas releases, the release velocity is independent of the containment pressure.

2.2.7 Single-phase Liquid Release (High Volatility)

A single-phase release of a high volatility liquid is a release of a material that, although a gas at ambient conditions, is stored in the liquid phase through refrigeration to a temperature below its boiling point (the material is "subcooled"). The release is a single-phase release if its release temperature is at or below the normal boiling point of the material, so that no flashing occurs.

Figure 2-4 illustrates a single-phase high volatility liquid release. The released liquid will form a pool which will volatilize as it absorbs heat from the surroundings and the spill surface. The temperature of the pool will be reduced as material evaporates. As previously discussed, the tendency for aerosol formation from a refrigerated liquid may be minimal since the release energy is typically relatively low. When calculating the atmospheric emission rate (the rate of vapor cloud formation) for a single-phase high volatility liquid, it is assumed that immediate volatilization of the material occurs (for model input calculations, see Section 4.0).

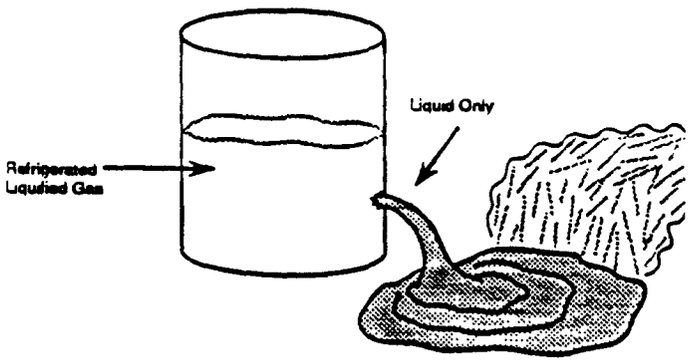


Figure 2-4. Single-phase High Volatility Liquid Release

2.2.8 Single-phase Liquid Release (Low Volatility)

A single-phase release of a low volatility liquid is a release of a material that is a liquid at ambient conditions. Neither refrigeration nor pressurization is needed to hold the material in liquid form. Figure 2-5 shows the single-phase low volatility liquid release.

A low volatility liquid will form a liquid pool upon release. The rate of ejection of mass from the container into the pool depends on the release size and height of the liquid level above the hole in the containment vessel. The atmospheric emission rate (the rate of vapor cloud formation) is only dependent on evaporation. Therefore, the area of the pool, the ambient temperature and wind speed, and the volatility (vapor pressure) of the released liquid determine the atmospheric emission rate.

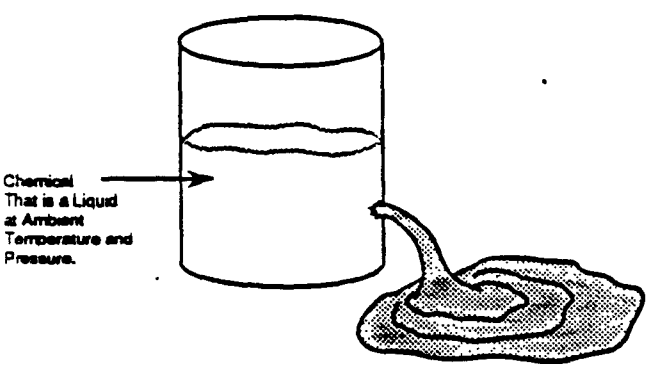


Figure 2-5. Single-phase Low Volatility Liquid Release

To determine the rate of atmospheric emission (rate of vapor cloud formation) of a low volatility liquid, the calculated liquid ejection rate must be compared to the atmospheric emission (volatilization) rate to establish the limiting condition. Section 4.0 explains how this comparison is made to determine the atmospheric emission rate for use as model input.

2.2.9 Additional Release Class Considerations

A given "release scenario" may simultaneously or sequentially produce a release that fits more than one of the release classes described in the preceding sections. To define the term "release scenario", and to illustrate

how multiple release classes may develop, the following example scenario is provided.

> A hazardous chemical which is a dense vapor at ambient conditions is stored as a liquid under pressure. A pipe leading from the bottom of the tank is severed, and the pressurized liquid flows toward the open pipe. The pressure of the liquid drops as it flows through the pipe, resulting in vaporization of part of the liquid within the pipe (adiabatic flash) before it reaches the point where it is released to the atmosphere. Once all of the liquid within the vessel is released, the remaining compressed vapor is expelled through the release opening.

Figure 2-6 illustrates this scenario. As shown, this type of release scenario initially results in a two-phase pressurized liquid release. The liquid fraction may form an aerosol, a short-lived liquid pool, or a combination of the two. If all of the liquid fraction is assumed to form aerosol, the atmospheric emission rate (vapor cloud formation rate) is assumed to be equal to the mass emission rate of both the liquid and vapor phases. If all of the liquid fraction is assumed to form a pool, the emission rate would be a combination of the rate of the vapor release rate and the rate at which the pool evaporates. If partial aerosol formation is assumed, a combination of the two calculations would be used.

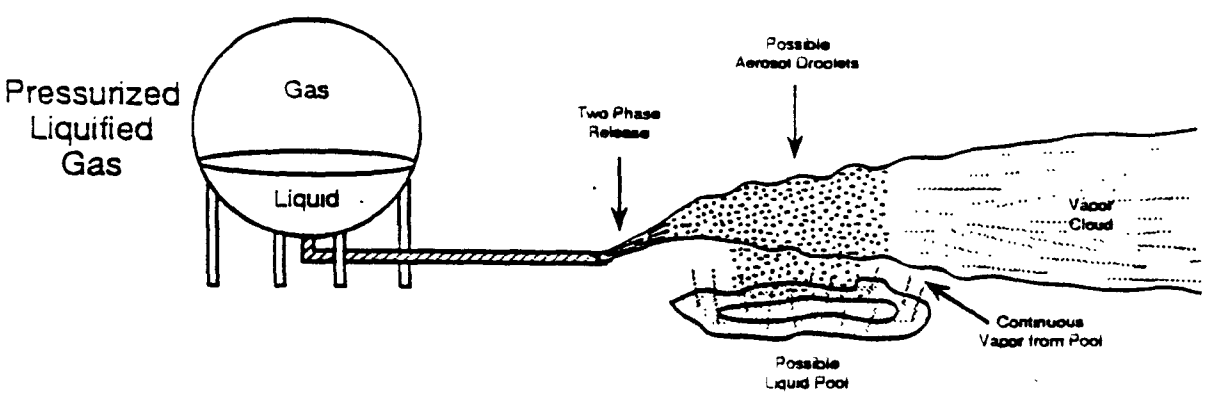


Figure 2-6. Example Release Scenario

It should be noted that, for the purposes of this modeling study, the rate of vapor cloud formation from a two-phase pressurized liquid release is assumed to be equal to the sum of the vapor and liquid release rates from the vessel. The basis for this assumption is that any pool that forms will evaporate very quickly, and the assumption of immediate vaporization results in a maximum vapor cloud generation rate which tends to produce conservative modeling results.

A second distinct release class results when all of the liquid is released from the vessel. The remaining compressed vapor will be expelled from the tank under either two-phase or single-phase gas release conditions, which may be either choked or unchoked. The specific gas release class and rate is determined by the pressure of the gas within the vessel. Under actual conditions, the tank pressure will decrease as the gas is expelled. For purposes of this study, however, the initial pressure is used to calculate the maximum release rate, which is assumed to be constant for the duration of the release. A maximum release rate tends to produce conservative modeling results.

A dense gas modeling analysis of scenarios involving multiple release classes may require combining results from multiple modeling runs. Where multiple release classes occur simultaneously, the vapor cloud generation rates from each class may be added to determine model input. Sequential or overlapping release classes may need to be considered individually and in combination to determine the most reasonable approach for interpreting results.

Table 2-1 shows the possible release classes which can result from common storage configurations. The table summarizes the criteria for determining the initial release class, and lists potential subsequent release classes that might develop for each storage situation. Most release scenarios chosen for this study are based on common storage configurations.

TABLE 2-1. POSSIBLE RELEASE CLASSES RESULTING FROM TYPICAL STORAGE CONDITIONS

Storage Condition	Initial Release Class	Release Class Considerations
Liquified Gas (Pressurized)	Two-phase Pressurized Liquid (hole below liquid level)	Liquid phase of release may form aerosol droplets and/or liquid pool, which will vaporize very quickly. Vapor release will result after liquid level falls below height of hole, or after all liquid is released from the vessel. Vapor release could be two-phase or single-phase, choked or unchoked, depending on release pressure.
Liquified Gas (Pressurized)	Single- or Two-phase Gas (hole above liquid level)	Release will be two-phase if condensation occurs, choked or unchoked. Subsequent release classes could involve transition from two-phase to single-phase, and/or choked to unchoked if vessel pressure drops over time. While liquid is in vessel, however, pressure will remain relatively constant unless substantial liquid cooling results from vaporization in vessel.
Liquified Gas (Refrigerated)	Single-phase, High Volatility	Liquid will remain single-phase if release temperature is below boiling point. Liquid will form short-lived pool which evaporates as heat is absorbed from surroundings. Vapor release will occur after material liquid level drops below hole. Pressure of vapor release will depend on liquid temperature in vessel, but will normally be below condensation and choked flow pressures.
Liquified Gas (Refrigerated)	Two-phase Liquid (hole below liquid level)	Two-phase release occurs if release temperature is above material's boiling point. Release is normally mildly flashing since release temperature is normally near boiling temperature. Possible subsequent release classes are same as for two-phase liquid release from pressurized vessel.

TABLE 2-1. (CONTINUED)

Storage Condition	Initial Release Class	Release Class Considerations
Liquified Gas (Refrigerated)	Single-phase Gas (hole above liquid level)	Since storage condition dictates that material is cooled to below boiling point, vapor pressure of liquid will be less than one atmosphere. Thus, vapor will be released relatively slowly as single-phase gas (as long as liquid remains cooled). Pressures will most likely be below minimum required for either condensation or choked flow conditions. No subsequent release classes will develop.
Compressed Gas	Single- or Two-phase Gas	Condensation will depend on material properties and storage pressure. Flow could be choked or unchoked. Subsequent release classes are same as for single- or two-phase gas release from pressurized liquified gas vessel. Since no liquid is in container, the vessel pressure will continuously drop during release.
Liquid (Chemical is liquid at ambient temperature)	Single-phase, Low Volatility Liquid	Released liquid will form pool that will volatilize at a rate depending on material's vapor pressure. Minor vapor release from vessel will occur after liquid is expelled.

2.3 SELECTION OF RELEASE SCENARIOS FOR MODELING

A total of eight release scenarios covering each of the release classes described in Section 2.2 were assembled for the purposes of this study. Most of the scenarios were selected from a larger general list, which covers most of the release class possibilities for each selected material in a typical storage condition.

Table 2-2 lists the eight release classes covered in the modeling analysis, as well as general release scenarios which could produce each of the release classes for a given chemical. Also included in Table 2-2 are the normal boiling temperatures of the each material, and a summary of the post-release state and dense gas vapor cloud hazards for each material.

Several "in-process" scenarios were selected since not all release classes could be covered using reasonable storage conditions with materials in vapor-liquid equilibrium (a condition which exists for nearly all storage conditions). In addition, a stack release was selected to produce a suitable example of a waste gas stream which is a combination of a hazardous material, air, and water vapor. This scenario was selected primarily to illustrate the determination of release density for a typical stack release.

Table 2-3 summarizes the release scenarios selected as examples for discussion in this document. A description of the release scenario is provided, along with the release class each scenario represents. The ehtylene oxide saturated vapor phase pipeline release scenario is used for two release classes (two-phase gas release, choked and unchoked) . Although some of the selected release scenarios could produce multiple release classes, only one class was addressed for each. Each of the eight release classes described in Section 2.2 was included to provide an example of model input determination for each class.

TABLE 2-2. STORAGE RELEASE SCENARIOS AND POST-RELEASE CHARACTERISTICS OF SELECTED CHEMICALS

Release Class	Ammonia, Anhydrous and Aqueous	Chlorine	Hydrogen fluoride, Anhydrous and Aqueous	Hydrogen Chloride, Anhydrous and Aqueous	Ethylene Oxide	Sulfur Dioxide
Boiling Point (for Anhydrous Material)	-33.4°C (28.1°F)	-34.6°C (-30.3°F)	19.4°C (66.9°F)	-85°C (-121°F)	10.6°C (50.1°F)	-10°C (14°F)
Single-phase Gas (Choked or Unchoked) or Two-phase Gas (Choked or Unchoked)	1. Hole in NH_3 (anhydrous) pressurized liquid storage vessel above liquid level, or 2. Hole in NH_3 (anhydrous) vapor storage vessel.	1. Hole in liquid storage vessel above liquid level, or 2. Hole in vapor storage vessel.	1. Hole in HF (anhydrous) pressurized liquid storage vessel above liquid level, or 2. Hole in HF (anhydrous) vapor storage vessel.	Hole in pressurized HCl (anhydrous) storage vessel.	1. Hole in liquid storage vessel above liquid level, or 2. Hole in vapor storage vessel.	1. Hole in liquid storage vessel above liquid line, or 2. Hole in vapor storage vessel.
Two-phase Refrigerated Liquid	Hole in NH_3 (anhydrous) refrigerated liquid storage vessel.	N/A	Hole in HF (anhydrous) refrigerated liquid storage vessel.	N/A	N/A	N/A
Single-phase, High Volatility Liquid	Hole in NH_3 (anhydrous) refrigerated liquid storage vessel.	N/A	Hole in HF (anhydrous) refrigerated liquid storage vessel.	N/A	N/A	N/A
Two-phase Pressurized Liquid	Hole in NH_3 (anhydrous) pressurized liquid storage vessel below liquid level. Also may form a pool.	Hole in pressurized liquid storage vessel below liquid level. Also may form a liquid pool.	Hole in HF (anhydrous) pressurized liquid storage vessel below liquid line. Also may form liquid pool.	N/A	Hole in EO pressurized liquid storage vessel below liquid level.	Hole in pressurized liquid storage vessel below liquid line. Also may form liquid pool.
Single-phase Low Volatility Liquid	Hole in NH_3 (aqueous) tank below liquid level. Liquid pool formed.	N/A	Hole in HF (aqueous) tank below liquid level. Liquid pool formed.	Hole in HF (aqueous) vessel below liquid level. Liquid pool formed.	N/A	N/A

TABLE 2-2. (CONTINUED)

Release Class	Ammonia, Anhydrous and Aqueous	Chlorine	Hydrogen fluoride, Anhydrous and Aqueous	Hydrogen Chloride, Anhydrous and Aqueous	Ethylene Oxide	Sulfur Dioxide
Single-phase High Volatility Liquid	Hole in NH_3 (anhydrous) refrigerated liquid storage vessel.	N/A	Hole in HF (anhydrous) refrigerated liquid storage vessel.	N/A	N/A	N/A
Post-Release State						
	Gas, normally lighter than air. Can be heavier than air due to aerosol effect: liquid droplets and cooling from a flash. Also, a brief-lived boiling liquid release is possible. or Aqueous NH_3 liquid	Gas (2.5 times heavier than air) plus aerosol. Also, a brief-lived boiling liquid release is possible.	Gas which is lighter than air but could be heavier than air due to self-association of HF at low P, T, and due to aerosol effect. Also, a boiling liquid release is possible. or Aqueous HF liquid	Gas (1.3 times heavier than air). or Aqueous HCl liquid	Gas (1.5 times heavier than air).	Gas (2.2 times heavier than air).
Post-Release Hazards and Changes						
	Toxic, flammable (but high minimum ignition temp.--1562°F and narrow flammable concentration range, 16-25% volume). Reactive and corrosive when combined with water.	Toxic, but not flammable. Corrosive when combined with moisture (HCl formation).	Toxic, hygroscopic: heat evolves and forms corrosive hydrofluoric acid when combined with water.	Toxic, non-flammable, highly corrosive.	Toxic, highly flammable.	Toxic. Noncombustible. Combines with water to form sulfurous acid (H_2SO_3). Also may be reduced by H_2 in the presence of water to form H_2S.

N/A indicates that release class does not occur for typical storage conditions of the material.

TABLE 2-3. DESCRIPTIVE SCENARIOS FOR MODELING

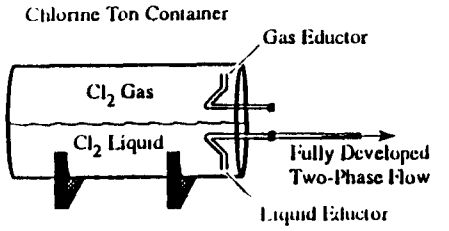
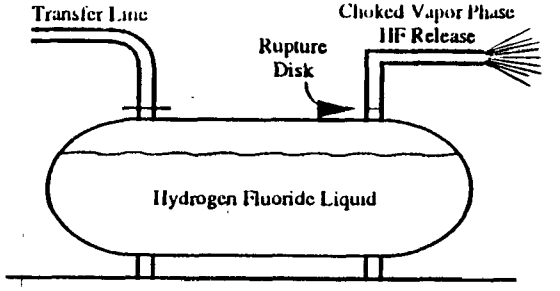
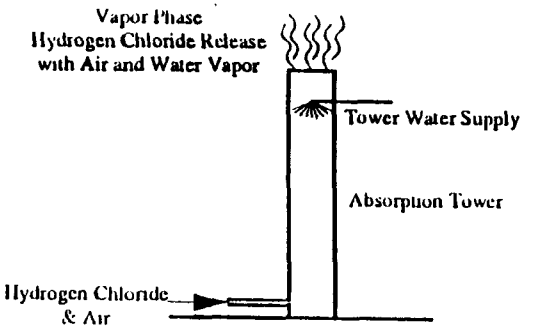
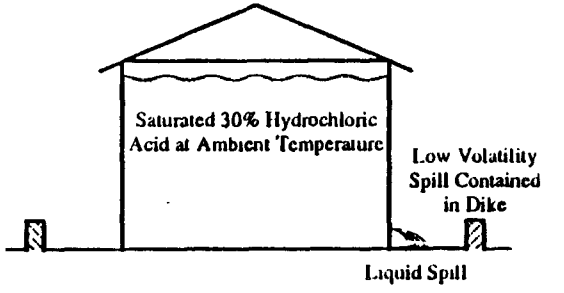
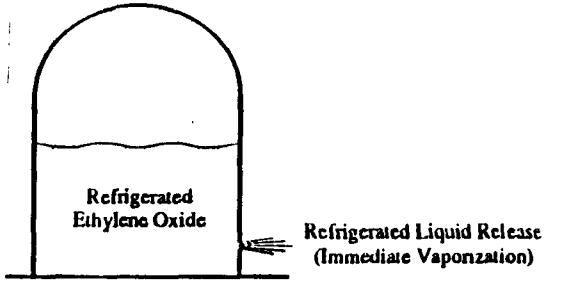
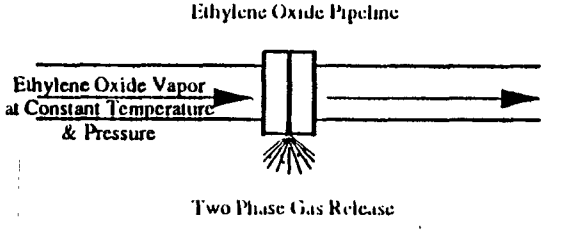
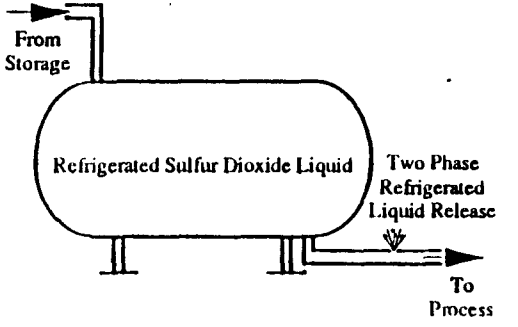
Chemical	Scenario Description	Illustration
Chlorine	Tubing from bottom of pressurized, ambient temperature vessel storing liquified chloring is broken off. This produces initial two-phase pressurized liquid release.	
Hydrogen Fluoride, anhydrous	Rupture disk breaks and relieves material from vapor space of pressurized, ambient temperature tank storing liquid HF. This produces an initial single-phase gas release (choked)	
Hydrogen Chloride, anhydrous	Water flow is lost to tower absorbing HCl from vent stream. This results in single-phase gas release (unchoked).	

TABLE 2-3. (CONTINUED)

Chemical	Scenario Description	Illustration
Hydrogen Chloride, aqueous	Hole develops in side of atmospheric pressure tank storing 30 wt.% hydrochloric acid in liquid phase. This results in a single-phase, low volatility liquid release.	
Ethylene Oxide	Hole develops in refrigerated vessel storing liquid EO at atmospheric pressure. Since hole is below the liquid level, the initial release is a single-phase, high volatility liquid release.	
Ethylene Oxide	Hole develops in saturated vapor phase pipeline. This leak results in two-phase gas release. The release flow rate may be choked or unchoked. This scenario is used in two release class examples.	
Sulfur Dioxide	A hole develops in a pipe from the bottom of a vessel storing liquid SO_2. Initial release is a two-phase refrigerated liquid release.	

The selection of release scenarios for hazardous material release impact modeling for an actual modeling submittal is not a trivial matter. Scenarios are most frequently selected as a result of a formal "hazard analysis" study. One of the goals of a hazard analysis is to produce a set of release scenarios meeting predetermined criteria for probability of their occurrence. The process of combining scenario probability (which may be determined qualitatively or quantitatively) with consequence analysis results (determined by applying impact modeling results) is termed "risk assessment". The final result provides useful qualitative and/or quantitative data on which emergency planning or other risk management decisions (e.g. whether to invest in risk reduction measures) are based.

2.4 VERIFICATION OF RELEASE SCENARIOS IN THE REVIEW OF MODELING SUBMITTALS

The starting point for any modeling submittal is the release scenario(s) chosen for modeling. The level of detail used to describe the release scenario(s) in the submittal may vary widely depending on specific regulatory requirements. At a minimum, the storage, processing, or transportation conditions necessary to define all model input should be included in the submittal to allow for complete model input verification.

The purpose of this section is to outline some procedures that can be used to check and verify pre-release conditions defined in scenario descriptions. Also, this section includes some basic guidance for determining an initial release class. The final determination of release class should, however, be made using the procedures outlined in Section 4.3.

Table 2-4 provides a listing of typically-encountered storage conditions for each of the chemicals chosen for this modeling study. For releases involving storage of any of the chemicals, the storage phases and volumes can

TABLE 2-4. TYPICAL STORAGE QUANTITIES FOR SELECTED CHEMICALS (ANHYDROUS)

Storage	Ammonia[8]		Chlorine[9]		Sulfur Dioxide[10]		Ethylene Oxide[11]		Hydrogen Fluoride[12]		Hydrogen Chloride[11]	
	Quantity	Stored Phase*	Quantity	Stored Phase*	Quantity	Stored Phase*	Quantity	Stored Phase*	Quantity	Stored Phase*	Quantity	Stored Phase*
Cylinders	100, 150 lb	L_P	100, 150 lb	L_P	100, 150 lb	L_P	176 lb	L_P	150 lb	L_P	150 lb	G
Ton Containers	2000 lb	L_P	2000 lb	L_P	2000 lb	L_P						
Single Unit Tanks	26.5 tons	L_P	16, 30, 55, 85, 90 tons	L_P	20, 30, 40, 50 tons	L_P	72.5 tons (20,000 gallons)	L_P	20-90 tons	L_P		
Tank Trucks	15-20 tons	L_P	15-20 tons	L_P	15-20 tons	L_P			20-90 tons	L_P		
Barges	600, 1100 tons	L_P	600, 1100 tons	L_P	600, 1100 tons	L_P						
Fixed Storage Vessels	25+ tons	L_P or L_R	25+ tons	L_P	25+ tons	L_P	25 tons	L_P				

* Stored Phase Types:
- L_P - Liquid phase held by pressurization
- L_R - Liquid phase held by refrigeration
- G - Gas

be checked against Table 2-4. While the list does not include all conceivable storage configurations, it will allow reviewers of modeling submittals to determine if the described condition should be questioned or whether it is within the range of normal conditions.

The best indicator of the types of release classes that can be expected from a given release scenario is the boiling point of the chemical. The boiling point determines both the material's pre-release state and the potential release class. A material with a boiling point above ambient temperature may be stored or processed as a liquid without the aid of pressurization or refrigeration. Conversely, a material with a boiling point below ambient temperature is a gas that must be compressed or cooled to be held in the liquid phase. For pressurized liquid releases, a simple check for flashing can be made by comparing the boiling point of the material to ambient temperature. If the ambient temperature is higher than the boiling point, there will be some flashing during the release.

The boiling point of the material can be used to make an initial determination of the reasonableness of modeling submittals. For instance, if a submittal is based on a scenario resulting in a vapor release of benzene (normal boiling point 80.1°C or 176.1°F) from the bottom of a process vessel, the pre-release condition is not possible unless the vessel is heated above benzene's boiling point or the vessel operates under substantial vacuum. The boiling points of the chemicals selected for the modeling study are given in Table 2-2.

The boiling point of a material represents the equilibrium temperature at which its vapor pressure is equal to atmospheric pressure. The equilibrium relationship between all three phases (liquid, gas, and solid) at any given pressure and temperature is conveniently represented by a triple-point diagram. For storage scenarios, which almost always involve liquid-vapor equilibrium conditions, the use of the triple-point diagram provides a simple and accurate method for verifying the reasonableness of pre-release conditions. Triple-point diagrams for each chemical selected for the modeling study are included in Appendix B.

The use of triple-point diagrams to check pre-release conditions is best illustrated by the following example.

Model input is calculated based on pre-release conditions for anhydrous ammonia stored as a liquid under pressure. The storage vessel is isolated from the process at the time of the release and, therefore, the liquid ammonia is in equilibrium with its vapor at ambient temperature (specified as 30°C, or 86°F). A hole develops in the vapor space of the vessel resulting in a single-phase gas release. The emission rate, as input to the model, is calculated using a containment pressure of 152 kPa absolute (1.5 atmospheres).

Figure 2-7 shows the triple-point diagram for anhydrous ammonia. To check the reasonableness of the pre-release conditions, a point is located on the liquid-gas equilibrium line at the specified release temperature of 30°C. Figure 2-7 shows that the corresponding equilibrium pressure is 11 atm, which is well above the 1.5 atmospheres used to calculate the vapor emission rate in the example. Since vapor release emission rates increase with increasing storage pressure, the example analysis results in an underprediction of the emission rate, and most likely an underestimation of vapor cloud impacts.

The triple-point diagram represents equilibrium conditions at which materials can exist in multiple phases. Conversely, the diagram can be used to show where only a single phase is possible. If the pressure-temperature combination given in the above example were accurate, the triple-point diagram shows that the stored ammonia would exist exclusively as a vapor. Thus, the diagrams can be used to check for the proper material phase, as well as for consistency between pressure and temperature for liquid/vapor equilibrium conditions.

To verify the pre-release conditions of a material in vapor-liquid equilibrium, any two of the following conditions must be known: 1) the temperature, 2) the pressure, and 3) the phase of the material. With two conditions known, the third condition can be readily determined using the triple-point diagram as in the preceding example. When only one condition is known, the parameter which is known can be used to intuitively estimate the pre-release state using the method given in Figure 2-8. Figures 2-8 and 2-9

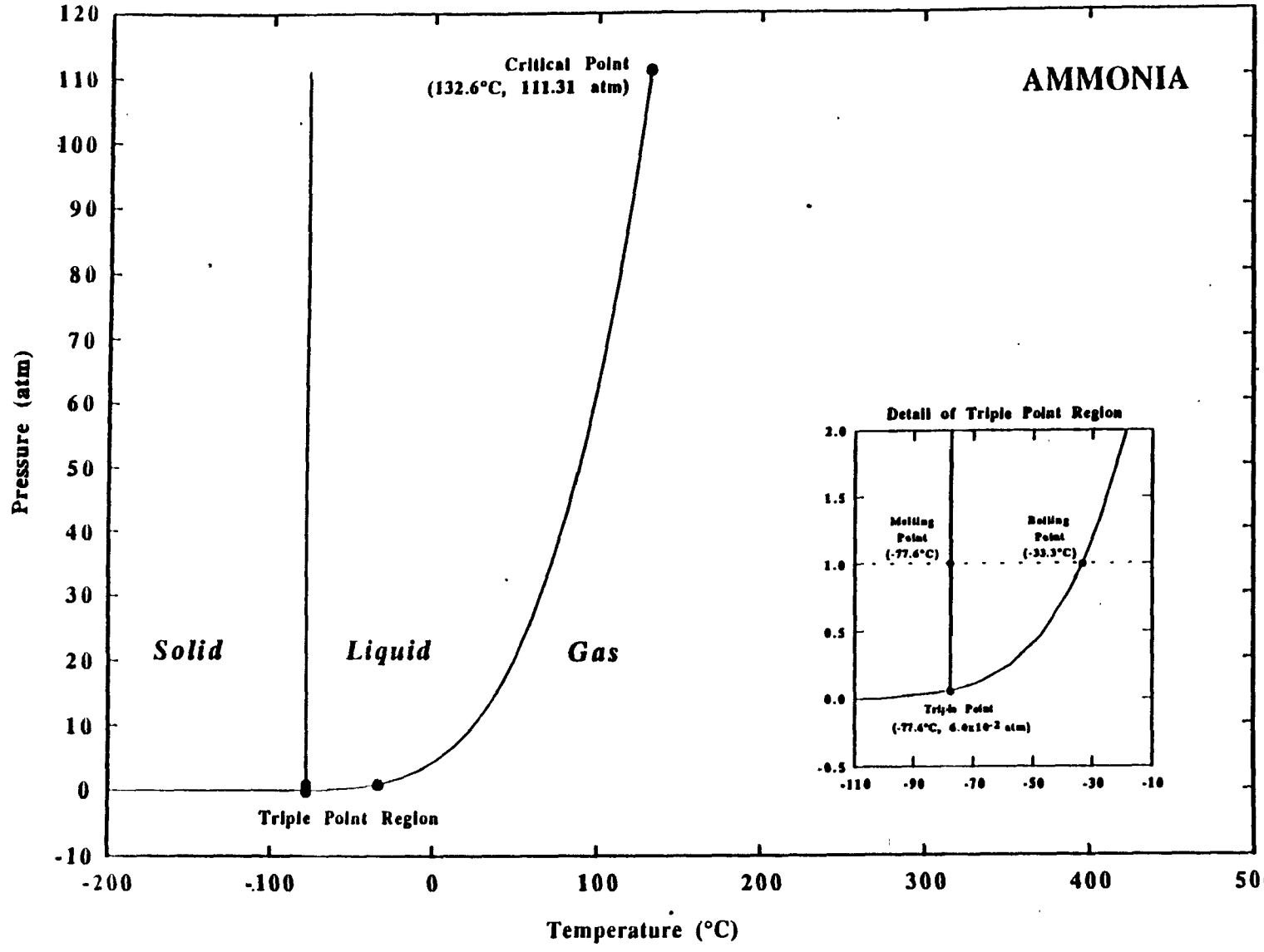


Figure 2-7. Triple Point Diagram for Anhydrous Ammonia

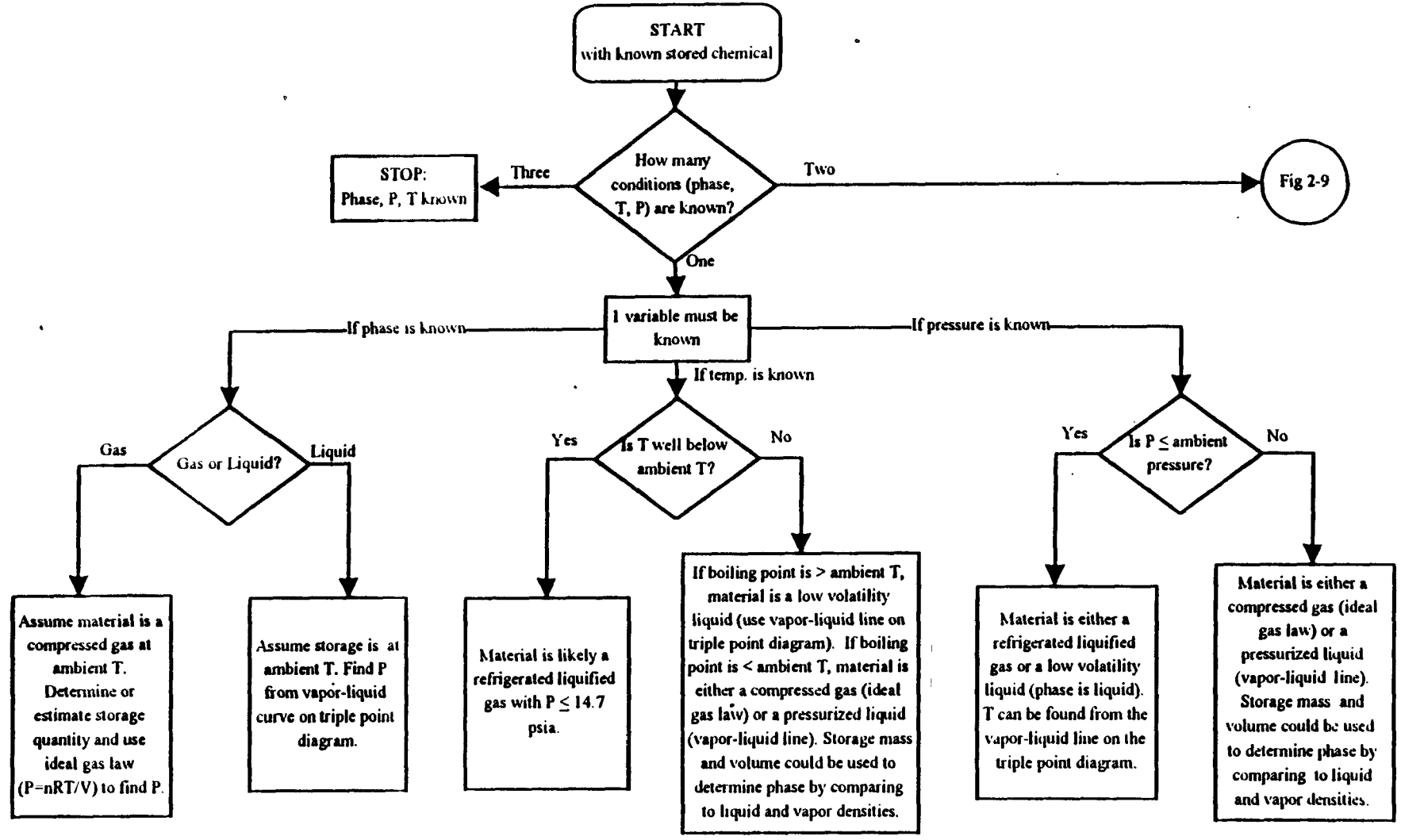


Figure 2-8. Method for Determination of Pre-Release Conditions Where One Condition is Known

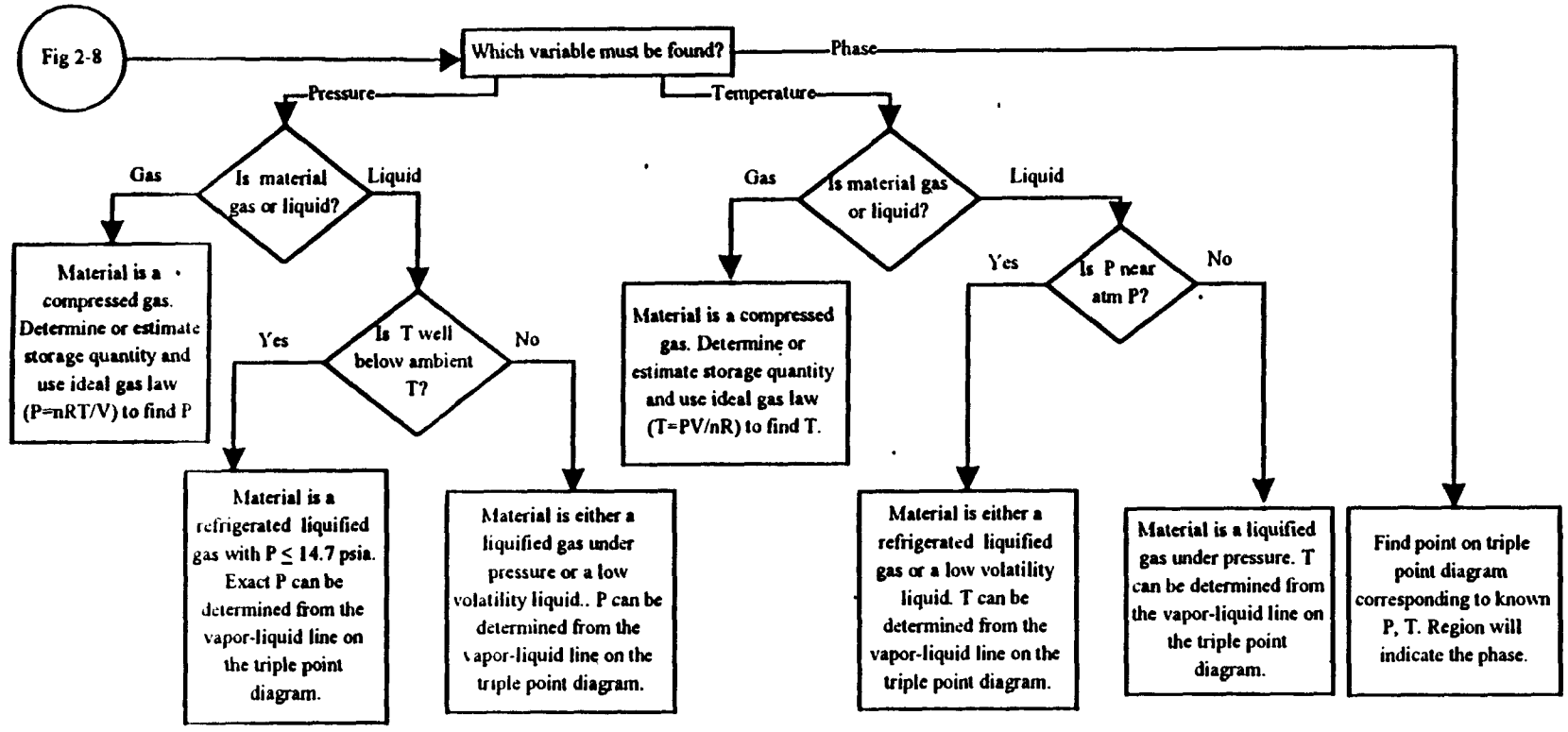


Figure 2-9. Method for Determination of Pre-Release Conditions Where Two Conditions are Known

Include the logic used to check pre-release conditions when only partial information is available in a modeling submittal.

The triple-point diagram can be used to determine unknown parameters only when the material is in liquid-vapor equilibrium. For materials that are stored only in the gas phase (not in equilibrium with its liquid), the exact pre-release conditions can be defined only if the stored quantity is known. The assumption that the stored quantity is equal to the capacity of the vessel will most likely result in a conservative emission rate estimate. For compressed gases, the assumption of maximum storage quantity results in maximum storage pressure, which produces the maximum initial emission rate. A maximum quantity assumption tends to produce more conservative vapor cloud impacts since the release duration will also tend to be maximized. Figures 2-8 and 2-9 provide a method to define or intuitively estimate pre-release conditions for compressed gasses, as well as for materials in vapor-liquid equilibrium.

Figures 2-8 and 2-9 apply to conditions where the material is contained in the gas phase or under liquid-gas equilibrium conditions. Where in-process release scenarios are specified, the material may or may not be at equilibrium conditions just before the release. Where non-equilibrium releases are specified, the pressure and temperature are usually measured or can be estimated from the design limits of the vessel. For example, a pressure relief valve is designed to open when the pressure reaches a predetermined value. If the consequences of a release are to be investigated, the pressure of the release can be assumed to be that predetermined value.

Some components of the release class can be readily determined after the pre-release conditions have been verified. As previously described, the material's boiling point provides an indication of the types of release classes that can be expected to result from a given release scenario. Further determination of the release class, specifically, the degree of flashing of a pressurized liquid release, can also be verified. A "flash diagram" may be used to determine the approximate fraction of liquid that will flash to vapor during a release. Use of the flash diagram is best illustrated through the

use of the following example.

> **A modeling submittal specifies a release of chlorine from a failure at the bottom of a pressurized liquid storage vessel. The scenario description states that an emergency containment/sump system is in place that removes 90 percent by mass of the released liquid chlorine before it vaporizes from a pool which presumably has formed. The storage temperature is specified as 25°C (77°F).**

Figure 2-10 is the "flash diagram" for chlorine showing the degree of immediate vaporization of liquid chlorine as it is released from containment. According to the specified release temperature, (25°C), 20% of the liquid chlorine flashes as it is released from the vessel. The flashed material immediately forms a vapor cloud, rather than forming a liquid pool. The flashed fraction determined from Figure 2-10 exceeds the 10% assumed in the example scenario as the amount ultimately entering the atmosphere as a dense gas vapor cloud. The assumption in the example scenario thus results in a substantial underprediction of the atmospheric emission rate of chlorine and, most likely, an underprediction of the downwind vapor cloud impacts.

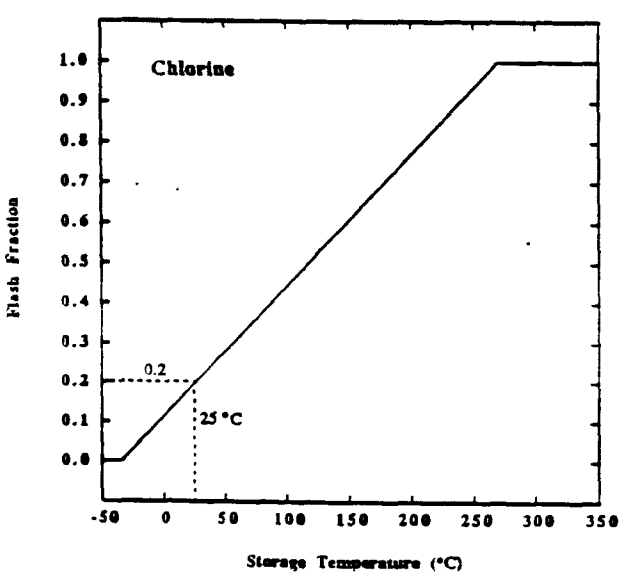


Figure 2-10. Flash Diagram for Chlorine

The procedures outlined in this section provide a method to estimate pre-release conditions for a given release scenario and a simple technique to

SECTION 3

MODELS

This section contains short descriptions of the five models illustrated in this document. Those models are:

- ADAM;
- ALOHA;
- DEGADIS;
- HGSYSTEM; and
- SLAB.

It is assumed that, before a model is exercised, the user will become familiar with the chosen model through use of technical references and user's guides written for that model. This document is not meant to be a replacement for a given model's documentation. Descriptions are provided here simply to allow prospective users to learn the general features of those models with which they may be unfamiliar.

3.1 ADAM[13]

ADAM is a PC-based dispersion model. It allows the user to specify the source-term right after a release or select from a menu of source-term options. However, the source-term must be either an instantaneous release or a steady-state continuous release; the model cannot handle a limited-duration release. Also, ADAM is not intended for elevated releases. Furthermore, ADAM does contain an algorithm for dealing with releases from jets, it treats the jet as being on the ground, and horizontally aligned with the wind.

ADAM has a database of chemicals, from which the user must select the chemical input for the model run. The database contains eight chemicals. It

is possible, however, to increase the database to include more than the original eight chemicals. Other input the user provides are the concentration contour of interest, and the averaging time.

ADAM will output a single contour showing the location of the gas cloud at the specified concentration level, along with a table showing the amount of time travelled by the cloud, its velocity, and the width of the contour. ADAM will also provide peak concentrations as a function of distance and, if the release is instantaneous, a peak dose may be calculated as a function of distance for the specified averaging time. In both cases, the information is calculated for the centerline of the contour. ADAM is unable to determine a time-history of concentration at specific points.

3.2 ALOHA[14]

ALOHA is a PC-based, menu-driven model, which employs a graphical user interface (GUI). There are five menus from which the user may select input for a model run. These menus are: "Chemical," "Site Data," "Atmospheric," "Source," and "Computational." The release type may be selected from the "Source" menu. There are three options: 1) pool evaporation; 2) liquid or gas leaks from a tank; or 3) a gas leak from a ruptured pipe. The user does not have to enter the release type if he or she knows the amount of chemical entering the atmosphere as a gas, along with other information, such as the temperature of the gas.

If the chemical desired is in the database, only the name need be specified; otherwise, all the data necessary can be input from the "Chemical" menu.

Output from the model includes a text summary, a plot of the "footprint" of concentrations that are greater than a user-specified concentration, time-series plots of concentration and dose at a particular location, and a time-series plot of the release site.

ALOHA also has a version of DEGADIS imbedded in it. ALOHA's formulation is almost identical to the stand-alone DEGADIS. However, some of the numerical techniques to solve the conservation equations are not the same. Also, the two models' output formats are quite different. The "official" name of the ALOHA dense gas model is "ALOHA-DEGADIS."

3.3 DEGADIS[4]

DEGADIS is a PC-based model that can be applied to a wide range of releases including: gases and aerosols; continuous, instantaneous, finite-duration, and time-variant releases; ground-level, low-momentum area releases, and ground-level or elevated upwardly-directed stack jet releases.

For aerosol releases, the user must characterize the density of the release, because the model is not capable of doing so itself. The model only simulates one set of meteorological conditions and does not accept any type of real-time meteorological data. Data, including chemical properties, must be input interactively, or from a file, for each run, since there is no chemical database. Terrain is assumed to be flat and unobstructed. Input required includes: emission rate; release area and release duration; chemical characteristics; stack parameters; and standard meteorological data. Receptor input includes: desired averaging time; above-ground height of receptors; and maximum distance between receptors.

The model automatically writes an output file; no graphical representations are provided. The contents of the file are: input data; plume centerline elevation, mole fraction, concentration, density, and temperature at each downwind distance; sigma y and sigma z values at each specified downwind distance; off-center line distances for two specified concentrations at a user-specified receptor height at each specified downwind distance; and concentration vs. time histories for finite-duration releases.

3.4 HGSYSTEM[15]

HGSYSTEM is a PC-based system consisting of seven distinct models, each of which represents a different type of release. The seven models are: 1) spillage of HF from a vessel (HFSPILL); 2) spreading/evaporation from a liquid pool (EVAP); 3) flashing of HF (HFFLASH); 4) jet flow, near-field dispersion of HF (HFPLUME); 5) jet flow, near-field dispersion of an ideal gas (PLUME); 6) ground-level heavy gas dispersion (HEGADIS); and 7) elevated passive dispersion (PGPLUME). In some cases, the models may be used together in sequence. That is, the output from one model may be used as the input to another model. Because several models may be involved with any particular scenario, modeling possibilities can be complex.

HGSYSTEM contains scripts that guide the user through the process. The model involving pool evaporation (number 2 above) requires the most input concerning properties of a liquid release. HF modeling (models 3 and 4) requires less input since the chemical information already exists in the model itself. Modeling of a jet flow, near-field dispersion (number 5 above) requires a description of the release and the ambient conditions. Finally, modeling of elevated passive dispersion (number 7) requires input from a near-field model, along with selected data on ambient conditions and dispersion.

For each of the seven models, detailed input is required on the thermal properties of the gas, its initial concentration and areal extent, and a complete description of ambient conditions and site characteristics. HEGADIS, which is the heavy gas atmospheric dispersion model, should be implemented after a source-term model has been specified. There are three choices: 1) steady-state; 2) finite-duration; or 3) transient. For the jet model, a jet may be elevated and inclined in the vertical; however, it is assumed that the jet points "downwind."

For output PGPLUME generates tabular data for distances downwind of the source, whereby the mole-concentration is reported in a vertical cross-section of the plume that is normal to the transport direction. Being a steady-state

or finite duration release model, no time-histories are reported. HEGADIS uses two postprocessing algorithms to calculate output. The algorithm, HSPOST, (used for steady-state releases) is used to determine concentrations at any point (x,y,z). It also reports concentrations, geometrical parameters, and temperature for points which are along the ground in line with the axis of the plume. This postprocessor may also calculate tabular or plotted results for releases of finite duration. HTPOST (used for transient releases) averages the time-series concentrations described from the transient version of HEGADIS. This postprocessor can output data at a particular time, or the user may specify a particular point and obtain a time-series of concentration.

3.5 SLAB[16]

SLAB is a PC-based dispersion model of denser-than-air releases. It can be applied to four types of releases including: a ground level evaporating pool, an elevated horizontal jet, a stack or elevated vertical jet, and an instantaneous volume source. All sources except the evaporating pool may be characterized as aerosols. The model can simulate multiple sets of meteorological conditions in a single run, but it does not accept any type of real time meteorological data. Data is input directly into the model from an external file. Input data include source type, source properties, spill properties, field properties, and standard meteorological parameters. There is no chemical database, but some chemical properties are available in the user's guide.

The model does not generate any type of graphical output, but rather automatically sends the tabular results to a printer file. These results include: input data; instantaneous spatially-average cloud parameters; time-averaged cloud parameters; and time-averaged concentration values at the plume centerline and at five off-centerline distances at four user-specified heights and at the height of the plume.

SECTION 4

MODEL INPUT

This section provides an overview of the input required by hazardous air pollutant dispersion models. The overview includes descriptions of the decision-making process and calculations required for determining model input. Most of the input for the models was developed using techniques described in the EPA Workbook[2].

This section is organized to lead the user from a physical description of the release (called observable data here) to input parameters which are calculated for the various models. Section 4.1 describes the observable data at the release site that are required to perform the input calculations. Section 4.2 lists the data required to define a chemical for a model. It also describes methods which can be used to approximate the data for a chemical mixture. Section 4.3 details the methods used to determine the basic release class of a given scenario. Section 4.4 discusses the differences between continuous and instantaneous releases.

Section 4.5 presents a series of flow charts which illustrate the approach used to calculate various input for the models. The techniques used depend on the release class of a given scenario. Sections 4.6 through 4.13 provide calculation methods for the following input:

- Choked/unchoked flow (4.6);
- Emission rate (4.7);
- Release temperature (4.8);
- Vapor fraction (4.9);
- Initial concentration (4.10);
- Density (4.11);
- Release diameter or area (4.12); and
- Release buoyancy (4.13).

Sections 4.14 through 4.17 discuss other input considerations which require little, if any, calculation. This input is: release height, ground temperature, averaging time, and meteorological data. The final section, 4.18, briefly describes model output concerns.

When a scenario is defined, the first thing to do is determine the release class that best represents the scenario. To determine the release class, a series of calculations may be required. The determination of a release class may be performed through a process of assumption and calculation. For example, in determining whether a release is two-phase or not, the assumption is made that it is single phase. Calculations of release parameters are performed for the single-phase release class. The results of the calculations are then checked for consistency. If the consistency checks fail, the release must be a two-phase class. Since input parameters must be calculated before the release class can be determined, this section is organized by the calculated parameters (e.g. the emission rate), with release class sub-headings.

The order of the parameters presented in Sections 4.6 through 4.13 is not necessarily consistent with the order of calculation. Each release class requires a specific order of calculation. If a prior calculation is required, it will be noted in the section. For instance, the emission rate calculation for the "two-phase gas release (unchoked)" in Section 4.7.2 requires the prior calculation of a change in enthalpy (ΔH) and release density(ρ_{rel}). These parameters are listed at the beginning of Section 4.7.2, along with the sections in which those calculations are detailed.

4.1 OBSERVABLE DATA

The initial step in preparing the input required for any air release model is to gather the observable data. Observable data are the physical descriptions of a release before and at the time of the release. As far as input is concerned, there are two types of models: source-term and non-source-term.

Source-term models can estimate the conditions of the gas state of a release entering the atmosphere. If the release is a liquid, the source-term model calculates the rate of emission of the liquid from the container and the rate of the gas and aerosol injection into the atmosphere. If the release is a gas, the source-term model can calculate the injection of the gas into the atmosphere, along with any aerosol that may form due to expansion cooling. As a gas de-pressurizes it cools. If the cooling is sufficient, the gas may condense into droplets. Besides emission rate, parameters such as temperature, initial concentration, initial density, etc., are also calculated by source-term models.

Models which cannot calculate release conditions based on storage conditions are called non-source-term models. Models rely on the user to supply the release condition information. The user, therefore, must perform these calculations outside of the model. The model then uses a dispersion model to predict impacts based on the user-calculated input.

Both source-term and non-source-term models require observable data to perform the calculations. Thus, the only difference is whether the user or the model carries out the calculations of input concerning release conditions. For both the non-source-term and source-term models, the following information is required:

- Chemical;
- Storage temperature;
- Storage pressure;
- Hole size;
- Depth of liquid in container above hole;
- Maximum pool size; and
- Meteorological conditions.

The ADAM, ALOHA, and HGSYSTEM (HF only) models contain source-term models. Therefore, many input values are calculated internally by these models.

The calculations in this section are designed, for the most part, to provide input to non-source-term models. However, some calculations may still be required for some of the source-term models. For example, a model may still require the emitted gas temperature for some release classes.

4.1.1 Vessel Shape and Dimensions

In the models described in this document, three general shapes of vessels are allowed. These are a horizontal cylinder, a vertical cylinder, and a sphere. The ADAM model, however, assumes only vertical cylinders. If a spherical vessel is involved, it can be conservatively modeled by assuming a vertical cylinder with a diameter equal to the sphere diameter.

4.1.2 Hole Location and Orientation

Besides hole size, a source-term model requires information on the height of the hole both with respect to the ground and with respect to the vessel bottom. The height above ground determines the height at which the gas escaping the vessel will enter the atmosphere. The height of the hole from the vessel bottom determines the amount of liquid that can be released and the pressure due to the liquid depth above the hole location.

A release may be from a pipe connected to a vessel. Some resistance to flow may occur due to the condition and size of the pipe.

The vertical orientation of the hole will determine if a release is a vertical, horizontal, or intermediate release. The azimuthal orientation of the hole will determine the initial direction of a release. Generally, higher concentrations can be expected downwind if a jet release is in the same direction as the ambient wind. The larger the vector difference in a jet velocity and the ambient wind velocity, the more mixing will occur. For example, a jet escaping directly into the wind will create more turbulence than a jet released in the same direction as the wind. This is especially true if the wind speed is comparable to the jet exit speed.

4.1.3 Diking

If the release is a liquid, the liquid may spread as the release continues. If there are dikes or terrain features in the area, the pool that forms may be restricted to a maximum size. This maximum size would limit the surface area of the spill available for evaporation into the atmosphere. Generally, the larger the surface area of the pool, the larger the total emission rate. This parameter is also used in the Workbook calculation for a low volatility release. In the Workbook, the total area of the pool is required. Source-term models may take into account the shape (circular, rectangular, etc.) of the diked area.

4.1.4 Surface Description

For liquid pools heat is transferred from the surface on which the spill occurred. At a minimum, the ground temperature is required for the calculation of the heat transfer rate. A more complete calculation would allow the specification of other parameters describing the surface. Examples of such parameters are: thermal conductivity, specific heat, and porosity.

4.1.5 Solar Radiation

Another factor in determining heat transfer to a pool of liquid is solar radiation. Direct insolation onto the pool surface can be a significant source of energy. Rather than asking for the value directly, a location (latitude and longitude) and time of day may be specified. The model then can estimate the location of the sun with respect to the spill location, and hence, a thermal radiation value. Sometimes a cloud transmittance factor is also requested to account for attenuation of the sunlight by the clouds. Although, strictly speaking, this parameter should be included in the meteorological section, it is almost solely used in the source-term calculation. The other meteorological parameters affect the transport and dispersion of the emission in addition to the source-term calculation.

4.2 CHEMICAL DATA REQUIREMENTS

Normally, data for some chemicals are supplied by the model. If a chemical is not already in the model's database, it must be added. The most often required chemical data are:

- Molecular weight;
- Heat capacity;
- Boiling point;
- Heat of vaporization;
- Liquid density;
- Vapor pressure;
- Critical values (temperature, pressure, and volume); and
- Enthalpy.

Values are available for many pure substances in sources listing many of the parameters describing a chemical. There are also techniques available for estimating physical and chemical properties for uncommon pure substances. Some of the sources are:

Perry's Chemical Engineers' Handbook, 6th ed., edited by Robert H. Perry and Don W. Green, McGraw-Hill, Inc., New York, New York, 1984 (data and estimation techniques);

The Properties of Gases & Liquids, 4th ed., Reid, Prausnitz, and Poling, McGraw-Hill, Inc., New York, New York, 1987 (data and estimation techniques);

Data Compilation Tables of Properties of Pure Compounds, T.E. Daubert and R.P. Danner, Design Institute for Physical Property Data, American Institute of Chemical Engineers, New York, New York, 1985 (data); and

CRC Handbook of Chemistry and Physics, 71st ed., edited by David R. Lide, PhD, CRC Press, Inc. Boca Raton, Florida, 1990 (data).

Most of the available data are for pure chemicals. Often a chemical mixture is the substance of concern. Models require a single set of chemical data for the material released. A chemical mixture is treated as a pure chemical by developing the parameters of a fictitious or "pseudo-chemical." For a gas or liquid mixture, the parameters describing the gas or liquid phase

of the pseudo-chemical are made up from using the parameters of the individual components of the mixture and their molar or mass fractions. The first pseudo-chemical parameter calculated is usually the molecular weight of the mixture. The mixture molecular weight is calculated using either mole fractions (f_i) or mass fractions (w_i) of the individual component i along with each component's molecular weight (M_i). The formula for calculating molecular weight (M) of a mixture using the mole fraction is:

$$M = \sum_C f_i M_i$$

The formula for calculating molecular weight of a mixture using the mass fraction is:

$$M = \left(\sum_C \frac{w_i}{M_i} \right)^{-1}$$

The relationship between the mass and molar fractions is:

$$w_i M = f_i M_i$$

In general, the parameters for a mixture (P) are calculated with the use of one of the following equations:

$$P = \sum_C f_i P_i$$

$$P = \sum_C w_i P_i$$

The first equation applies if the parameter is in units of inverse moles [or has no mole or mass units (such as temperature)]. The second equation applies when the parameter is in units of inverse mass. Vapor pressure is, however, a special case. The vapor pressure of a mixture is the sum of the vapor pressures (in equilibrium with the liquid mixture) of the individual

components. The boiling point is defined as the temperature when the mixture vapor pressure is equal to 1 atmosphere.

The gas-phase mixture in equilibrium with the liquid-phase mixture probably will not have the same proportions of components as the liquid-phase mixture. The pseudo-chemical parameters for the two phases should be kept separate. The liquid-phase parameters influence the emission rate but have little or no effect on the dispersion of the gas phase after it leaves the source.

For these pseudo-chemicals there are two methods of generating the required thermodynamic data. In both methods, the data describing the liquid mixture would represent the weighted average of the mixture, as described above. For example, the boiling point of a mixture could be given as the temperature at which the sum of the partial pressures of the constituents is equal to 1 atmosphere.

The first approach for calculating thermodynamic data for the vapor state is to use the weighted average scheme described above. When determining the concentration of a specific species in the vapor mixture, the model-calculated concentration needs to be modified by multiplying it by the molar fraction (f_i).

In the second method, the data describing the vapor state must be specific to the chemical of interest. The vapor mixture in equilibrium with the liquid mixture will be made up of many, if not all, of the components in the liquid. The relative concentrations (partial pressures) of the vapor mixtures will be different than those of the liquid mixture. The vapor pressure data would represent the vapor pressure of only a single constituent in equilibrium with the liquid mixture.

A pure substance may have varying parameters describing the substance. An example is hydrogen fluoride. At high concentrations, the individual molecules can form oligomers (polymers which contain two, three, or four

monomers). The dynamic effect is to increase the molecular weight of the release. It may be desirable to have different data sets for a compound such as hydrogen fluoride. One set of parameters could be used for low concentration releases, the other for pure releases. From previous work[17], there is sufficient data to create a table relating the apparent molecular weight of hydrogen fluoride to the temperature and concentration of the hydrogen fluoride gas. Such a table is included in the database for hydrogen fluoride in Appendix B. As that table shows, in pure concentration (1,000,000 ppm) hydrogen fluoride at 20°C has an apparent molecular weight of 51.6. Above 70 °C, however, hydrogen fluoride is present as a monomer at all concentrations giving a molecular weight of 20.

4.3 RELEASE CLASS

Probably the most important part of determining the impacts from a release is determining the manner in which the release occurs. The release classes covered in this document are:

- Two-phase gas (choked or unchoked gas released as gas and liquid);
- Two-phase liquid (liquid released as gas and liquid);
- Single-phase gas (choked or unchoked gas released as gas);
- Single-phase, high-volatility liquid (liquid released as gas); and
- Single-phase, low-volatility liquid (liquid evaporating as gas).

A release class is a categorization of a release scenario based on the chemical's physical storage conditions (gas or liquid) and initial vaporization (single- or two-phase) during the release from storage. The release class and chemical determine the parameters required for a model to carry out a simulation. Chemicals may be stored as a gas or as a liquid. A chemical stored as a gas under pressure may enter the atmosphere in both liquid and gaseous form. Liquid droplets may form due to cooling from expansion after a release. Such a suspended phase mixture is called an aerosol. A chemical with a boiling point below the ambient temperature that is stored either under pressure at the ambient temperature or refrigerated to a temperature below its boiling point may also form an aerosol upon release.

If no aerosol forms when such a liquid is released, it would be considered a high-volatility liquid. A chemical with a boiling point above the ambient temperature that is released will most likely form a liquid pool, except when the chemical is stored under high pressure (the high pressure release may emit the liquid as droplets). This pool will evaporate into the atmosphere. Chemicals with lower volatility or vapor pressure will evaporate more slowly than chemicals with a higher volatility, given that all other conditions are the same.

The question of aerosol formation and fate is not yet clearly answered. For screening purposes it is suggested for two phase releases that all the liquid in the release be assumed to be entrained with the vapor phase as an aerosol. As mentioned above, aerosols can form due to cooling. They can also form when a liquid comes out at high pressure, by splashing or impacting on surrounding objects, or comes from superheated storage.

The steps in determining the release class are given in Figure 4-1. Before the determination can be made, the storage phase must be known. A flow diagram (Figure 2-8) given in Section 2.4 which can be used to determine the storage phase. As mentioned in the introduction to this section, determining the release class using the flow diagram in Figure 4-1 requires some calculations. These calculations are described in the sections referenced in parentheses in Figure 4-1. The same calculations required to determine the release class may also be used as model input for the selected release class. Flow charts outlining the required calculations for each release class are presented with the discussion of each release class.

In Figure 4-1, the initial question is the storage state (gas or liquid which can be determined from Figure 2-8).

For material stored in the gas phase, you must determine if there is choked flow. The calculation for determining if there is choked flow is described in Section 4.6. A choked flow can limit the emission rate.

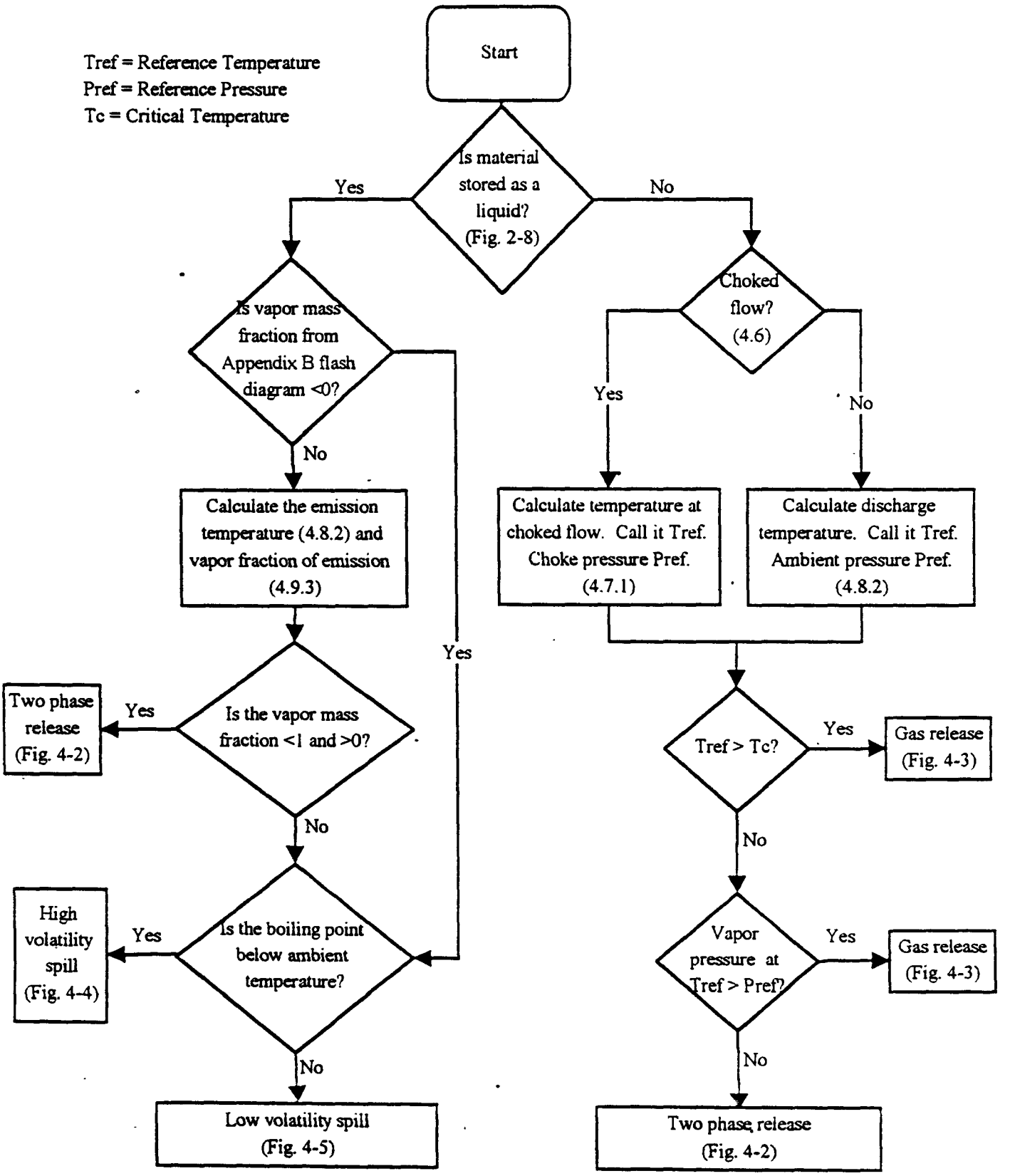


Figure 4-1. Determining Initial Release Class

Next, a reference temperature (T_{ref}) and reference pressure (p_{ref}), indicative of the conditions at the hole must be determined. The method of determining the reference temperature and pressure depends on whether the flow is choked or not. If the flow is choked, then the pressure (p_*) and temperature (T_*) at choke conditions must be determined. This calculation is described in Section 4.7.1. The values of p_* and T_* could then be set to reference values p_{ref} and T_{ref}. If the flow is unchoked, the reference pressure, p_{ref}, is equal to the ambient pressure (p_a). The reference temperature, T_{ref}, is set to the unchoked release temperature (T_{rel}) calculated in Section 4.8.2.

Once the reference temperature and reference pressure have been determined, they can be used to determine if the release is two-phase (i.e., whether any condensation occurs during the release). This is done by performing two checks to determine if the release is single-phase. If both checks prove negative, the release is two-phase. The first check is to compare the reference temperature to the critical temperature of the chemical. If $T_{ref} > T_c$, the release is single phase. If not, the second check is be performed. In this check, if the vapor pressure of the chemical (from the data in Appendix B) at T_{ref} is greater than p_{ref}, then the release is single-phase. Otherwise, the release is two-phase.

For material stored in the liquid phase, a preliminary check may be carried out as indicated in Figure 4-1. This preliminary check is a graphical determination of whether the release may result in flashing (a two-phase release). The equation used to determine the flash fraction diagrams in Appendix B is based on the assumption that the temperature after the emitted chemical is out of the container is equal to the boiling point temperature.

If there is still uncertainty as to whether a flash occurs after referring to the flash diagram in Appendix B, a calculation for the flash fraction must be carried out. The flash fraction (F_{rel}) calculation is described in Section 4.9.3. This calculation is the same whether the release

is a pressurized or a refrigerated liquid. When a flash is occurring, the release temperature (T_{rel}) is the boiling point.

If no flash occurs ($F_{rel} = 0$), then the boiling point of the chemical determines whether the release is of a high or low volatility chemical. If the boiling point is lower than the ambient temperature, the release should be considered one of high volatility. If the boiling point is higher than the ambient temperature, assume a low volatility release.

4.4 CONTINUOUS OR INSTANTANEOUS RELEASE CATEGORIES

For a source-term model, the words "instantaneous" and "continuous" normally describe the manner in which the chemical gets out of the container. For a non-source-term model, the words "instantaneous" and "continuous" describe the manner in which the chemical enters the atmosphere. In some models the emission rate (either from the container or into the atmosphere) can be time varying.

All of the models allow the user to specify whether the release is instantaneous or continuous. However, as stated above, these terms are interpreted differently depending on whether a source-term model is being used or not. If a specific model provides guidance on the determination of whether a release is continuous or instantaneous, that guidance should be followed.

Some of the models also allow a finite duration release. A finite duration release is one that only exists for a limited period of time. That is, a finite duration release is neither instantaneous, nor does it go on without ceasing. For example, if a relief valve opened and the entire contents of the vessel escaped in 15 minutes, a finite duration release of 15 minutes would have occurred. If a model allows a finite duration release, the actual time of duration (rather than specifying an instantaneous or continuous release) should always be used.

Most models do not take into account mitigation efforts during a release (for example, if an automatic or human-activated shutoff valve is turned on during a release). In this case, the release duration would be limited to the time from the beginning of the release to the closing of the valve. If the actual release time is significantly different from the model computed release time, the release may be better simulated by assuming it is instantaneous or by using a finite release duration model.

When a gas is released from a container, it goes from the container immediately into the air. An aerosol may form, but it also is positioned in the air. A liquid release, on the other hand, can actually be two releases. One is the release from the container. If the liquid entirely flashes or all the liquid is suspended as an aerosol, that is the only release. But, if the liquid forms a pool on the ground, a second release would occur involving release of the chemical from the liquid state to the vapor state and its injection into the atmosphere.

4.4.1 Non-source-term Model

To decide whether the release should be considered continuous or instantaneous two factors need to be known: 1) the release duration, and 2) the location of the nearest receptors or the maximum distance to the lowest concentration of interest. To determine the category, if a concentration of interest is specified, the release first needs to be simulated as a continuous release. Then the travel time to the maximum distance of the concentration of interest is compared to the actual release duration. If only receptor locations are of interest, their distance from the source can be substituted for the maximum distance of the concentration of interest.

In practice, a continuous release initially should be assumed. The time required for the material to reach a specific downwind distance is then compared to the actual emission duration. If the emission duration is longer than the time it took for the material to reach a downwind point, the release

may be considered continuous. Otherwise, the release should be considered instantaneous. The travel time (t_{trav}) to some site at a downwind distance (X) from the release site can be approximated using this formula:

$$t_{trav} = \frac{2X}{u}$$

where: u = ambient wind speed.

If the model allows a finite duration release, the release duration should also be compared to the desired averaging time. If the release duration is less than the averaging time of concern, then a transient model should be used to reflect average concentrations more accurately. For example, if the release duration is 5 minutes and the averaging time of concern is 15 minutes, it is important to use a finite duration model to simulate the proper average concentrations.

4.4.2 Source-term Model

Source-term models normally use the words "continuous" and "instantaneous" to describe how the material escapes from confinement. If the model has guidance on determining whether a release is continuous or instantaneous, it should be followed. If such guidance is not available, the following is provided.

For a source-term model, the general rule of thumb is if the chemical escapes in less than one minute, it is assumed to be an instantaneous release. If the release is of longer duration, another approach is used, which is related to the emission rates from the two releases that a liquid goes through. If the emission rate from the container is much faster than the rate of evaporation from the formed liquid pool, the emission from the container can be assumed to be instantaneous. In this case, a pool forms, and the container emission just makes the pool deeper. The limiting emission for entry of the gas phase into the atmosphere is the evaporation.

If the emission from the container is such that the pool formed has an evaporation rate that is the same as the rate of emission from the container, the release should be considered continuous. In this case, if the emission rate from the container increases, the size of the pool would increase.

4.5 RELEASE-CLASS-SPECIFIC CALCULATIONS

Each release class requires a series of calculations to determine the initial emission conditions:

- Rate;
- Temperature;
- Vapor/liquid fraction;
- Concentration (air, water vapor, and chemical); and
- Density.

The method for determining each value, even the order of the calculation, changes with the release class. In addition, a specific calculation may be needed in determining the release class and used as model input. This section describes the overall flow of calculating the input for each release class. The following sections describe the input calculations in more detail for each of the release classes. The Workbook[4], from which these calculation techniques were taken, presents the calculations in detail by release class.

The overall approach for determining model input is to first use Figure 4-1 to determine the release class. Second, use the appropriate flow chart (Figures 4-2 through 4-5) for the release class-dependent calculations. When the release-class-dependent calculations have been completed, the common input requirements, presented in flow chart form in Figure 4-6, should be determined.

It is assumed that, before the calculations listed in the flow charts for the individual release classes are completed, the approach given in Figure 4-1 has been used to determine the release class. Note that some of

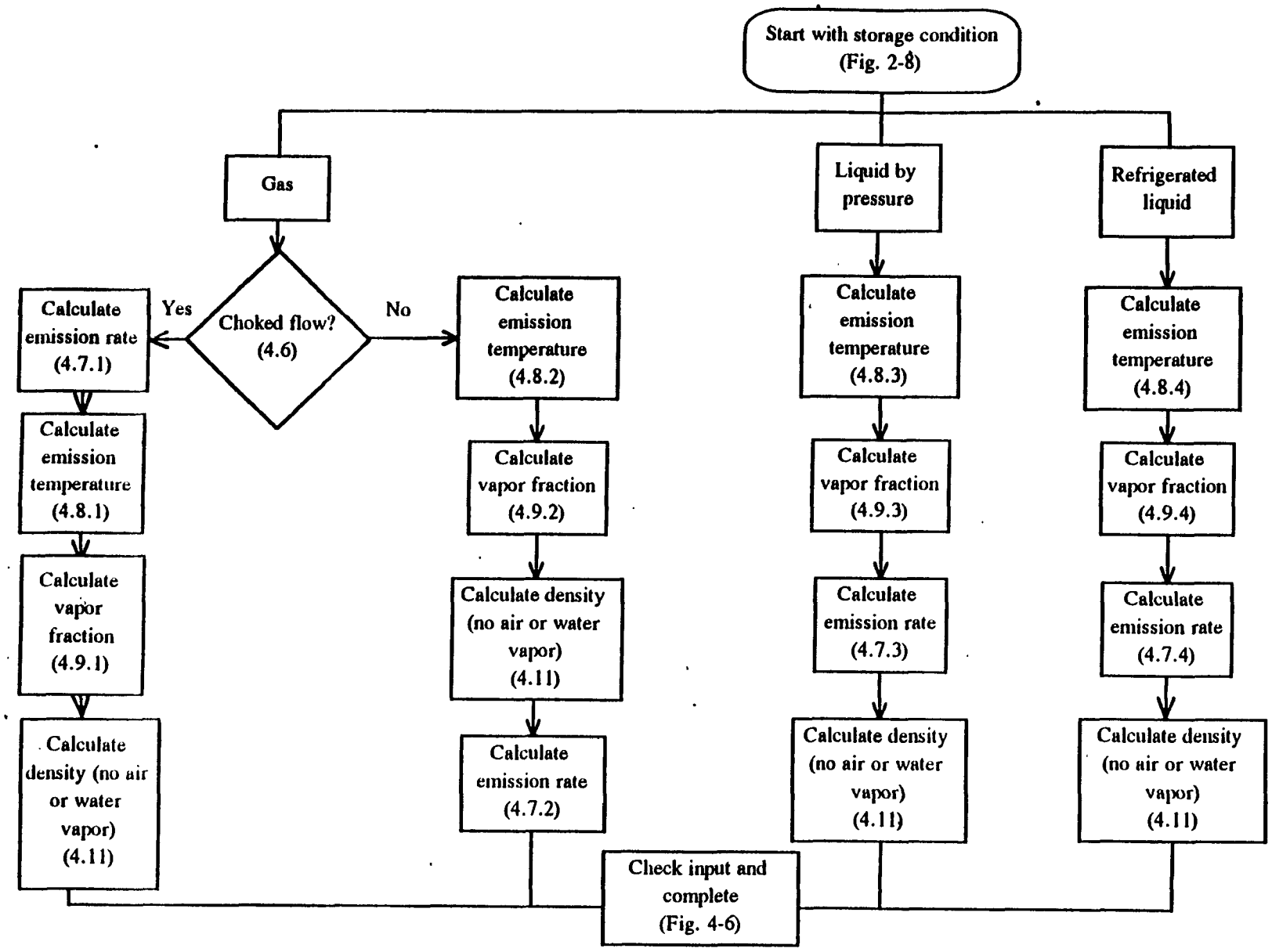


Figure 4-2. Two-Phase Input

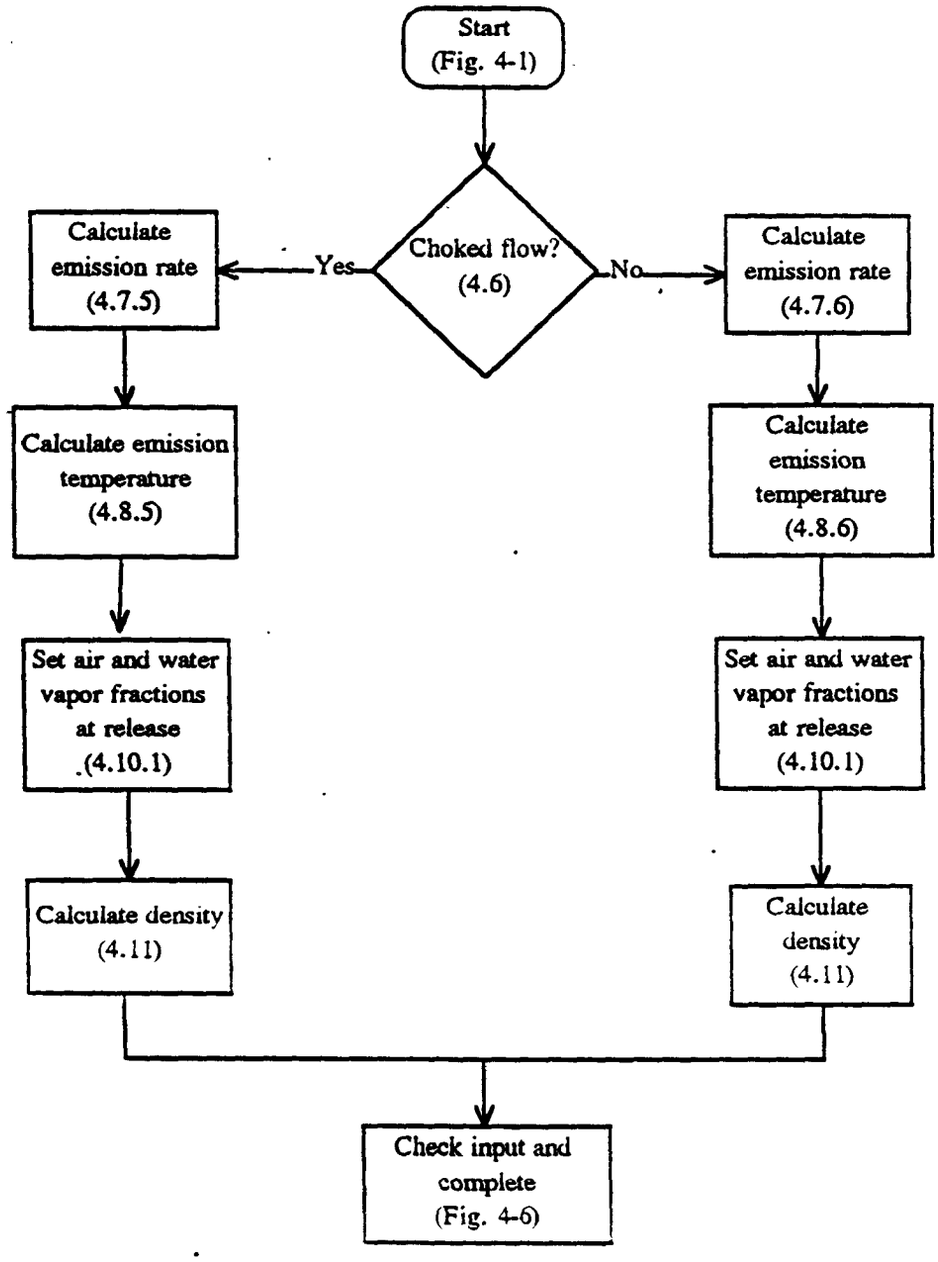


Figure 4-3. Gas to Gas Release Input

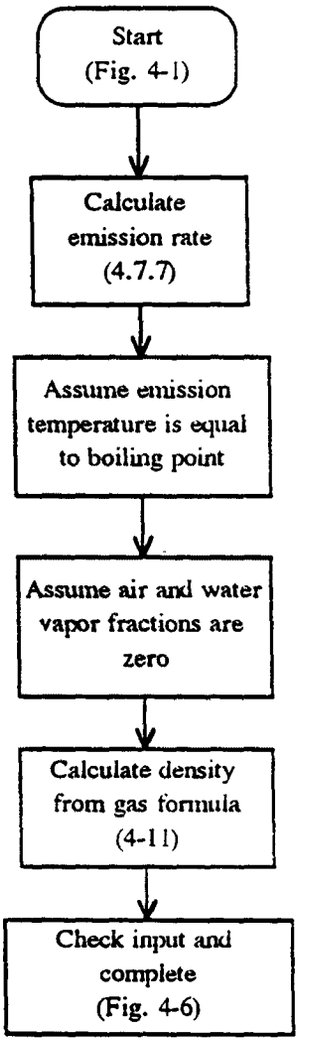


Figure 4-4. High-Volatility Release Input (Not Two-Phase)

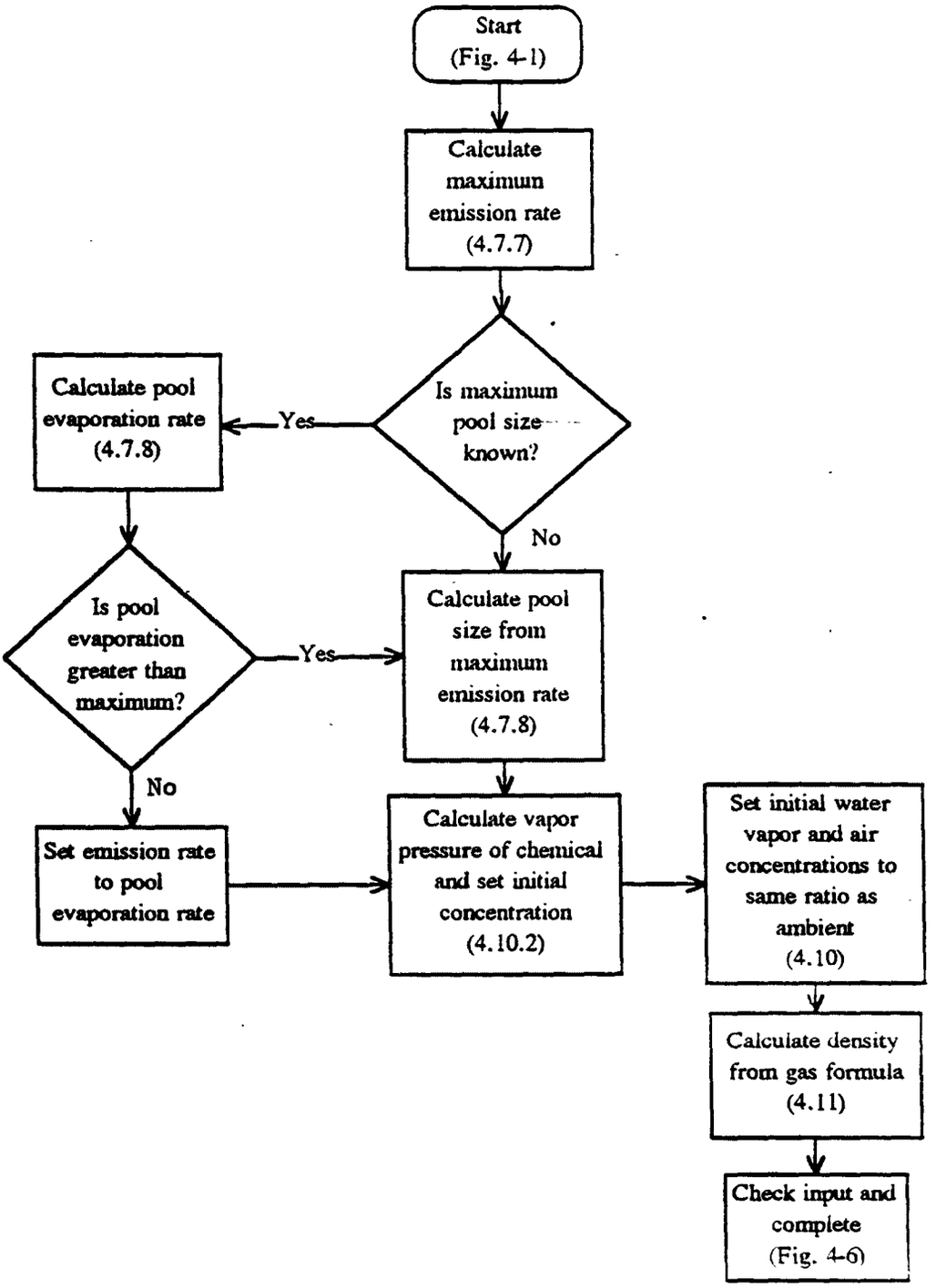


Figure 4-5. Low-Volatility Release Input

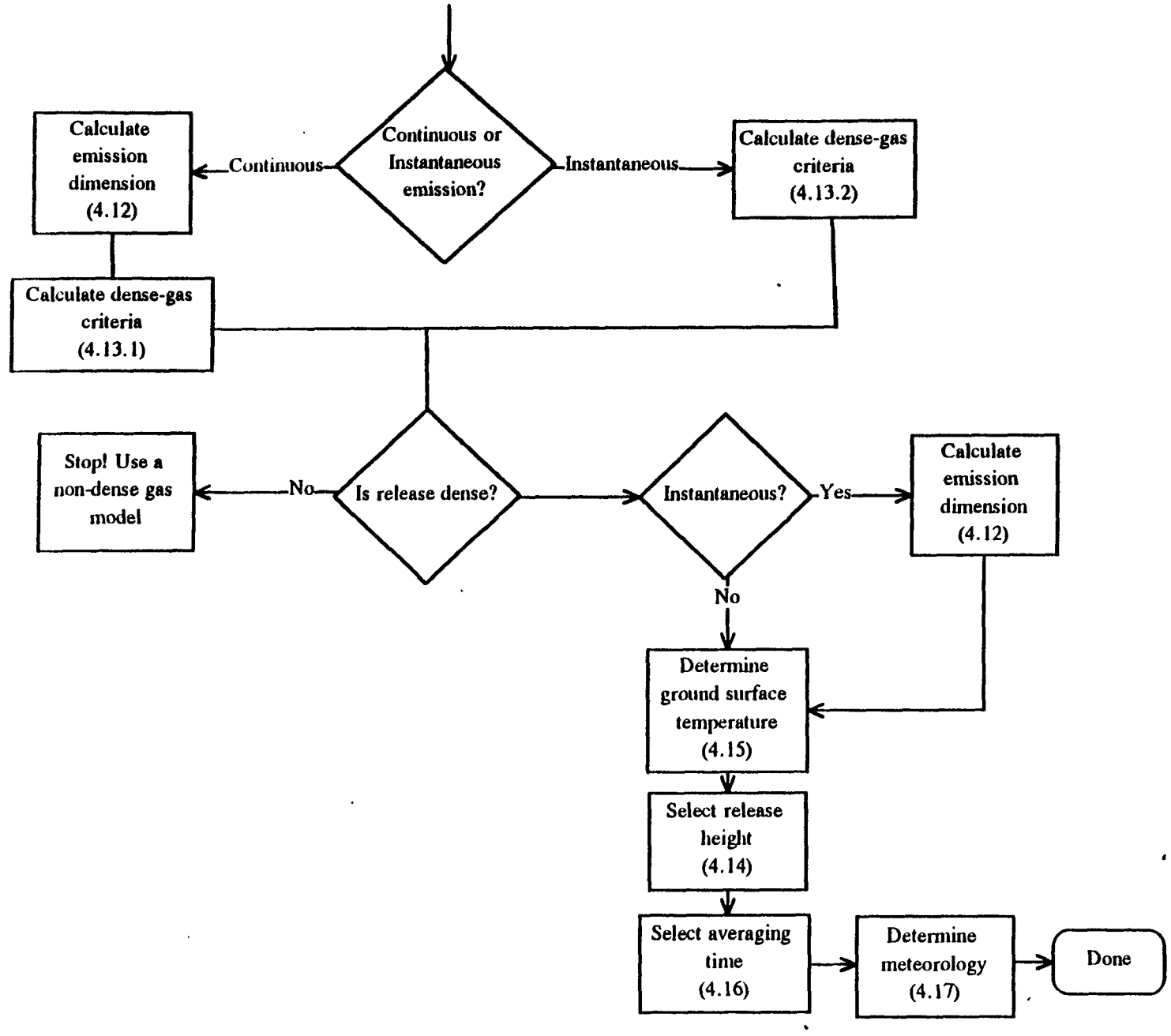


Figure 4-6. Check Input and Complete

the calculations required for a specific release class may have already been performed when using Figure 4-1.

4.5.1 Two-phase Releases (Gas and Liquid)

A flow diagram showing the steps required to calculate the input for the two-phase releases is shown in Figure 4-2.

The gas release becomes two-phase through condensation of the material due to cooling by expansion. The flow may be choked, which limits the emission rate and the amount of condensation that can occur.

Liquids with boiling points lower than the ambient temperature are stored either under pressure or are refrigerated to a temperature that is lower than their individual boiling points. In many cases, the liquid is stored in a container in which there is a combination of pressure and refrigeration. In those cases, it is suggested that the calculations be performed for the pressurized case. The pressurized case may have aerosolization occurring because of jetting at the exit. Refrigeration-only releases would not tend to have aerosolization. The presence of aerosols tend to keep the emitted cloud cooler longer than if there are no aerosol. The cloud should be at boiling point until all the aerosols have evaporated.

4.5.2 Single-phase Gas

A flow diagram showing the steps required to calculate model input to simulate a non-condensing gas release is shown in Figure 4-3. The release may exhibit choked flow. As the flow diagram shows, different paths of calculation must be followed for choked flow and unchoked flow. Although the same quantities are calculated for both the choked and unchoked flows, the methods used for the calculations are different.

4.5.3 Single-phase, High Volatility Liquid

Figure 4-4 shows a flow diagram for calculating the input for a release of a highly volatile liquid. This is the simplest of the flow charts, with no decision branches. The released material is assumed to be in a pure vapor state. The density can be calculated using the perfect gas law.

4.5.4 Single-phase, Low Volatility Liquid

Figure 4-5 shows the flow diagram for calculating input for a low-volatility liquid release. In this case, the release rate into the atmosphere is controlled by the pool size. The pool size, in turn, may be limited by the rate at which the liquid exits the container or by containment from a dike or bund.

4.6 DETERMINATION OF CHOKED FLOW FOR GAS RELEASES

Gases may be stored at high enough pressures that, if the gas is escaping through a hole rather than the container failing, the gas escape velocity may reach the speed of sound. However, the escape velocity can not be greater than the speed of sound no matter how high the pressure under which the material is stored. The pressure at the exit point of the gas (p_*) is calculated by:

$$\frac{p_*}{p_s} = \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{(\gamma-1)}}$$

where: γ = the ratio of the specific heat at constant pressure to that at constant volume; and

p_s = storage pressure (Pa).

If $p_* \geq p_a$, then the flow should be considered choked. If $p_* < p_a$, then the flow is not choked. For the calculations in this document, the units of p_*

should be Pascals (Pa). The standard atmosphere at sea level has a pressure of 101325 Pa.

Whether a flow is choked or not is important for determining which sets of equations to use for the calculation of emission rate and temperature. In the following sections, the gas release calculations will be divided into those for critical or choked flow and those for subcritical, or unchoked, flow.

In the case of gases from stacks, the calculations given here are not required. The determination of whether a flow is choked or not assumes that a storage pressure is known, but for a stack release, this may not be the case. Stack release volume rates may be governed more by a release temperature or mechanical device (such as exhaust fans). In those cases, a storage pressure is not specified. Normally, the emission rate is known through measurement, assumed based on design limitations, or estimated from emission factors. Temperature, if not known, can be estimated as the ambient temperature.

4.7 EMISSION RATE

The emission rate input to the model is often known when calculating impacts from a release that occurred in the past. The amount of mass that was lost from the system and the duration of the release are normally known or calculable. In planning or in a real-time release, the emission rate normally requires a calculation using the design criteria of the container involved in the release.

The emission rate is not always calculated before the other parameters discussed in this section. The flow charts of input calculations given for the various release classes can be used as a guide to the proper order of calculation. Where a prior calculation is required, it is noted along with the section in which to find that calculation.

4.7.1 Two-phase Gas Release (Choked)

Prior calculations required:

p_* - critical pressure (Pa) (4.6).

Flow chart reference: Figure 4-2

A series of calculations is required to determine the conditions at choked flow. The parameters describing the conditions can then be used to calculate the emission rate.

The first of these parameters is the temperature (T_*) corresponding to the critical pressure. It can be calculated from:

$$p_* = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_*}\right)\right]$$

where: M = molecular weight (kg/kmol);
λ = heat of vaporization at T_b (J/kg);
R = gas constant = 8314 J/kmol °K;
T_b = normal boiling point (°K); and
T_* = temperature at choked conditions (°K).

The vapor fraction at choked flow conditions (F_*) can be estimated from:

$$F_* = 1 + \frac{T_*}{M\lambda}\left[MC_p \ln\left(\frac{T_s}{T_*}\right) - R \ln\left(\frac{p_s}{p_*}\right)\right]$$

where: C_p = gas heat capacity at T_s (J/kg °K); and
T_s = storage temperature (°K).

The change in enthalpy (ΔH_*) from storage conditions to the choked flow conditions is given by:

$$\Delta H_* = C_p(T_s - T_*) + \lambda(1 - F_*)$$

The last choked flow parameter required before the emission rate can be calculated is the density at choked flow conditions (ρ_*). It is given by:

$$\rho_* = \left[F_*\left(\frac{RT_*}{p_*M}\right) + \left(\frac{1 - F_*}{\rho_l}\right)\right]^{-1}$$

where ρ_l = liquid density at T_b (kg/m^3).

With the choked flow parameters, the emission rate can be calculated as:

$$E^{\cdot} = A_o\rho_*\left[2(0.85)\left(\frac{\Delta H_*}{\left(1 + \frac{4fL_p}{D_p}\right)}\right)\right]^{\frac{1}{2}}$$

where: E = emission rate (kg/s);
A_o = area of hole (m^2);
f = 0.0045, estimated (dimensionless);
L_p = pipe length (m); and
D_p = pipe diameter (m).

4.7.2 Two-phase Gas Release (Unchoked)

Prior calculations required:

ΔH - change in enthalpy between storage and release conditions (J/kg) (4.9.2); and

ρ_{rel} - density at release temperature (kg/m^3) (4.11).

Flow chart reference: Figure 4-2

The intermediate calculations required for the emission rate of an unchoked gas flow to be calculated are very similar to the calculations required for the choked flow. In the case of choked flow, the calculations

are carried out at the choked conditions. For the unchoked case, the calculations are carried out at the release temperature and ambient pressure.

The emission rate (E) is calculated from:

$$E = A_o \rho_{rel} \left[2(0.85) \left(\frac{\Delta H}{\left(1 + \frac{4fL_p}{D_p}\right)} \right) \right]^{\frac{1}{2}}$$

where:
- E = emission rate (kg/s);
- A_o = area of hole (m^2);
- f = 0.0045, estimated (dimensionless);
- L_p = pipe length (m); and
- D_p = pipe diameter (m).

4.7.3 Two-phase Pressurized Liquid

Prior calculations required: None.

Flow chart reference: Figure 4-2

The emission rate for a pressurized liquid can take into account a length of pipe through which a release may occur. If the pipe length is zero (the emission is directly from a tank), the emission rate will become that calculated from the standard orifice equation for incompressible flow. If the pipe length is greater than the length of pipe required to establish an equilibrium flow, a different equation (presented below in this section) is required. The longer a pipe the more the resistance to the flow of the chemical is encountered. By ignoring the pipe length the emission rate will be maximized.

The expression for the emission rate from a system with a pipe shorter than the pipe length required for equilibrium flow ($L_p/L_e \leq 1$) is:
where: E = emission rate (kg/s);

$$E = A_o\left(\frac{\lambda M p_s}{RT_s^2}\right)\left(\frac{T_s}{NC_{pl}}\right)^{\frac{1}{2}}$$

A_o = area of hole (m^2);

M = molecular weight (kg/kmol);

λ = heat of vaporization at T_b (J/kg);

R = gas constant = 8314 J/kmol °K;

$$N = \frac{R(\lambda M p_s)^2}{2(p_s - p_a)\rho_l C^2 (RT_s)^3 C_{pl}} + \frac{L_p}{L_e}$$

T_s = storage temperature (°K);

p_s = storage pressure (Pa);

C_{pl} = liquid heat capacity at T_s;

p_a = ambient pressure (Pa);

ρ_l = liquid density at T_b;

T_b = normal boiling point (°K);

C = discharge coefficient, 0.6 (dimensionless);

L_p = pipe length (m); and

L_e = pipe length required for equilibrium flow (m), assumed 0.1 m.

If $L_p/L_e > 1$, the expression becomes:

$$E = A_o F\left(\frac{\lambda M p_s}{RT_s^2}\right)\left(\frac{T_s}{C_{pl}}\right)^{\frac{1}{2}}$$

where: F = a pipe friction factor given by

$$F^2 = \frac{1}{\left(1 + \frac{4fL_p}{D_p}\right)}$$

where: f = 0.0015, estimated (dimensionless); and

D_p = pipe diameter (m).

4.7.4 Two-phase Refrigerated Liquid

Prior calculations required: None.

Flow chart reference: Figure 4-2

The emission rate for a refrigerated liquid can be calculated from:

$$E = A_o\left[2C^2(p_s - p_{sv})\rho_l + \frac{F^2}{C_{pl}T_s}\left(\frac{\lambda M p_s}{RT_s}\right)^2\right]^{\frac{1}{2}}$$

where: E = emission rate (kg/s);

A_o = area of hole (m^2);

M = molecular weight (kg/kmol);

λ = heat of vaporization at T_b (J/kg);

R = gas constant = 8314 J/kmol °K;

T_s = storage temperature (°K);

p_s = storage pressure (Pa);

C_{pl} = liquid heat capacity at T_s;

ρ_l = liquid density at T_b;

T_b = normal boiling point (°K);

C = discharge coefficient, 0.6 (dimensionless);

p_{sv} = the vapor pressure of the chemical at T_s (Pa);

$$p_{sv} = 101325\text{Pa}\ \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_s}\right)\right]$$

and F = a pipe friction factor given by

$$F^2 = \frac{1}{\left(1 + \frac{4fL_p}{D_p}\right)}$$

where: f = 0.0015, estimated (dimensionless);

L_p = pipe length (m); and

D_p = pipe diameter (m).

4.7.5 Single-phase Gas Release (Choked)

Prior calculations required: None.

Flow chart reference: Figure 4-3

The estimate for the emission rate can be calculated from:

$$E = CA_o\left[p_s\rho_s\gamma\left(\frac{2}{\gamma + 1}\right)^{\frac{(\gamma+1)}{(\gamma-1)}}\right]^{\frac{1}{2}}$$

where: E = emission rate (kg/s);

A_o = area of hole (m^2);

p_s = storage pressure (Pa);

ρ_s = storage density (kg/m^3);

C = discharge coefficient, 0.75 (dimensionless); and

γ = the ratio of the specific heat at constant pressure to that at constant volume.

4.7.6 Single-phase Gas Release (Unchoked)

Prior calculations required: None.

Flow chart reference: Figure 4-3

The emission rate estimate for unchoked gas flow that is not condensing can be calculated from:

$$E = KYA_o[2\rho_s(p_s - p_a)]^{\frac{1}{2}}$$

where: E = emission rate (kg/s);

A_o = area of hole(m^2);

ρ_s = storage density (kg/m^3);

p_s = storage pressure (Pa);

p_a = ambient pressure (Pa);

$$K = \frac{C}{\sqrt{1 - \beta^4}}$$

and

$$Y = 1 - \left(\frac{p_s - p_a}{p_s \gamma}\right) (0.41 + 0.35\ \beta^4)$$

$C = 0.62$;

$\beta^2 = A_o / A_1$; and

A_1 = cross-sectional area of gas container in direction of flow.

4.7.7 <u>Single-phase Liquid Release (High Volatility)</u>

Prior calculations required: None.

Flow chart reference: Figures 4-4 and 4-5

A high volatility liquid can have a range of release rates of its gas phase into the air. The largest injection rate would occur if the liquid vaporizes immediately upon release. However, if the liquid is refrigerated, a pool of the liquid may form. In that case the vapor emission would be from a combination of the vaporization of the liquid occurring straight from the hole and evaporation from the boiling liquid pool. Since the calculations in this document and the Workbook are intended to be done using only a hand-calculator and the purpose of this document is to provide screening or conservative calculations for input to models, the most conservative case, which is immediate vaporization of the liquid, is assumed.

Two steps are required to calculate the emission rate for a high volatility liquid. The first part of the calculation is to estimate the pressure at the hole from which the liquid is being released. This is done using the following formulas:

where: p_h = pressure at the hole (Pa);

$$p_h = \max(p_a, p_s) + \rho_s g H_1$$

p_a = ambient pressure (Pa);

ρ_s = storage density (kg/m^3);

g = acceleration due to gravity (9.806 m/s^2); and

H_1 = vertical distance between hole and the top of liquid level (m).

p_s = the vapor pressure of the chemical at T_s (Pa);

$$p_s = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_s}\right)\right]$$

M = molecular weight (kg/kmol);

λ = heat of vaporization at T_b (J/kg);

R = gas constant = 8314 J/kmol °K;

T_s = storage temperature (°K); and

T_b = normal boiling point (°K).

With the value of the pressure at the hole known, the emission rate can be estimated by:

$$E = KA_o[2\rho_s(p_h - p_a)]^{\frac{1}{2}}$$

where: A_o = area of hole (m^2);

$$K = \frac{C}{\sqrt{1 - \beta^4}}$$

and C = 0.65 (dimensionless).

$\beta^2 = A_o / A_1$; and

A_1 = cross-sectional area of gas container in direction of flow.

4.7.8 Single-phase Liquid Release (Low Volatility)

Prior calculations required:

E - emission rate of liquid from hole (kg/s) (4.7.7); and

T_{rel} - temperature of the liquid after release (°K).

Flow chart reference: Figure 4-5

The calculation of the emission rate for the low volatility case begins just the same as the high volatility case, by calculating the liquid release rate from the container. In the high volatility case, it is assumed that the liquid vaporizes as it comes out. However, for the low volatility case, another emission rate from the evaporating pool (E_{pool}) is calculated and compared to the container emission rate.

The emission rate from a pool can be estimated as:

$$E_{pool} = 6.94\times10^{-7}(1 + 0.0043(T_2 - 273.15)^{*2})U_r^{0.75}A_pM\frac{p_v}{p_{vh}}$$

where:

E_{pool}	= pool emission rate (kg/s);
U_r	= ambient wind speed at 10 m altitude (m/s);
A_p	= pool size (m^2);
M	= molecular weight (kg/kmol);
T_2	= T_{rel} or T_a (°K);
T_a	= ambient temperature (°K);
$[T_2\text{-}273.15]^*$	= 0 if $[T_2\text{-}273.15] < 0$
	= $[T_2\text{-}273.15]$ if $[T_2\text{-}273.15] \geq 0$;
p_{vh}	= vapor pressure of hydrazine at T_2 (Pa)

$$p_{vh} = \exp\left[76.8580 - \frac{7245.2}{T_2} - 8.22\ln(T_2) + 0.0061557T_2\right]$$

p_v = vapor pressure of chemical at T_2 (Pa):

$$p_v = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_2}\right)\right]$$

λ = heat of vaporization at T_b (J/kg);

T_b = normal boiling point (°K); and

R = gas constant = 8314 J/kmol °K.

Note that T_2 can be either of two values. The value of E_{pool} should be calculated for each value of T_2. The higher E_{pool} should be used in the subsequent calculations. Normally the higher value of T_2 will provide the highest pool emission rate. However, this may not always be the case since the vapor pressure of hydrazine is used as a scaling factor and enters as an inverse.

If the value of $E_{pool} < E$, then the pool's evaporation determines the rate at which material enters the atmosphere. In that case, E_{pool} and A_p should be used in calculating the emission rate and source size.

If $E_{pool} > E$, then the container discharge determines the rate at which the chemical enters the air. As the chemical is released, a pool is formed that is smaller than A_p. The evaporation from the formed pool is equal to E. A new pool size should be calculated using the equation for E_{pool} but setting the value of E_{pool} equal to E. This new pool size should be used as the source size.

4.8 RELEASE TEMPERATURE

Source-term models require the storage temperature of the chemical just before release. The source-term model calculates the change in temperature after the release. Non-source-term models require the emission temperature after depressurization has occurred. An external calculation is required for determining the depressurized temperature.

If the material release is colder than the ambient air, its density may be increased enough that it acts as a dense gas, even if its molecular weight is less than air's molecular weight. If the material released is warmer than the ambient air, its density may be less than that of the ambient air and it will act as a buoyant release. As the release moves downwind, entrainment of the ambient air and contact of the plume with a surface can change the plume temperature. Entrainment with ambient air makes the plume temperature approach that of the ambient air. Contact with a surface makes the plume temperature approach that of the surface.

There are many effects that temperature can have on a release. For example, in an actual release, a pressurized gas was initially escaping through a small hole. The cooling due to expansion was so great that not only did water vapor in the air condense, it froze. The hole became clogged with ice, reducing the flow rate. As the flow rate decreased, the ice melted. Some of the liquid water reacted with the escaping material which, in this case, formed an acid. The acid dissolved some of the container wall which made the hole larger. The release rate increased, the cooling increased, and a cycle of large emissions and low emissions began. This is an extreme case, and probably no model will ever take into account such detailed effects. However, it is important to realize some of the effects that temperature can have, not only on the dispersion, but on the source itself.

4.8.1 Two-phase Gas Release (Choked)

Prior calculations required:

F_{rel} - flash fraction of chemical of interest (dimensionless) (4.9.1) (as a check);

T_* - temperature at choked conditions (°K) (4.7.1); and

F_* - mass vapor fraction at choked conditions (dimensionless) (4.7.1).

Flow chart reference: Figure 4-2

Note that in this case, a two-step solution may be required. The release temperature is calculated here using the value of F_{rel} calculated in Section 4.9.1. The first time calculating release temperature assume that $F_{rel} < 1$. If the subsequent calculation in Section 4.9.1 indicates that F_{rel} is equal to 1, recalculate the release temperature.

If $F_{rel} < 1$, the release temperature can be estimated using the Clausius-Clapeyron equation:

$$p_a = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_{rel}}\right)\right]$$

where: T_{rel} = release temperature (°K);
M = molecular weight (kg/kmol);
λ = heat of vaporization at T_b (J/kg);
R = gas constant = 8314 J/kmol °K;
T_b = normal boiling point (°K); and
p_a = ambient pressure (Pa).

If $F_{rel} \geq 1$, it should be set to 1 for later calculations, and the following equation should be used for the release temperature:

$$T_{rel} = T_* + \frac{\lambda(1 - F_*)}{C_{pl}}$$

where: λ = heat of vaporization at T_b (J/kg); and
C_{pl} = liquid heat capacity at T_s (J/kg °K).

Note that the value of C_{pl} is to be at T_s. The data in Appendix B is for C_{pl} at a fixed temperature. Using the value of C_{pl} in the Appendix rather than correcting for temperature, considering other uncertainties in the screening approach, will not add significant error to the results.

4.8.2 Two-phase Gas Release (Unchoked)

Prior calculations required: None.

Flow chart reference: Figure 4-2

The release temperature can be estimated using the Clausius-Clapeyron equation:

$$p_a = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_{rel}}\right)\right]$$

where: T_{rel} = release temperature (°K);
M = molecular weight (kg/kmol);
λ = heat of vaporization at T_b (J/kg);
R = gas constant = 8314 J/kmol °K;
T_b = normal boiling point (°K); and
p_a = ambient pressure (Pa).

4.8.3 Two-phase Pressurized Liquid

Prior calculations required: None.

Flow chart reference: Figure 4-2

For this release class, the same calculation is used for release temperature as the calculation given for "Two-Phase Gas Release (Unchoked)." See Section 4.8.2.

4.8.4 Two-phase Refrigerated Liquid

Prior calculations required: None.

Flow chart reference: Figure 4-2

For this release class, the same calculation is used for release temperature as the calculation given for "Two-Phase Gas Release (Unchoked)." See Section 4.8.2.

4.8.5 Single-phase Gas Release (Choked)

Prior calculations required: None.

Flow chart reference: Figure 4-3

The temperature is calculated based on the assumption that the change occurs in two steps. The first step is when the release goes to choked flow conditions (adiabatic and reversible temperature change). The second occurs between the choked flow conditions and ambient pressure conditions (adiabatic but not reversible). The equation to use in estimating the discharge temperature is:

$$T_{rel} = T_s\left[1 - 0.85\left(\frac{\gamma - 1}{\gamma + 1}\right)\right]$$

where: T_{rel} = release temperature (°K);

T_s = storage temperature (°K); and

γ = the ratio of the specific heat at constant pressure to that at constant volume.

4.8.6 Single-phase Gas Release (Unchoked)

Prior calculations required:

E - emission rate (kg/s) (4.7.2).

Flow chart reference: Figure 4-3

The calculation of the release temperature for the unchoked case depends on the rate of emission, which is less than that in the choked flow case. The equation to use is:

$$T_{rel} = \frac{2T_s}{[1 + \sqrt{(1 + 4aT_s)}]}$$

where:

$$a = \frac{1}{2C_p}\left(\frac{ER}{p_a M A_o}\right)^2$$

and E = emission rate (kg/s);

A_o = area of hole(m^2);

p_a = ambient pressure (Pa);

M = molecular weight (kg/kmol);

R = gas constant = 8314 J/kmol °K; and

C_p = gas heat capacity at T_s (J/kg °K).

4.8.7 Single-phase Liquid Release (High Volatility)

Prior calculations required: None.

Flow chart reference: Figure 4-4

This release class is based on the assumption that, as soon as the liquid leaves the container, it vaporizes. The release temperature can be assumed to be the normal boiling point of the chemical.

4.8.8 Single-phase Liquid Release (Low Volatility)

Prior calculations required: None.

Flow chart reference: Figure 4-5

This release class is based on the assumption that the spilled material evaporates from a pool. The normal boiling point of the chemical is higher than the ambient temperature. The release temperature into the air can be assumed to be the same as the ambient temperature or the storage temperature, whichever is lower. This enhances any heavier-than-air effects on the dispersion.

In reality, the temperature from an evaporating pool may be less than the ambient temperature because of the cooling effect due to evaporation. Such a temperature calculation requires more than a simple formula; it requires a complete model for an evaporating liquid. Many models assume that the temperature is the same as the ambient temperature in calculating the emission rate. This is a conservative assumption, since higher temperatures lead to higher emission predictions. In summary, for a conservative approach, assume that the liquid is evaporating due to a high surface temperature but entering the atmosphere at a low temperature (the lower of ambient or pool temperature).

Low volatility liquid releases should always be continuous or of finite duration. Evaporation is the primary method in which the material enters the air. Unless the release is very small, evaporation may take a while. If a low volatility release is small enough to evaporate quickly into the atmosphere, it is probably small enough to ignore.

4.9 VAPOR FRACTION

The vapor fraction of a release is always a required calculation for a two-phase release class. For single-phase releases, it is assumed that all the material enters the air in the vapor phase because: 1) the material is stored in the vapor state and cooling due to expansion is insufficient to cause condensation; 2) the release is of a high volatility liquid that vaporizes instantly upon release to the environment; or 3) the release is from a low volatility liquid emitted to the air through evaporation.

Since the two-phase releases are the only classes exhibiting a mixture of liquid and vapor fractions, they are the only ones for which calculations are presented here. For all other cases, the vapor fraction of the release (F_{rel}) should be set to 1; that is, only vapor is assumed to enter the atmosphere.

4.9.1 Two-phase Gas Release (Choked)

Prior calculations required:

F_* - vapor fraction at choked flow conditions (dimensionless) (4.7.1);

T_* - temperature at choked flow conditions (°K) (4.7.1); and

T_{rel} - release temperature (°K) (4.8.1).

Flow chart reference: Figure 4-2

The vapor fraction after decompression (F_{rel}) is given, in this case, as:

$$F_{rel} = F_* + \frac{C_{pl}(T_* - T_{rel})}{\lambda}$$

where: C_{pl}= liquid heat capacity at T_s (J/kg °K); and
λ = heat of vaporization at T_b (J/kg).

If $F_{rel} > 1$, set it equal to 1 and correct the release temperature (T_{rel}) calculation in Section 4.8.1.

4.9.2 Two-phase Gas Release (Unchoked)

Prior calculations required:

T_{rel} - release temperature (°K) (4.8.2).

Flow chart reference: Figure 4-2

The vapor fraction after decompression (F_{rel}) for unchoked flow is estimated from:

$$F_{rel} = 1 + \frac{T_{rel}}{M\lambda}\left[MC_p \ln\left(\frac{T_s}{T_{rel}}\right) - R \ln\left(\frac{p_s}{p_a}\right)\right]$$

where: M = molecular weight (kg/kmol);
λ = heat of vaporization at T_b (J/kg);
R = gas constant = 8314 J/kmol °K;
T_s = storage temperature (°K);
C_p = gas heat capacity at T_s (J/kg °K);
p_s = storage pressure (Pa); and
p_a = ambient pressure (Pa).

This value is also used to calculate the change in enthalpy from storage conditions to ambient conditions (ΔH). The value for the change in enthalpy is given by:

$$\Delta H = C_{pl}(T_s - T_{rel}) + \lambda(1 - F_{rel})$$

4.9.3 <u>Two-phase Pressurized Liquid</u>

Prior calculations required:

T_{rel} - release temperature (°K) (4.8.2).

Flow chart reference: Figure 4-2

The vapor fraction after release (F_{rel}) is given as:

$$F_{rel} = \frac{C_{pl}(T_s - T_{rel})}{\lambda}$$

where: λ = heat of vaporization at T_b (J/kg);

T_s = storage temperature (°K); and

C_{pl}= liquid heat capacity at T_s (J/kg °K).

4.9.4 Two-phase Refrigerated Liquid

Prior calculations required: None.

Flow chart reference: Figure 4-2

This release class uses the same calculation for vapor fraction as the calculation given for "Two-Phase Pressurized Liquid" in Section 4.9.3.

4.10 INITIAL CONCENTRATION

The initial concentration sets an upper limit for the maximum concentration that may be seen downwind since the maximum concentration (considering all altitudes) cannot increase with downwind distance. If the initial concentration is low enough, it may also mean that the emission need not be treated as a denser-than-air release. The concentrations of emitted chemical, air, and water vapor are used in determining the density of the release. The concentrations are defined as:

f_a = molar fraction of air;

f_w = molar fraction of water vapor; and

f_i = molar fraction of chemical of interest.

The only release classes where the values of f_a, f_w, and f_i need to be calculated are the single-phase gas release and the low volatility liquid release. In all the other classes, the release is near the boiling point of the chemical. Either a gas cools to near its boiling point and condensation occurs or a liquid is vaporizing or flashing. For these near-boiling-point releases, the conservative assumption is that f_i is 1 and f_a and f_w are both zero. This, in fact, is the implicit assumption in most models.

In single phase gas or low volatility liquid releases the chemical of interest is in the gas phase and, in general, could be made up of multiple species. If the chemical of interest is a mixture, its data description should be created as described in Section 4.2. Knowing any two of the molar concentrations of the three constituents determines the third because:

$$f_a+f_w+f_i = 1$$

Measurement of the individual constituents would normally be required for determining the molar fractions. The water vapor fraction is the easiest to estimate or measure. If the temperature (T) of the release is known (in Kelvin) and it is less than about 370 °K, the saturated molar fraction of the water vapor (e_s) at 1 atmosphere of pressure is estimated as:

$$\log_{10} e_s = 6.3994 - \frac{2353}{T}$$

The value of e_s gives the maximum molar fraction of water vapor. At 298 °K, e_s is about 0.03. For releases near moderate atmospheric temperatures, the molar fraction of water vapor is small. However, in energy content calculations, the amount of water vapor present can be significant because of the greater heat capacity of water vapor versus dry air. If the relative humidity is also known, the molar fraction of water vapor can be calculated as:

$$f_w = \left(\frac{RH}{100}\right) e_s$$

where: RH = relative humidity in percent.

It should be noted that these equations for e_s and f_w are only strictly valid for a water vapor and air mixture. Adding a chemical to the mix can introduce error to the estimate. The amount of error and the direction of the error would depend on the chemical. However, for input screening purposes, these equations are adequate.

In reality, if a release has a jet phase where the emission is expanding, some air will be entrained. The calculation to estimate the amount of ambient air entrained is beyond the scope of this data screening study. When there is uncertainty, the assumption should be made to make f_i as close to 1 as possible.

4.10.1 Single-phase Gas Release

Prior calculations required: None.

Flow chart reference: Figure 4-3

If the release is from a vessel containing only the chemical of interest, the release should be treated as pure. This means that the value of f_i would be 1 and the other fractions would be zero. In most pressurized containers, this would be the case. The special case is that of a stack release.

A stack release is the most likely release to have all three constituents present. If a liquid water cloud is visibly being emitted from the stack, then f_w can be assumed to be equal to e_s. When water is used as a scrubbing media, the emission is often water saturated at the release point. The value for f_a or f_i must be determined from measurement or deduced from information about the release. An example of such a deduction is given below. The conservative assumption is that f_a is equal to zero; i.e. that the stack release is of chemical undiluted by air.

An example of a deduction from release information would be the case where a release of a known amount of chemical occurred over a known amount of

time inside a building. The ventilation system would carry the spilled material out to a vent. If the volume flow rate of the ventilation system (V_{rv}) (from design documents) and the volume emission rate of the chemical of interest (V_r) are known, then the value of f_i could be estimated from:

$$f_i = \frac{V_{ri}}{V_{rv}}$$

The value of f_w would be assumed to be consistent with the humidity in the vessel. In other words, the values of f_w and f_a would be prorated over $(1 - f_i)$ at the same relative proportions that were in the air within the building. If the molar fractions of water vapor and air inside the building were f_w' and f_a', respectively, the values for f_w and f_a would be calculated by:

$$f_w = f_w'(1 - f_i)$$

and

$$f_a = f_a'(1 - f_i)$$

4.10.2 <u>Single-phase Liquid Release (Low Volatility)</u>

Prior calculations required:

T_{rel} - release temperature (°K) (4.8.8).

Flow chart reference: Figure 4-5

This release class is for a pool of evaporating liquid. The chemical has a boiling point higher than the ambient temperature. The initial molar

concentration of the chemical that is directly over a pool of evaporating liquid can be estimated by:

$$f_i = \frac{p_v}{p_a}$$

where: p_v = vapor pressure of chemical at T_{rel} (Pa); and
p_a = ambient pressure (Pa).

For pools of liquid that are not boiling, the value of f_i is less than 1. The rest of the emission can be assumed to include air and water vapor in the same proportions as those found in the ambient air, unless some process is going on that alters these proportions. For example, if a water spray were in use during a spill, the value of f_w could be assumed to be equal to e_s, the saturation mole fraction of water.

4.11 DENSITY

Prior calculations required:

T_{rel}	-	release temperature (°K) (4.8);
F_{rel}	-	initial mass vapor fraction of chemical of interest (dimensionless) (4.9);
f_i	-	initial molar fraction of chemical of interest (dimensionless) (4.10);
f_a	-	initial molar fraction of air (dimensionless) (4.10); and
f_w	-	initial molar fraction of water vapor (dimensionless) (4.10).

Flow chart reference: Figure 4-6

Among the models used in this study, the DEGADIS model requires the user to input the release density. The specific use of this value in DEGADIS is described below. Cloud density is also used in determining whether a release

is to be treated as a dense gas, as described in Section 4.13. The molar fractions of each of the constituents respectively are f_a, f_w, and f_i for air, water vapor, and chemical of interest. Descriptions and relationships of these molar fractions are given in Section 4.10. In calculating the density of the initial release, the partitioning of the cloud into air, water vapor, and the chemical of interest should be taken into account . Also, the chemical of interest should be allowed to be in both liquid and gas phases. The chemical of interest may be in the form of an aerosol (liquid droplets and vapor phase chemical). The initial partitioning of liquid and gas phases of the chemical of interest is determined by calculating the flash fraction, described in Section 4.9. The fraction of a two-phase release in the gas state is given as F_{rel}. The density for each constituent is required to calculate the overall density of the release. The density of the chemical of interest can be determined by:

$$\rho_i = \left(\frac{F_{rel}}{\rho_g} + \frac{(1-F_{rel})}{\rho_l} \right)^{-1}$$

where the density of the gas phase can be calculated assuming it is a perfect gas.

The density would be given by:

$$\rho_g = \frac{p_a M_i}{RT_{rel}}$$

where: p_a = ambient pressure (Pa); and
R = gas constant = 8314 J/kmol °K.

The density of the liquid phase for specific chemicals is available in Appendix B.

The densities of the air and the water vapor in the cloud can be determined by also assuming a perfect gas. These densities (kg/m^3) are:

$$\rho_a = \frac{p_a M_a}{RT_e}$$

$$\rho_w = \frac{p_a M_w}{RT_e}$$

where: M_a = molecular weight of air (kg/kmol); and
M_w = molecular weight of water (kg/kmol).

Once the individual component densities have been determined, the overall density (ρ_{rel}) of the released cloud can be determined by calculating:

$$\rho_{rel} = \left(\frac{f_a M_a}{M_T \rho_a} + \frac{f_w M_w}{M_T \rho_w} + \frac{f_i M_i}{M_T \rho_i} \right)^{-1}$$

where: M_T = mean molecular weight of all material released (air, water vapor, and chemical of interest) (kg/kmol) and given by the formula:

$$M_T = f_a M_a + f_w M_w + f_i M_i$$

Note that if f_a and f_w are both zero (a release of pure chemical), then f_i is equal to 1. In that case, ρ_{rel} is equal to ρ_i.

The DEGADIS model requires density triplets when aerosol is present in the release. Each triplet consists of:

- Mole fraction of chemical of interest (f_i);
- Mass concentration of chemical of interest (ρ_i); and
- Mass density of the mixture (ρ_{mix}).

In the DEGADIS model, the values for f_a and f_w are based on the relative proportion of these constituents in the ambient air. The assumption is made

that all air and water vapor come directly from the atmosphere and that none come from the chemical source. The DEGADIS model would prefer a schedule of triplets for various air and chemical mixtures. Since the temperature, liquid content, vapor content, and chemical concentrations vary as air is entrained into the release, it is not a trivial calculation to create such a schedule.

A simpler approach is to provide the model with only two triplets in the schedule. The first triplet would be for cases where only air is present in the release (f_a is 1 and f_i and f_w are both zero). This triplet would be: 0.0, 0.0, ρ_a. Because there is no contaminant in this triplet, the ρ_a entered here should be evaluated at the ambient temperature T_a, rather than the release temperature T_e. The second triplet would be for cases where there is no air present in the release (f_i is 1 and f_a and f_w are both zero). The second triplet would then become: 1.0, ρ_{rel}, ρ_{rel}. DEGADIS will linearly interpolate the air contaminant mixture for all chemical concentrations.

4.12 RELEASE DIAMETER OR AREA

Source-term models normally require the hole size, stack diameter, or pool area of a release. Non-source-term models require a source size that represents the size of the release after any expansion has taken place. For the source-term model, the input requirement is fulfilled from the list of observables. For the non-source term model, some calculations may be required.

In the case of a liquid pool evaporating, the release area is simply the area of the pool. This is because the emission velocity into the atmosphere is low and there is no expansion of the vapor coming from the liquid surface. In the case of a jet release, some expansion can take place, and a calculation should be done to provide an estimate of the expansion effect.

There are two methods that can be used to estimate the post-expansion dimension of a release. One can be used in cases with low release momentum. The other can be used in the case of high momentum releases such as jets.

If the release is a choked gas the diameter of the hole used in non-source term models should be changed. In this case the high momentum release formula should be used, but the value of ρ_s should be replaced with the density at choked conditions (ρ_*). If the release is unchoked and the exit velocity is of the same order or less than the ambient wind velocity, the low momentum formula should be used. For a continuous release, if the exit velocity is unknown, the smaller diameter calculated from the two formulae should be used. Using the smaller diameter will minimize the release buoyancy criteria discussed in Section 4.13.1. The smaller the release diameter, the more likely that the release will behave as a denser-than-air release.

If the exit velocity (u) is unknown, but the emission rate (E), density in the container (ρ_s), and hole or emission area (A) are known, an exit velocity can be estimated. The formula to use is:

$$u = \frac{E}{A\rho_s}$$

With an approximation, the exit velocity can be compared to the ambient wind speed. The exit velocity for evaporating pools is negligible and need not be estimated.

Instantaneous releases normally are not associated with an exit velocity and the low momentum formula should be used. If the released volume of an instantaneous release is known, the release diameter can be assumed 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 base on ground) with the height equal to the diameter. If the release is not at ground level assume the cloud is shaped like a sphere.

4.12.1 Low-momentum Release

Prior calculations required:

E - emission rate (kg/s) (4.7); and

ρ_{rel} - release density (kg/m^3) (4.11).

Flow chart reference: Figure 4-6

The diameter of a source after expansion can be estimated as:

$$D_{rel} = \sqrt{\frac{2}{U_r}\left(\frac{E}{\rho_{rel}}\right)}$$

where: D_{rel} = diameter (m); and

U_r = ambient wind speed (m/s).

4.12.2 High-momentum Release

Prior calculations required:

ρ_{rel} - release density (kg/m^3) (4.11).

Flow chart reference: Figure 4-6

The diameter after expansion can be estimated as:

$$D_{rel} = D_s \sqrt{\frac{\rho_s}{\rho_{rel}}}$$

where: D_{rel} = diameter (m);

D_s = hole or stack diameter (m); and

ρ_s = density at hole (kg/m^3).

4.13 RELEASE BUOYANCY

The models discussed in this document handle dense gas releases. If a release can be considered not to be denser than air, standard passive dispersion modeling or a model capable of handling neutrally buoyant releases should be applied. To determine whether a release should be considered denser than air, a comparison is done of the Richardson number describing the release to a selected value. The formulation of the Richardson number, and thus the calculation, depends on whether the release is instantaneous or continuous.

4.13.1 Continuous Release

Prior calculations required:

E - emission rate (kg/s) (4.7);

ρ_{rel} - release density (kg/m^3) (4.11); and

D_{rel} - release diameter (m) (4.12).

The criteria (C_ρ)for determining whether a continuous release should be considered denser than air is if:

$$C_\rho \equiv \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}} \leq 6$$

where: U_r = ambient wind speed (m/s);

g = acceleration due to gravity (9.806 m/s^2); and

ρ_a = air density (kg/m^3).

4.13.2 Instantaneous Release

Prior calculations required:

E - emission rate (kg/s) (4.7);

ρ_{rel} - release density (kg/m^3) (4.11); and

The criteria (C_ρ) for determining whether an instantaneous release should be considered denser than air is if:

$$C_\rho \equiv \left[\frac{g(E_t/\rho_{rel})^{1/3}}{U_r^2}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{2}} > 0.2$$

where: U_r = ambient wind speed (m/s);

g = acceleration due to gravity (9.806 m/s^2);

E_t = total amount of material released (kg);

ρ_a = air density (kg/m^3).

The value of E_t must be calculated from the emission rate (E) and duration of the release as:

$$E_t = E\,\Delta t$$

where: Δt = release duration (s).

The value of E_t can also be calculated if the volume of the vessel is known by:

$$E_t = \frac{V_t}{\rho_s}$$

where: V_t = total volume of the vessel (m^3); and

ρ_s = storage density (kg/m^3).

4.14 RELEASE HEIGHT

The release height represents the altitude above ground that the emission enters the atmosphere. For liquid releases with evaporating pools, this height should be that of the liquid-air interface, which is typically at ground level.

4.15 GROUND SURFACE TEMPERATURE

An appropriate input value for ground surface temperature should be that from routine on-site measurements. If such data are not available, ground surface temperature may be approximated to be equal to the ambient temperature measured at the standard height for most applications. Experience to date indicates little, if any, sensitivity in predicted model concentrations due to changes in this parameter.

4.16 AVERAGING TIME

Hazardous chemical releases are often of short duration, and the concentrations of interest are short-term averages. Typical concerns from a hazardous air release are the maximum short-term concentration and the maximum dose. Many hazardous air pollutant models are designed to provide concentration predictions for unit averaging times ranging from 1 second to 1 hour. By contrast, regulatory models for most criteria pollutants have a basic averaging time of 1 hour for concentration estimates.

Refined dense gas models can typically provide concentration estimates for user-specified averaging times of 1 hour or less. Due to entrainment with ambient air, a dense gas release typically does not remain significantly dense for travel times longer than 1 hour. Meteorological input, however, is often based on an hourly average. To determine the appropriate averaging time, the user should examine the release duration and the concentration levels of concern (keeping health or other reference levels in mind).

If a concentration exposure to population is of concern, the averaging time should be determined from the concentration limit selected. For example, Short Term Exposure Limits (STEL) have an implicit time interval of 15 minutes, the Immediately Dangerous to Life and Health limit (IDLH) has an implicit interval of 30 minutes, and the Emergency Response Planning Guideline (ERPG) concentrations have a 60-minute implied exposure time. If flammability or possibility of explosion is of concern, the averaging time should be on the

order of seconds since an ignition can occur when the instantaneous concentration is within the flammable limits of the chemical.

Defining an appropriate averaging time for dense gas modeling applications is complicated. Large averaging times allow for more plume meander, and therefore, lower average concentrations. Thus, a 5-minute ensemble average concentration is generally less then a 1-minute ensemble average since more meander can generally occur in 5 minutes than in 1 minute. Thus, some researchers use much shorter averaging times (i.e., 5-10 seconds) than the release duration, especially when comparing model predictions with field measurements when these field measurements are made with shorter averaging times. However, meteorological input (i.e., stability classification) used in conjunction with these models is based on a longer duration, usually 60 minutes.

The time scales relevant to determining the averaging time to be used in the models can be designated as:

t_{haz} = averaging time associated with the hazard being assessed;
t_{rel} = duration of the contaminant release into the atmosphere; and
t_{trav} = travel time from the release site to a receptor.

If t_a is the averaging time that represents the effect of plume meander, then the largest recommended t_a is the minimum of t_{haz}, t_{rel}, and t_{trav} (for steady-state or transient releases); smaller values of t_a can be chosen to compare with field observations or to obtain a conservative estimate of downwind impacts. If $t_{a,t}$ is the averaging time that accounts for transient effects (not pertinent for steady-state releases), $t_{a,t}$ is recommended to be t_{haz}.

When the averaging time used is less than the requested averaging time, the output must be converted to represent the requested averaging time. To extrapolate from a reported average concentration to the requested averaging time, multiply the reported average concentration by the ratio of the actual averaging time to the requested averaging time. This means that to find a

concentration averaged over the requested time, a higher concentration may need to be found in the output. For example, if the release duration is 500 seconds and the requested averaging time is 1000 seconds, the averaging time of 500 seconds should be used. To convert the concentrations reported in the output to concentrations for the requested averaging time, each reported concentration must be multiplied by (500 s/1000 s) or 0.5. This means that if a 1000 second average concentration of 1 ppm is of interest, the output will have to be searched for a concentration of (1 ppm/0.5) or 2 ppm.

An alternative to average concentrations being used to determine impact is the use of dose. Dose is an indication of total exposure at a point. It is usually expressed in units of ppm-minutes. The simplest dose (D) calculation is given by:

$$D = \int_{t_0}^{t} C \, dt$$

where: C = concentration (ppm);
t = time (min); and
t_0 = time the release began (min).

Some expressions for dose give an increased weighting to the chemical by raising the concentration to some power N (change C to C^N in the above equation). In the simple dose calculation, N has the value of one. When N is not equal to one, dose should actually be referred to as toxic load or some other name since the units would no longer be ppm-minutes. The values of N for the chemicals in this document are[18]:

Species	N
Ammonia	2
Chlorine	2
Ethylene Oxide	Not available

Species	N
Hydrogen chloride	1
Hydrogen fluoride	1
Sulfur dioxide	1

4.17 METEOROLOGY

Much of the input discussed above is only weakly dependent on the meteorological conditions. Meteorology is most important to the transport and dispersion of material after it has been released. Many releases can be considered as having two independent input streams: one is the description of the source term, and the other is the meteorological conditions at the time of and following the release.

4.17.1 Wind Speed and Direction

Wind speed is used in determining: 1) plume rise, 2) plume dilution, and 3) mass transfer in evaporation models. In very light winds, dense gases tend to form "pancake-shaped" clouds near the source, and the dense cloud may not be very deep until further downwind. At higher wind speeds, the rate of air mixing is increased (more energy is added to the mixture), and the maximum concentrations can decrease. For releases from liquid pool spills, high wind speed increases the rate of evaporation, and thus, the plume source strength. However, high wind speed also results in more dilution due to increased entrainment of outside air, which can lead to a lowering of maximum concentrations.

Concentration estimates predicted by air dispersion models decrease as the wind speed increases. However, most dense gas models are less sensitive to this increase in wind speed at close-in distances, where gravity effects are dominant. Further downwind, the behavior of dense gas models and non-dense gas models is more similar.

If the user wishes to assess the hazard of a past event, wind speed should be obtained from on-site measurements usually made at the standard 10 m level height. The wind speed at release height is frequently adjusted internally by the model using a power law equation. Guidance for on-site meteorological data collection is available in an EPA document[19]. On-site meteorological data are normally averaged over a 1-hour interval.

The wind direction is used to approximate the direction of transport of the plume. The variability of the direction of transport over a period of time is a major factor in estimating ground-level concentrations averaged over that time period, i.e., plume meandering. For response analyses, wind direction should be estimated from on-site or nearby measurements. For planning analyses, wind direction should be chosen to maximize potential off-site impacts.

The wind speed and direction used can have large effects on jet releases. In the extreme case, if a high velocity horizontal release is in the direction that the ambient wind is blowing toward and the wind speed is comparable to the release velocity, the release would have a relative minimum of mixing with the ambient air.

4.17.2 Stability Class

Stability conditions are typically assessed by means of the Pasquill-Gifford (PG) stability categories where Category A represents extremely unstable conditions and Category F represents moderately stable conditions. The modeling guideline[1] recommends several methods for determining the PG stability category. For example, in urban areas the stability class is often assumed to be at least one class level less stable than for rural areas. As guidance documents continue to be created, new methods may become available.

For a given wind speed, stable atmospheric conditions provide smaller levels of atmospheric turbulence than unstable conditions. The influence of atmospheric stability on the dispersion of a dense gas (as a result of altered

levels of ambient turbulence) may be similar to that for neutrally buoyant releases, but may also be much less. As in the case of wind speed, various models exhibit different sensitivity levels in concentration prediction due to changes in stability class[20].

For planning analyses, where there is a need to obtain conservative estimates from models, it may be necessary to make a number of refined model simulations using various stability and wind speed combinations. If a release is at ground level and is not an upwardly directed jet, the F stability class will most likely lead to the largest concentration impacts downwind. In all other cases, multiple simulations with varying stability class will be needed.

For near-field impacts, dense gas and jet releases will be only weakly sensitive to stability class. As the release becomes neutrally buoyant or a non-jet, the plume is more influenced by the atmospheric conditions such as stability class.

Also see Section 8.0, "Modeling 'Worst Case'," for some discussion on stability effects for the specific models.

4.17.3 Surface Roughness Length

In principle, the surface roughness length is a measure of the roughness of a surface over which a fluid is flowing. For a homogeneous surface, its value is sometimes approximated as 1/10th of the average height of the surface irregularity. When the landscape contains any obstructions (i.e., nonhomogeneous), an effective roughness length must be determined. Typical values of surface roughness are shown in Table 4-1.

The overall effects of increasing surface roughness are to retard the horizontal, buoyancy-induced spreading of the plume or cloud and to enhance the mixing between plume and environment as a result of the ambient and plume turbulence[21]. As in the case of wind speed and stability class, various models exhibit different capabilities to incorporate the effect of surface

TABLE 4-1. REPRESENTATIVE VALUES OF SURFACE ROUGHNESS FOR A UNIFORM DISTRIBUTION OF SELECTED TYPES OF GROUND COVER[21]

Surface	Surface Roughness (m)
Ice	0.00001
Snow	0.00005 to 0.0001
Sand	0.0003
Soils	0.001 to 0.01
Short grass	0.003 to 0.01
Long grass	0.04 to 0.10
Agricultural crops	0.04 to 0.20

roughness in predicted concentrations[22]. Because releases of a dense gas may occur in industrial settings where the presence of a wide variety of structure heights and shapes is common, some users have input large surface roughness values into a model to account for the presence of such obstacles. However, these large surface roughness values can significantly decrease modeled concentrations. For low or ground-level releases, increasing the surface roughness value by a factor of 10 may result in concentration reductions by about a factor of 2[22]. The use of "enhanced" roughness values for simulating the effects of obstacles in an industrial setting has yet to be thoroughly tested and justified. For planning analyses where there is a need for obtaining conservative estimates from these models, the use of a surface roughness value characteristic of the smallest roughness element in the vicinity of the release is probably most appropriate. If no information is available on the surface roughness, a value of 0.01 m is suggested.

4.17.4 Wind Speed at 10 m Altitude

The stability class and surface roughness length can also alter the vertical wind profile assumed in a model. The wind speed at any height can be estimated by[23]:

$$u = u_1\left(\frac{z}{z_1}\right)^p$$

where: u = wind speed at height z;

u_1 = wind speed measured at height z_1; and

p = stability and surface roughness related exponent.

Some example values of p are given in Table 4-2.

The stability class determination requires the wind speed at 10 meters altitude. However, in the above formula the stability class is used to calculate the 10 meter altitude wind. When the 10 meter wind speed calculation is complete, the stability class should be confirmed.

TABLE 4-2. VALUES FOR THE EXPONENT IN THE WIND PROFILE CURVE AS A FUNCTION OF STABILITY CLASS AND SURFACE ROUGHNESS (z_0)[23]

Stability/z_0	0.01 m	0.10 m	1.00 m	3.00 m
A	0.05	0.08	0.17	0.27
B	0.06	0.09	0.17	0.28
C	0.06	0.11	0.20	0.31
D	0.12	0.16	0.27	0.37
E	0.34	0.32	0.38	0.47
F	0.53	0.54	0.61	0.69

4.17.5 Ambient Temperature, Relative Humidity, and Pressure

To assess the consequences of a past event, input parameters should be used that are representative of the conditions at the time of the release. An appropriate input value for each of these parameters should be obtained from on-site measurements at the time of release. Guidance on methods for collecting these data are presented in the meteorological data guidance document[19]. If on-site data are not available for these parameters, observations from nearby National Weather Service (NWS) stations may be used instead.

These parameters can have some marked effects on hazardous releases. For instance, if the ambient temperature is above or below the boiling point of a chemical, it will determine whether the liquid may flash, boil, or evaporate from the wind. Similarly, the relative humidity can affect the dynamics of elevated jet releases[15]. Varying the humidity can result in altering the plume height above the ground. Models are not normally as sensitive to the pressure. Since the pressure is used to determine release criteria (two-phase versus single-phase releases), some variations in simulations could be expected for a spill in Denver as opposed to a spill at sea level.

4.18 OUTPUT DEFINITION

When running a model, a set of output parameters of interest are normally specified. The basic parameters are concentrations of interest and receptor locations. The ERPGs for each chemical are listed in Appendix B. Some STEL and IDLH values are also listed in the Appendix. The receptor locations need to be determined on a case-by-case basis. Normally all receptors are at ground level. The distance from the release site is determined by whether on-site or off-site (or both) impacts are being studied.

A number of outputs may be desired. The outputs that are most often requested and those available from the models in this study are discussed in Section 7.

SECTION 5

MODEL INPUT DEVELOPMENT FOR RELEASE CLASS EXAMPLES

In the previous section methods for determining input to hazardous air pollutant simulation models were provided. In this section, examples of the eight release classes described in Section 2 are presented to illustrate model input requirements. For each example, a release scenario is presented followed by a description of how the input values are developed. Although in reality there may be more than one release class associated with a single release scenario, only one release class is covered in this section for each release scenario. If a scenario is made up of more than one release class, each class should be modeled separately.

Not all of the input presented here for a given release class are used by every model. Section 6.0 of this document gives, for each model, the input actually used in each release class.

Two key assumptions have been made for all examples presented in this section. First, it is assumed in all the scenarios that the release takes place in the direction with the wind. A release against the wind would have more turbulence and mixing, which would reduce maximum concentrations downwind. Second, the release is assumed to occur at or near the ground, which keeps the emission closer to the ground than does a vertical release.

The examples presented in this section are organized by release class. As explained in Section 4, calculation of some release parameters is required before a release class determination can be made. Determining a release class is often an iterative procedure. A release class is assumed, calculations are carried out, and a self-consistency check is made. If the self-consistency check fails the actual release class must be different than the one assumed.

The release class determination for each example is described in each subsection 5.X.3 (where X is 1 through 8).

The calculations performed in the examples presented in this section are discussed in detail in Section 4. The subsections in this Section are related to the subsections in Section 4 such that the calculation performed in subsection 5.X.N is described in subsection 4.N.X. For example, emission rate calculations are described in Section 4.7. The calculation for the emission rate in the first example release scenario is given in subsection 5.1.7 and the corresponding calculation technique is described in subsection 4.7.1.

5.1 TWO-PHASE GAS RELEASE (CHOKED) EXAMPLE

The scenario for this example is as follows. A 3-inch pipe delivers saturated vapor-phase ethylene oxide from a storage area to a process area. The temperature and pressure within the pipe are 86.9°F (303.67 °K) and 2.0 atmospheres absolute (202,650 Pa), respectively. The pipe is supported on a pipe rack 12 ft (3.66 m) above grade level. The pipe's length for this scenario is assumed to be zero. (The longer a pipe is the greater the resistance in the pipe to the flow of the chemical inside. Thus, by ignoring the pipe length, the emission rate will be maximized.)

A leak develops in the flange of the pipe with a size equivalent to a round hole of 0.5 inches (0.0127 m) in diameter. The release of vapor-phase ethylene oxide continues until the pipe flow is manually isolated, 8 minutes after its inception. The pressure and temperature within the pipe remain constant throughout the duration of the release. Ethylene oxide is in its vapor phase at the release point (See Section 5.1.3 for the determination). The material flows through the release opening under critical (choked) conditions (also shown in Section 5.1.3). Upon cooling due to expansion, part of the material condenses as it enters the atmosphere, thereby forming a two-phase release. Figure 5-1 provides a simple sketch of the release.

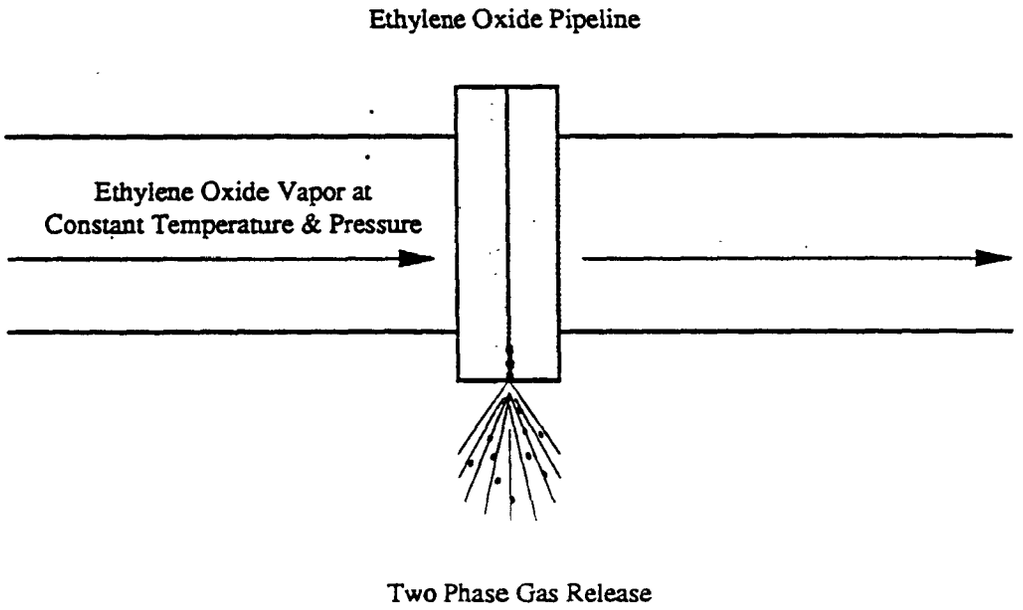


Figure 5-1. Two-Phase Gas Release (Choked)

The meteorological conditions at the time of release are:

- Northeast wind at 12 mph;
- Temperature at 57.2°F;
- Relative Humidity of 62%;
- Pressure of 1 atm (sea level);
- 3/8 cloud cover;
- Early-afternoon release; and
- Measurement height of 15 ft.

The nearest public boundary is 200 m from the release point.

A summary of the model input is provided in Table 5-1. Each of the following sections describes how these input values were developed.

5.1.1 Observable Data

The observable data input were listed in the scenario description. Table 5-2 summarizes this information.

5.1.2 Chemical Data Requirements

The data for ethylene oxide is in Appendix B.

5.1.3 Release Class

This section describes the calculations required to determine the release class for this example. The flow diagram in Figure 4-1 is used as a guide.

Note that some assumptions made in the process of determining the release class conflict with the description of the release scenario. Also note that many of the calculations required to determine the release class are also required for other model input. Rather than presenting all these calculations on one section, reference is made to the appropriate section for each calculation.

TABLE 5-1. INPUT SUMMARY FOR THE TWO-PHASE CHOKED GAS RELEASE EXAMPLE

Chemical Data (5.1.2)
From Appendix B

Release Type (5.1.3)
Two-phase choked flow

Continuous or Instantaneous Release Categories (5.1.4)
Continuous

Emission Rate (5.1.7)
0.06340 kg/s

Release Temperature (5.1.8)
283.85 °K (T_b)

Vapor Fraction (5.1.9)
F_{rel} = 0.9867

Initial Concentration (5.1.10)
f_a = 0.0
f_w = 0.0
f_i = 1.0

Density (5.1.11)
ρ_{rel} = 1.916 kg/m^3
ρ_a' = 1.220 kg/m^3 (at ambient temperature)

Release Diameter or Area (5.1.12)
Diameter = 0.01347 m (choke point)
Diameter = 0.01725 m (expanded)

Release Buoyancy (5.1.13)
C_ρ = 2.435 < 6 (use dense gas model)

Release Height (5.1.14)
3.66 m

Ground Surface Temperature (5.1.15)
Same as ambient

Averaging Time (5.1.16)
5 seconds

TABLE 5-1. (CONTINUED)

Meteorology (5.1.17)

Wind Speed and Direction
45° @ 12 mph (5.37 m/s)
Measurement height = 15 ft (4.57 m)
Speed @ 10 m = 5.63 m/s

Stability Class
C

Surface Roughness Length
Z0 = 0.01 m

Ambient Temperature, Relative Humidity, and Pressure
Temperature = 57.2°F (287.52 °K)
Relative Humidity = 62%
Pressure = 1 atm (101325 Pa)

Output Definition (5.1.18)
LEL (3%) and UEL (100%) concentrations
Minimum distance of concern = 200 m

Observable Data (5.1.1)
See Table 5-2

TABLE 5-2. OBSERVABLE DATA SUMMARY FOR THE TWO PHASE CHOKED GAS RELEASE EXAMPLE

Release Description

Species: Ethylene oxide
Container: Horizontal pipe
- Diameter: 3 inches (0.0762 m)
- Temperature: 87°F (303.67 °K)
- Pressure: 2.0 atm (absolute) (2.0265×10^5 Pa)

Hole site:
- Inner diameter: 0.5 inch (0.0127 m)
- Hole area: 1.267×10^{-4} m^2
- Height of hole: 12 ft (3.66 m)
- Duration: 8 min

Nearest boundary: 656.2 ft (200 m)

Meteorology:
- Temperature: 57.2°F (287.52 °K)
- Relative Humidity: 62%
- Pressure: 1 atm (101325 Pa)
- Wind Speed: 12 mph (5.37 m/s)
- Wind Direction: Northeast (45°)
- Measurement hgt: 15 ft (4.57 m)
- Surface Roughness: 0.01 m
- Cloud cover: 3/8
- Time: Early-afternoon

The ethylene oxide in the pipe is in gas phase. To select the release class, it must be determined whether the release is choked or not and whether the gas cools enough for condensation to occur.

The release flow is choked (see Section 5.1.6) when the pressure at the exit (p_*) is calculated as being higher than the ambient pressure (p_a). In determining the release class, first it is assumed that the release is single phase. The value of the temperature at choked conditions (T_*) is estimated by the equation:

$$T_* = T_s \left[\frac{2}{\gamma + 1}\right]$$

$$= (303.67°K)\left[\frac{2}{1.2126 + 1}\right]$$

$$= 274.5°K$$

Thus, in this example, the value of T_* is less than the critical temperature of ethylene oxide, 469.2 °K, which is given in Appendix B. Using the vapor pressure equation for ethylene oxide in the Appendix, the temperature T_* gives a pressure of 70211 Pa. Since this vapor pressure is less than p_*, the release class is a two-phase gas release. The calculation technique to use is presented in the flow chart in Figure 4-2.

5.1.4 Continuous or Instantaneous Release Categories

In this example, the emission duration (t_d) is 8 minutes. This is the time elapsed before a valve was closed or the release was ended in some other manner.

For non-source term models, to determine whether the source should be characterized as a continuous or finite release, the value of t_d must be compared to either the advection time of the plume to a receptor or to the maximum downwind distance reached by a specific concentration of interest. Using the formula given in Section 4.4 for t_{trav}, the advection time for this

example is 74 seconds. This advection time was calculated using a wind speed of 12 mph (5.37 m/s) and a distance of 200 meters. Since the emission duration is longer than the time required to reach the downwind point of interest, this release is considered continuous.

For a source-term model, the value of t_d is also sufficiently long to treat this release as a continuous release for most receptors.

5.1.5 Release-class-specific Calculations

The flow chart for the calculations of input for a choked two-phase gas release is shown in Figures 4-2 and 4-6.

5.1.6 Determination of Choked Flow for Gas Releases

To determine whether the flow is choked or not, (see Section 4.6) the exit pressure (p_*) must be estimated using the formula:

$$\frac{p_*}{p_s} = \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{(\gamma-1)}}$$

where: γ = the ratio of the specific heat at constant pressure to that at constant volume (1077.96 J/kg °K / 888.96 J/kg °K) = 1.2126.

$$p_* = (2.0265\text{x}10^5\text{Pa})\left(\frac{2}{1.2126 + 1}\right)^{\frac{1.2126}{(1.2126 - 1)}}$$

$$= 1.1389\text{x}10^5\text{Pa}$$

Since $p_* > p_a$ ($1.01325\text{x}10^5$ Pa), flow is choked.

5.1.7 Emission Rate

As described in Section 4.7.1, a number of parameters are required to calculate the emission rate for this release class. These are the temperature (T_*), vapor fraction (F_*), change in enthalpy (ΔH_*), and density (ρ_*) at choke flow. The first of these is calculated by solving:

$$p_* = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_*}\right)\right]$$

or

$$1.1389\text{x}10^5\text{Pa} = 101325\text{Pa} \exp\left[\frac{(5.6900\text{x}10^5\text{J/kg})(44.053\text{kg/kmol})}{8314\text{J/kmol°K}}\left(\frac{1}{283.85°\text{K}} - \frac{1}{T_*}\right)\right]$$

which yields a T_* of 287.01 °K.

The value for F_* is estimated from:

$$F_* = 1 + \frac{T_*}{M\lambda}\left[MC_p \ln\left(\frac{T_s}{T_*}\right) - R \ln\left(\frac{p_s}{p_*}\right)\right]$$

or

$$F_* = 1 + \frac{287.01°\text{K}}{(44.053\text{kg/kmol})(5.6900\text{x}10^5\text{J/kg})}\left[(44.053\text{kg/kmol})(1077.96\text{J/kg°K}) \ln\left(\frac{303.67°\text{K}}{287.01°\text{K}}\right) - (8314\text{J/kmol°K}) \ln\left(\frac{2.0265\text{x}10^5\text{Pa}}{1.1389\text{x}10^5\text{Pa}}\right)\right]$$

$$= 0.9758$$

The change in enthalpy from storage conditions to choke conditions is calculated by:

$$\Delta H_* = C_p(T_s - T_*) + \lambda(1 - F_*)$$

or

$$\Delta H_* = (1077.96 J/kg°K)(303.67°K - 287.01°K) + (5.6900x10^5 J/kg)(1 - 0.9758)$$

$$= 3.1729x10^4 J/kg$$

The emission density at choke flow is given as:

$$\rho_* = \left[F_*\left(\frac{RT_*}{p_*M}\right) + \left(\frac{1 - F_*}{\rho_l}\right)\right]^{-1}$$

or

$$\rho_* = \left[(0.9758)\left(\frac{(8314 J/kmol°K)(287.01°K)}{(1.1389x10^5 Pa)(44.053 kg/kmol)}\right) + \left(\frac{1 - 0.9758}{882.67 kg/m^3}\right)\right]^{-1}$$

$$= 2.1546 kg/m^3$$

Finally, the emission rate for choked flow is:

$$E = A_o\rho_*\left[2(0.85)\left(\frac{\Delta H_*}{\left(1 + \frac{4fL_p}{D_p}\right)}\right)\right]^{\frac{1}{2}}$$

Thus , using a zero-length pipe (L_p) to give a conservative estimate:

$$E = (1.267\text{x}10^{-4}\text{m}^2)(2.1546\text{kg/m}^3)$$

$$\left[2(0.85)\left(\frac{3.1729\text{x}10^4\text{J/kg}}{\left(1 + \frac{4(0.0045)(0.0\text{m})}{0.0762\text{m}}\right)}\right)\right]^{\frac{1}{2}}$$

$$= 0.06340\text{kg/s}$$

5.1.8 Release Temperature

The calculation of release temperature for this release class is described in Section 4.8.1. The first attempt at calculating the release temperature should be with the assumption that the value of F_{rel} is less than 1. If the value of F_{rel} later is calculated to be greater than 1, the value of T_{rel} must be modified. The release temperature is calculated from:

$$p_a = 101325\text{Pa}\ \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_{rel}}\right)\right]$$

thus,

$$101325\text{Pa} = 101325\text{Pa}\ \exp\left[\frac{(5.6900\text{x}10^5\text{J/kg})(44.053\text{kg/kmol})}{8314\text{J/kmol}^\circ\text{K}}\left(\frac{1}{283.85^\circ\text{K}} - \frac{1}{T_{rel}}\right)\right]$$

Since the pressure in this example is 1 atm, the release temperature is the boiling point. Thus, T_{rel} is 283.85 °K.

5.1.9 Vapor Fraction

From Section 4.9.1, the vapor fraction can be calculated from:

$$F_{rel} = F_* + \frac{C_{pl}(T_* - T_{rel})}{\lambda}$$

thus,

$$F_{rel} = 0.9758 + \frac{(1971.56 J/kg°K)(287.01°K - 283.85°K)}{5.6900x10^5 J/kg}$$

$$= 0.9867$$

Since the value of F_{rel} is between zero and one, recalculation of T_{rel} is not required.

5.1.10 Initial Concentration

Since this is a two-phase flow, it is safe to assume that the release is of the liquid and vapor states of the chemical in equilibrium. Since the release temperature is at the boiling point, the vapor pressure is 1 atm. This means that in this release only ethylene oxide is emitted. Thus, under this assumption, the concentration levels (described in Section 4.10) are:

$f_a = 0.0$
$f_w = 0.0$
$f_l = 1.0$

5.1.11 Density

The release starts as aerosol and vapor of ethylene oxide. The water vapor molar fraction is assumed to be zero. The density of the water vapor component of the atmosphere is also assumed to be negligible. As explained in Section 4.11, when aerosol is present, the DEGADIS model will require two triplets, one describing pure air and one describing the aerosol and vapor mix. The density of air (including water vapor) at the ambient temperature is

required to be able to provide one of the triplets. Assuming that air behaves as a perfect gas:

$$\rho_a = \frac{p_a M_a}{RT_a}$$

$$= \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol°K})(287.52\text{°K})}$$

$$= 1.225\text{kg/m}^3$$

Similarly, the water vapor density is given as:

$$\rho_w = \frac{p_a M_w}{RT_a} = \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol°K})(287.52\text{°K})}$$

$$= 0.7638\ \text{kg/m}^3$$

The mole fractions of ambient water vapor (f_w') and air (f_a') are given as:

$$f_w' = \left(\frac{RH}{100}\right) 10^{\left(6.3994 - \frac{2353}{T_a}\right)}$$

$$= \left(\frac{62}{100}\right) 10^{\left(6.3994 - \frac{2353}{287.52\text{°K}}\right)}$$

$$= 0.01019$$

$$f_a' = 1 - f_w' = 1 - 0.01019 = 0.9898$$

The apparent molecular weight of the air and water vapor of the ambient atmosphere is:

$$M_T' = f_a' M_a + f_w' M_w$$

$$= (0.9898)(28.9\text{kg/kmol}) + (0.01019)(18.02\text{kg/kmol})$$

$$= 28.79\text{kg/kmol}$$

Finally, the ambient density ρ_a' is given as:

$$\rho_a' = \left(\frac{f_a' M_a}{M_T' \rho_a} + \frac{f_w' M_w}{M_T' \rho_w} \right)^{-1}$$

$$= \left(\frac{(0.9898)(28.9\text{kg/kmol})}{(28.79\text{kg/kmol})(1.225\text{kg/m}^3)} + \frac{(0.01019)(18.02\text{kg/kmol})}{(28.79\text{kg/kmol})(0.7638\text{kg/m}^3)} \right)^{-1}$$

$$= 1.220\text{kg/m}^3$$

For the second triplet, the density of the aerosol/vapor mixture (ρ_i) at the initial portion of the release is required. To calculate ρ_i, the densities of the vapor (ρ_g) and liquid (ρ_l) must be known. The temperature used in the calculation is the release temperature, which in this case, is the boiling point of ethylene oxide. Assuming a perfect gas, ρ_g is:

$$\rho_g = \frac{p_a M_i}{RT_e} = \frac{(101325\text{Pa})(44.053\text{kg/kmol})}{(8314\text{J/kmol°K})(283.85\text{°K})}$$

$$= 1.891 \text{ kg/m}^3$$

The liquid density at the boiling point is given in Appendix B as 882.67 kg/m^3. The overall aerosol/vapor mixture density then, from Section 4.11, is:

$$\rho_i = \left(\frac{F_{rel}}{\rho_g} + \frac{(1-F_{rel})}{\rho_l} \right)^{-1}$$

or

$$\rho_i = \left(\frac{0.9867}{1.891\text{kg/m}^3} + \frac{(1-0.9867)}{882.70\text{kg/m}^3}\right)^{-1}$$

$$= 1.916\text{kg/m}^3$$

As stated in Section 5.1.10, the release is of pure ethylene oxide. That is, both f_a and f_w are zero. Therefore, the release density (ρ_{rel}) is equal to the ethylene oxide density (ρ_i).

5.1.12 Release Diameter or Area

The release diameter can be calculated using the high momentum formula (Section 4.12.2) for the expansion size. Since this release is choked, there are two release diameters to be considered; which one is to be used depends on the model. The first release diameter considered is that of the choke conditions. This diameter will replace the actual hole size in models requiring input on hole size. If the actual hole size were used, a calculated exit velocity would be greater than sonic speed. The choke point release diameter from the high momentum formula is:

$$D_{rel} = D_s \sqrt{\frac{\rho_*}{\rho_{rel}}}$$

$$= 0.0127\text{m} \sqrt{\frac{2.1546\text{kg/m}^3}{1.916\text{kg/m}^3}}$$

$$= 0.01347\text{m}$$

The second release diameter is calculated using the storage density rather than the choke density. This release diameter is used in models requiring the after-expansion size of a release. To calculate this release

diameter, the gas density inside the container (ρ_s) is required. Assuming the perfect gas law:

$$\rho_s = \frac{p_s M_i}{RT_s} = \frac{(2.0265\text{x}10^5\text{Pa})(44.053\text{kg/kmol})}{(8314\text{J/kmol°K})(303.67\text{°K})}$$

$$= 3.536 \text{ kg/m}^3$$

The expanded release diameter is then:

$$D_{rel} = D_s \sqrt{\frac{\rho_s}{\rho_{rel}}}$$

$$= 0.0127\text{m} \sqrt{\frac{3.536\text{kg/m}^3}{1.916\text{kg/m}^3}}$$

$$= 0.01725\text{m}$$

5.1.13 Release Buoyancy

The release buoyancy is used to determine if a dense gas model should be used, rather than a neutral or positive buoyancy model. If ρ_{rel} is less than or equal to ρ_a, the release is not to be treated as a dense gas release. In this case, ρ_{rel} is 1.916 kg/m^3 and ρ_a' is 1.220 kg/m^3. Since ρ_{rel} is greater than ρ_a', the denser-than-air criteria should be calculated to determine whether this should be treated as a dense gas or not.

The formula in Section 4.13.1 is used to calculate the denser-than-air criterion, since this release is being considered a continuous release (Section 5.1.4). The larger D_{rel} from Section 5.1.12 will be used to maximize the criterion. The criterion (C_ρ) is given by:

$$C_\rho = \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}}$$

$$= (5.37\text{m/s})\left[\frac{(9.806\text{m/s}^2)(0.06340\text{kg/s}/1.916\text{kg/m}^3)}{0.01725\text{m}}\left(\frac{1.916\text{kg/m}^3 - 1.220\text{kg/m}^3}{1.220\text{kg/m}^3}\right)\right]^{-\frac{1}{3}}$$

$$= 2.435$$

Since $C_\rho < 6$, a dense gas model should be used.

5.1.14 Release Height

The flange with the leak is 12 ft (3.66 m) above grade. The gas and liquid droplets that form are both assumed to enter the atmosphere at that altitude.

5.1.15 Ground Surface Temperature

No direct information on the ground surface temperature was given. Therefore, the ground surface temperature is assumed to be equal to the ambient temperature, i.e., 87°F or 303.67 °K.

5.1.16 Averaging Time

The averaging time is specified as 5 seconds to make the model-predicted concentrations comparable to the Lower and Upper Explosion Limits.

5.1.17 Meteorology

Wind Speed and Direction

The wind speed and direction are either assumed to be available from on-site meteorological equipment or are average conditions at the site. The wind speed is given as 12 mph (5.37 m/s). The wind direction is given as northeast (45°). The measurement height is given as 15 ft (4.57 m). To determine the greatest specific impact, multiple wind speeds may be required in conjunction with multiple stability classes.

Stability Class

The stability class is not given explicitly. However, a stability class can be estimated from the information provided using the method described in the Workbook, Section 3.1.2. In this example, there is 3/8 cloud coverage and the release occurs in the early afternoon. These conditions indicate that insolation is strong. The stability class estimated in the Workbook Table 3-2 for a wind speed greater than 5.37 m/s at 10 m (assuming wind speed increases with height) during a day with strong insolation would be C.

Surface Roughness Length

In keeping with the value suggested to be used for planning, the surface roughness is assumed to be 0.01 m.

Wind Speed at 10 m Altitude

Given the previous estimates of surface roughness, stability class, and wind speed at 15 ft, the wind speed at 10 meters can be estimated using the equation in 4.17.3:

$$u = u_1\left(\frac{z}{z_1}\right)^p$$
$$= 5.37\text{m/s}\left(\frac{10.0\text{m}}{4.57\text{m}}\right)^{0.06}$$
$$= 5.63\text{m/s}$$

This wind speed at 10 meters altitude still indicates a C stability class.

Ambient Temperature, Relative Humidity, and Pressure

The ambient temperature, relative humidity, and pressure are all assumed to be available from on-site equipment. See the observable data, Table 5-2.

5.1.18 Output Definition

The concentrations to output should be for the LEL (3%) and UEL (100%). The actual impact values to be predicted are listed in Section 7.0. The specified point mentioned in Section 7.0 is assumed to be the site boundary, 200 m directly downwind of the release.

5.2 TWO-PHASE GAS RELEASE (UNCHOKED) EXAMPLE

In this example, the 3 inch ethylene oxide pipeline described in the previous example is now operating at a pressure of 1.58 atmospheres absolute (160,094 Pa) and the ethylene oxide within the pipe is a saturated vapor at 71.6°F (295.16 °K).

A leak develops in the flange of the pipe with a size equivalent to a round hole of 0.5 inches (0.0127 m) in diameter. As in the previous example, the release is 12 ft (3.66 m) above grade level. The release of vapor-phase ethylene oxide continues until the pipe flow is manually isolated, 8 minutes after its inception. The pressure and temperature within the pipe remain constant throughout the duration of the release. As shown below, the ethylene oxide is in its vapor phase at the release point. The flow of material

through the opening is under subcritical (unchoked) conditions. As the gas expands upon release, it cools, causing part of the material to condense as it enters the atmosphere, thereby forming a two-phase release situation. Since the release configuration is identical to that of the previous example, Figure 5-1 also represents this release scenario.

The meteorological conditions at the time of release are:

- Southwest wind at 6 mph;
- Temperature at 74°F;
- Relative Humidity of 37%;
- Pressure of 1 atm (sea level);
- 5/8 cloud cover;
- Early-morning release; and
- Measurement height of 20 ft.

The nearest public boundary is 300 meters from the release point.

Model input is summarized in Table 5-3. The following sections describe how specific input values were calculated.

5.2.1 Observable Data

The observable data input was provided in the scenario description. These data are summarized in Table 5-4.

5.2.2 Chemical Data Requirements

The data for ethylene oxide is in Appendix B.

5.2.3 Release Class

This section describes the calculations required to determine the release class for this example. The flow diagram in Figure 4-1 was used as a guide.

TABLE 5-3. INPUT SUMMARY FOR THE TWO PHASE UNCHOKED GAS RELEASE EXAMPLE

Chemical Data (5.2.2)
From Appendix B

Release Type (5.2.3)
Two-phase unchoked flow

Continuous or Instantaneous Release Categories (5.2.4)
Continuous

Emission Rate (5.2.7)
0.0503 kg/s

Release Temperature (5.2.8)
283.85 °K (T_b)

Vapor Fraction (5.2.9)
$F_{rel} = 0.9779$

Initial Concentration (5.2.10)
$f_a = 0.0$
$f_w = 0.0$
$f_i = 1.0$

Density (5.2.11)
$\rho_{rel} = 1.9336$ kg/m^3
$\rho_a' = 1.183$ kg/m^3 (at ambient temperature)

Release Diameter or Area (5.2.12)
Diameter = 0.01548 m

Release Buoyancy (5.2.13)
$C_\rho = 1.226 < 6$ (use dense gas model)

Release Height (5.2.14)
3.66 m

Ground Surface Temperature (5.2.15)
Same as ambient

Averaging Time (5.2.16)
5 seconds

TABLE 5-3. (CONTINUED)

Meteorology (5.2.17)

Wind Speed and Direction
225° @ 2.68 m/s
Measurement height = 20 ft (6.10 m)
Speed @ 10 m = 5.63 m/s

Stability Class
C

Surface Roughness Length
Z0 = 0.01 m

Ambient Temperature, Relative Humidity, and Pressure
Temperature = 74°F (296.48 °K)
Relative Humidity = 37%
Pressure = 1 atm (101325 Pa)

Output Definition (5.2.18)
LEL (3%) and UEL (100%) concentrations
Minimum distance of concern = 300 m

Observable Data (5.2.1)
See Table 5-4

TABLE 5-4. OBSERVABLE DATA SUMMARY FOR THE TWO PHASE UNCHOKED GAS RELEASE EXAMPLE

Release Description

Species: Ethylene oxide
Container: Horizontal pipe

Diameter:	3 inches (0.0762 m)
Temperature:	71.6°F (295.16 °K)
Pressure:	1.58 atm (absolute) (1.6009 x 10^5 Pa)

Hole site:

Inner diameter:	0.5 inch (0.0127 m)
Hole area:	1.267×10^{-4} m^2
Height of hole:	12 ft (3.66 m)
Duration:	8 min

Nearest boundary: 984 ft (300 m)

Meteorology:

Temperature:	74°F (296.48 °K)
Relative Humidity:	37%
Pressure:	1 atm (101325 Pa)
Wind Speed:	6 mph (2.68 m/s)
Wind Direction:	Southwest (225°)
Measurement hgt:	20 ft (6.10 m)
Surface Roughness:	0.01 m
Cloud cover:	5/8
Time:	Early-morning

Note that some assumptions made in the process of determining the release class conflict with the description of the release scenario in 5.2.1. Also note that many of the calculations required to determine release class are also required for other model input. Rather than presenting all these calculations in one section, reference is made to the appropriate section for each calculation.

The ethylene oxide in the pipe is in the gas phase. To select the release class, it must be determined whether the release is choked or not and whether the gas cools enough for condensation to occur.

The release flow is unchoked (as shown in Section 5.2.6) when the pressure at the exit (p_*) is calculated as being lower than the ambient pressure (p_a). In the determination of the release class, it is first assumed that the release is single phase. A discharge temperature (T_{rel}) is required so that the vapor pressure at that temperature can be compared to the ambient temperature. The equation for an unchoked single phase gas release is given in Section 4.8.6 as:

$$T_{rel} = \frac{2T_s}{[1 + \sqrt{(1 + 4aT_s)}]}$$

where:

$$a = \frac{1}{2C_p}\left(\frac{ER}{p_a MA_o}\right)^2$$

The emission rate is required to calculate the temperature. The emission rate calculation is described in Section 4.7.6. The expressions required for the emission rate are:

$$E = KYA_o[2\rho_s(p_s - p_a)]^{\frac{1}{2}}$$

$$K = \frac{C}{\sqrt{1 - \beta^4}}$$

$$Y = 1 - \left(\frac{p_s - p_a}{p_s\gamma}\right)(0.41 + 0.35\ \beta^4)$$

The β term is the square root of the ratio of the hole size to the area containing the volume of the ethylene oxide. The hole size in this example is 1.267×10^{-4} m^2. The surface area of the pipe containg the volume of ethylene oxide is the length of the pipe multiplied by the circumference of the pipe. The length of the pipe is not given in the scenario description. In the first release class example (Section 5.1), it was assumed that the pipe was zero in length which resulted in maximizing the emission rate. From Figure 5-1 it is apparent that the pipe is much longer than it is wide. Thus the surface area of the pipe is much larger that the area of the hole, which leads to the β term being assumed to be zero. Using the constants in Section 4.7.6, the value of γ (1.2126) from Section 5.2.6, and ethylene oxide data from Appendix B, this leads to the following:

$$K = C = 0.62$$

$$Y = 1 - \left(\frac{p_s - p_a}{p_s\gamma}\right) 0.41$$

$$= 1 - \left(\frac{1.6009\text{x}10^5\text{Pa} - 1.01325\text{x}10^5\text{Pa}}{(1.6009\text{x}10^5\text{Pa})\ (1.2126)}\right) 0.41$$

$$= 0.8759$$

$$E = KYA_o[2\rho_s(p_s - p_a)]^{\frac{1}{2}}$$

$$= (0.62)(0.8759)(1.267\text{x}10^{-4}\text{m}^2)[2(2.873\text{kg/m}^3)(1.6009\text{x}10^5\text{Pa} - 1.01325\text{x}10^5\text{Pa}$$

$$=0.0400\text{kg/s}$$

$$a = \frac{1}{2C_p}\left(\frac{ER}{p_a MA_o}\right)^2$$

$$= \frac{1}{2(1077.96\text{J/kg}^\circ\text{K})}\left(\frac{(0.0400\text{kg/s})(8314\text{J/kmol}^\circ\text{K})}{(1.01325\text{x}10^5\text{Pa})(44.053\text{kg/kmol})(1.267\text{x}10^{-4}\text{m}^2)}\right)^2$$

$$=1.604\text{x}10^{-4\circ}\text{K}^{-1}$$

$$T_{rel} = \frac{2T_s}{\left[1 + \sqrt{(1 + 4aT_s)}\right]}$$

$$= \frac{2(295.16^\circ\text{K})}{\left[1 + \sqrt{(1 + 4(1.604\text{x}10^{-4\circ}\text{K}^{-1})(295.16^\circ\text{K}))}\right]}$$

$$= 282.4^\circ\text{K}$$

The value of T_{rel} is less than the critical temperature of ethylene oxide (469.15 °K) given in Appendix B. T_{rel} is also less than the normal boiling point of ethylene oxide (283.85 °K). The ethylene oxide is at T_{rel} at atmospheric pressure. This means that the ethylene oxide vapor pressure is less than the ambient pressure. From the flow chart in Figure 4-1, the release class therefore must be a two-phase gas release. Use the flow chart in Figure 4-2 to calculate the rest of the input.

5.2.4 Continuous or Instantaneous Release Categories

In this example, the emission duration (t_d) is given as 8 minutes. This is the amount of time that elapsed before a valve was closed or the release was mitigated in some other manner.

For a non-source-term model, the value of t_d must be compared either to advection time to a receptor or to the maximum downwind distance reached by a concentration of interest. Using the formula in Section 4.4 for t_{trav}, and assuming a wind speed of 6 mph (2.68 m/s) and a distance of 300 meters, the advection time is calculated to be 223.8 seconds. Since the emission duration is longer than the time required to reach the downwind point of interest, the release is considered continuous.

For a source-term model, the value of t_d is also sufficient to treat this release as a continuous release for most receptors.

5.2.5 Release-class-specific Calculations

The flow chart of the calculations required for input for an unchoked two-phase gas release is shown in Figures 4-2 and 4-6.

5.2.6 Determination of Choked Flow for Gas Releases

As discussed in Section 4.6, to determine whether the flow is choked or not, the exit pressure (p_*) must be estimated using the formula:

$$\frac{p_*}{p_s} = \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{(\gamma-1)}}$$

In this example, the exit pressure (p_*) is:

$$p_* = (1.6009\text{x}10^5\text{Pa})\left(\frac{2}{1.2126 + 1}\right)^{\frac{1.2126}{(1.2126 - 1)}}$$

$$= 8.997\text{x}10^4\text{Pa}$$

where: γ = the ratio of the specific heat at constant pressure to that at constant volume (1077.96 J/kg °K / 888.96 J/kg °K) = 1.2126.

Since $p_* < p_a$ ($1.01325\text{x}10^5$ Pa), flow is unchoked.

5.2.7 Emission Rate

As indicated in Section 4.7.2, to calculate the emission rate, two parameters must be known. These are the change in enthalpy during the release (ΔH, Section 5.2.9) and the release density (ρ_{rel}, Section 5.2.11). Once these two parameters are known, the emission rate can be calculated using the following expression:

$$E = A_o \rho_{rel}\left[2(0.85)\left(\frac{\Delta H}{\left(1 + \frac{4fL_p}{D_p}\right)}\right)\right]^{\frac{1}{2}}$$

or, in this example, where the pipe length is zero:

$$E = (1.267\text{x}10^{-4}\text{m}^2)(1.9336\text{kg/m}^3)$$

$$\left[2(0.85)\left(\frac{2.4767\text{x}10^4\text{J/kg}}{\left(1 + \frac{4(0.0045)(0.0\text{m})}{D_p}\right)}\right)\right]^{\frac{1}{2}}$$

$$= 0.0503\text{kg/s}$$

5.2.8 Release Temperature

As discussed in Section 4.8.2, the release temperature (T_{rel})is calculated from the Clausius-Clapeyron equation:

$$p_{rel}=101325\text{Pa}\ \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_{rel}}\right)\right]$$

or, in this example,

$$101325\text{Pa} = 101325\text{Pa}\ \exp\left[\frac{(5.6900\text{x}10^5\text{J/kg})(44.053\text{kg/kmol})}{8314\text{J/kmol°K}}\left(\frac{1}{283.85\text{°K}} - \frac{1}{T_{rel}}\right)\right]$$

Since the pressure after release is one atmosphere, the release temperature is the boiling point. The fact that p_{rel} is equal to the atmospheric pressure (101325 Pa) means that the exponent must be zero. It is only zero if T_{rel} is equal to T_b. Thus, T_{rel} is 283.85 °K. Otherwise, the equation would have to be re-written solving for T_{rel}.

5.2.9 Vapor Fraction

As discussed in Section 4.9.2, the vapor fraction can be calculated from:

$$F_{rel} = 1 + \frac{T_{rel}}{M\lambda}\left[MC_p \ln\left(\frac{T_s}{T_{rel}}\right) - R \ln\left(\frac{p_s}{p_a}\right)\right]$$

or, in this example,

$$F_{rel} = 1 + \frac{283.85°K}{(44.053kg/kmol)(5.6900x10^5 J/kg)}$$

$$\left[(44.053kg/kmol)(1077.96J/kg°K)\ \ln\left(\frac{295.16°K}{283.85°K}\right)\right.$$

$$\left. - (8314J/kmol°K)\ \ln\left(\frac{1.6009x10^5 Pa}{1.01325x10^5 Pa}\right)\right]$$

$$= 0.9779$$

Now that the values of F_{rel} and T_{rel} are known, the change of enthalpy in the release can also be calculated. This change in enthalpy (ΔH) is given as:

$$\Delta H = C_p(T_s - T_{rel}) + \lambda(1 - F_{rel})$$

$$= (1077.96J/kg°K)(295.16°K - 283.85°K)$$

$$+ (5.6900x10^5 J/kg)(1 - 0.9779)$$

$$= 2.4767x10^4 J/kg$$

5.2.10 Initial Concentration

Since this release is a two-phase flow, it is safe to assume that all material being emitted is ethylene oxide. Therefore, it follows that the concentration values (described in Section 4.10) are:

$f_a = 0.0$
$f_w = 0.0$
$f_i = 1.0$

5.2.11 Density

The release starts as a mixture of aerosol and vapor. The water vapor molar fraction is assumed to be zero. The density of the water vapor

component of the atmosphere is also assumed to be negligible. As explained in Section 4.11, when aerosol is present, the DEGADIS model will require two triplets, one describing pure air and one describing the aerosol and vapor mixture. The density of air at ambient temperature (ρ_a) is required to calculate one of the triplets. Assuming the air behaves as a perfect gas:

$$\rho_a = \frac{p_a M_a}{RT_a} = \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol°K})(296.48\text{°K})}$$

$$= 1.188 \text{ kg/m}^3$$

Similarly, the water vapor density (ρ_w)is given as:

$$\rho_w' = \frac{p_a M_w}{RT_a} = \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol°K})(296.48\text{°K})}$$

$$= 0.7407 \text{ kg/m}^3$$

The mole fractions of ambient water vapor (f_w') and air (f_a') are given as:

$$f_w' = \left(\frac{RH}{100}\right) 10^{\left(6.3994 - \frac{2353}{T_a}\right)}$$

$$= \left(\frac{37}{100}\right) 10^{\left(6.3994 - \frac{2353}{296.48\text{°K}}\right)}$$

$$= 0.01074$$

and

$$f_a' = 1 - f_w' = 1 - 0.01074 = 0.9893$$

The apparent molecular weight (M'_T)of the air and water vapor of the ambient atmosphere is:

$$M_T' = f_a' M_a + f_w' M_w$$

$$= (0.9893)(28.9\text{kg/kmol}) + (0.01074)(18.02\text{kg/kmol})$$

$$= 28.78\text{kg/kmol}$$

Finally, the ambient density (ρ_a') is given as:

$$\rho_a' = \left(\frac{f_a' M_a}{M_T' \rho_a} + \frac{f_w' M_w}{M_T' \rho_w} \right)^{-1}.$$

or

$$\rho_a' = \left(\frac{(0.9893)(28.9\text{kg/kmol})}{(28.78\text{kg/kmol})(1.188\text{kg/m}^3)} + \frac{(0.01074)(18.02\text{kg/kmol})}{(28.78\text{kg/kmol})(0.7407\text{kg/m}^3)} \right)^{-1}$$

$$= 1.183\text{kg/m}^3$$

The density of the aerosol/vapor mixture at the initial portion of the release is required to calculate the second triplet. To calculate the density of the aerosol/vapor mixture (ρ_i), the densities of the vapor and liquid must be known. The temperature used in the calculation is the release temperature. In this example, the release temperature is the boiling point of ethylene oxide. Assuming a perfect gas, the density of the gas state (ρ_g) is:

$$\rho_g = \frac{p_a M_i}{RT_e} = \frac{(101325\text{Pa})(44.053\text{kg/kmol})}{(8314\text{J/kmol°K})(283.85\text{°K})}$$

$$= 1.891\ \text{kg/m}^3$$

The liquid density at the boiling point is given in Appendix B as 882.70 kg/m^3. The formula for calculating the overall aerosol/vapor mixture density is (from Section 4.11):

$$\rho_i = \left(\frac{F_{rel}}{\rho_g} + \frac{(1-F_{rel})}{\rho_l} \right)^{-1}$$

or

$$\rho_i = \left(\frac{0.9779}{1.891 kg/m^3} + \frac{(1-0.9779)}{882.70 kg/m^3} \right)^{-1} = 1.9336 kg/m^3$$

Since the release is of pure ethylene oxide (f_a and f_w are both zero), the release density (ρ_{rel}) is equal to that of the ethylene oxide density (ρ_i).

5.2.12 Release Diameter or Area

The release diameter is calculated as discussed in Section 4.12. Since this is not a choked flow release, an estimate is required for exit velocity. To estimate exit velocity, the formula requires the gas density inside the vessel (ρ_s). Assuming the perfect gas law yields:

$$\rho_s = \frac{p_s M_i}{RT_s} = \frac{(1.6009 \times 10^5 Pa)(44.053 kg/kmol)}{(8314 J/kmol°K)(295.16°K)}$$

$$= 2.874 kg/m^3$$

The exit velocity can then be estimated as:

$$u = \frac{E}{A\rho_s}$$

$$= \frac{0.0503 kg/s}{(1.267 \times 10^{-4} m^2)(2.874 kg/m^3)}$$

$$= 138 m/s$$

With such a high emission velocity, the release diameter can be calculated using the high momentum formula given in Section 4.12.2. The release diameter from the high momentum formula is then:

$$D_{rel} = D_s \sqrt{\frac{\rho_s}{\rho_{rel}}}$$

$$= 0.0127\text{m} \sqrt{\frac{2.874\text{kg/m}^3}{1.9336\text{kg/m}^3}}$$

$$= 0.01548\text{m}$$

5.2.13 Release Buoyancy

The release buoyancy is used to determine if a dense gas model should be used rather than a neutral or positive buoyancy model. If ρ_{rel} is less than or equal to ρ_a', the release is not to be treated as a dense gas release. In this case, ρ_{rel} is 1.934 kg/m^3 and ρ_a' is 1.183 kg/m^3. Since ρ_{rel} is greater than ρ_a', the next step is to apply the denser-than-air criterion to determine of whether this release should be treated as a dense gas or not.

The calculation of the denser-than-air criterion should use the formula given in Section 4.13.1, since this release is considered a continuous release (Section 5.2.4). The criterion (C_ρ) is calculated as:

$$C_\rho = \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}}$$

$$C_\rho = (2.68\text{m/s})\left[\frac{(9.806\text{m/s}^2)(0.0503\text{kg/s}/1.9336\text{kg/m}^3)}{0.01548\text{m}} \cdot \left(\frac{1.9336\text{kg/m}^3 - 1.183\text{kg/m}^3}{1.183\text{kg/m}^3}\right)\right]^{-\frac{1}{3}}$$

$$= 1.226$$

Since $C_\rho < 6$, a dense gas model should be used.

5.2.14 Release Height

The flange with the leak is 12 ft (3.66 m) above grade. Both the gas and liquid droplets that form are both assumed to enter the atmosphere at that altitude.

5.2.15 Ground Surface Temperature

There is no direct information on the ground surface temperature. Therefore, the ground surface temperature is assumed to be equal to the ambient temperature, which is given as 74°F or 295.16 °K.

5.2.16 Averaging Time

The averaging time is specified as 5 seconds. This averaging time was selected to make the model-predicted concentrations comparable to the Lower and Upper Explosion Limits.

5.2.17 Meteorology

Wind Speed and Direction

The wind speed and direction are either assumed to be available from on-site meteorological equipment or else represent average conditions at the site. The wind speed is given as 6 mph (2.68 m/s). The wind direction is given as southwest (225°). The measurement height is given as 12 ft (6.10 m). To determine the greatest specific impact, multiple wind speeds may be required in conjunction with multiple stability classes.

Stability Class

The stability class is not given explicitly; however, it can be estimated from the information provided using the method described in the Workbook, Section 3.1.2. In this example, there is 5/8 cloud coverage, and the release occurs in the early morning. These conditions indicate that the insolation is slight. The stability class indicated in Table 3-2 of the Workbook for a wind speed between 2 to 5 m/s at 10 m during a day with slight insolation is "C." The measurement height in this example is a little over 6 meters.

Surface Roughness Length

In keeping with the suggested value to be used for modeling done for planning purposes, the surface roughness is assumed to be 0.01 m.

Wind Speed at 10 m Altitude

The wind speed at 10 meters can be estimated using the surface roughness, stability class, and wind speed at 6.1 meters. Using the formula

given in Section 4.17.3 and assuming a stability class of "C," the predicted wind speed at 10 meters (u) is:

$$u = u_1\left(\frac{h}{z_1}\right)^p$$

$$= (2.68\text{m/s})\left(\frac{10\text{m}}{6.1\text{m}}\right)^{0.06}$$

$$= 2.76\text{m/s}$$

which falls within the wind speed limits for "C" stability class "C" conditions.

Ambient Temperature, Relative Humidity, and Pressure

The ambient temperature, relative humidity, and pressure are all assumed to be available from on-site equipment. See the observable data, presented in Table 5-4.

5.2.18 Output Definition

The appropriate concentrations to be specified for generating output are the LEL (Lower Explosive Limit) and UEL (Upper Explosive Limit) concentrations given in the ethylene oxide data table provided in Appendix B. The actual impact values to be predicted are listed in Section 7.0.

5.3 TWO-PHASE PRESSURIZED LIQUID EXAMPLE

In this example, chlorine is used in the biological control of cooling water at a chemical plant. A one-ton container is used to deliver chlorine to the cooling tower basin (see Figure 5-2). This container is a pressurized, atmospheric temperature vessel (70°F) containing both liquid- and vapor-phase chlorine. The vapor pressure (6.86 atmospheres absolute) of chlorine forces it through a connection to the lower valve on the ton container into the

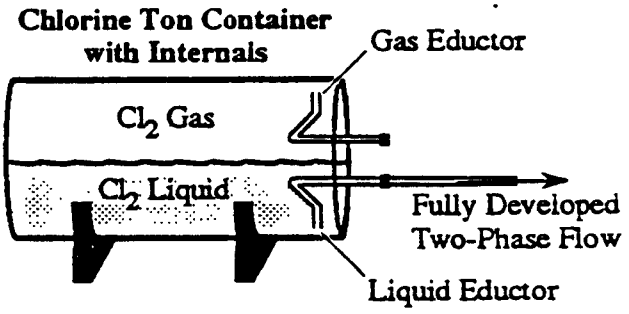


Figure 5-2. Two-Phase Pressurized Liquid

delivery header. The storage pressure can be determined from the triple point diagram for chlorine provided in Appendix B. A one-meter long, 3/8 inch diameter section of flexible tubing is used to deliver chlorine to the delivery header. This tubing is accidentally severed at the delivery header during routine maintenance. The tubing is two meters above the ground level.

At the time of the accident, the vessel contains 500 lbs of chlorine in the liquid phase. As liquid chlorine is released, its pressure drops and some of the liquid flashes to vapor (adiabatically) within the tubing. The existence of flashing (two-phase flow) can be determined by the flash diagram for chlorine given in Appendix B. The chlorine is released horizontally under fully developed, two-phase flow conditions. Since the release is somewhat remote from the vessel, the cooling effect of vaporization within the tubing does not result in cooling of the chlorine within the vessel.

The two-phase release continues until the liquid level within the container drops below the level of the passage to the liquid eductor (exit pipe). At this level, 30 lbs of chlorine remains within the vessel in the liquid phase. After the liquid level has reached the level of the liquid eductor, chlorine is emitted as a vapor for the duration of the release. A schematic of the vessel and tubing dimensions is given in Figure 5-2.

The meteorological conditions at the time of release are:

- South wind at 10 mph;
- Temperature at 70°F;
- Relative humidity of 50%;
- Pressure of 1 atm (sea level);
- 4/8 cloud cover;
- Mid-morning release; and
- Measurement height of 10 m.

The nearest public boundary is assumed to be 100 meters from the release site. Table 5-5 presents a summary of the model input. The following sections describe how the input values were developed.

TABLE 5-5. INPUT SUMMARY FOR THE TWO-PHASE PRESSURIZED LIQUID RELEASE EXAMPLE

Chemical Data (5.3.2)
From Appendix B

Release Type (5.3.3)
Two-phase

Continuous or Instantaneous Release Categories (5.3.4)
Continuous

Emission Rate (5.3.7)
0.3170 kg/s

Release Temperature (5.3.8)
239.09 °K (T_b)

Vapor Fraction (5.3.9)
F_{rel} = 0.1779

Initial Concentration (5.3.10)
f_a = 0.0
f_w = 0.0
f_i = 1.0

Density (5.3.11)
ρ_{rel} = 20.11 kg/m^3
ρ_a' = 1.191 kg/m^3 (at ambient temperature)

Release Diameter or Area (5.3.12)
Diameter = 0.06201 m

Release Buoyancy (5.3.13)
C_ρ = 1.311 < 6 (use dense gas model)

Release Height (5.3.14)
2 m

Ground Surface Temperature (5.3.15)
Same as ambient

Averaging Time (5.3.16)
15 minutes

TABLE 5-5. (CONTINUED)

Meteorology (5.3.17)

Wind Speed and Direction
180° @ 10 mph (4.47 m/s)
Measurement height = 10 m
Speed @ 10 m = 4.47 m/s

Stability Class
C

Surface Roughness Length
Z0 = 0.01 m

Ambient Temperature, Relative Humidity, and Pressure
Temperature = 70°F (294.3 °K)
Relative Humidity = 50%
Pressure = 1 atm (101325 Pa)

Output Definition (5.3.18)
STEL
Minimum distance of concern = 100 m

Observable Data (5.3.1)
See Table 5-6

5.3.1 Observable Data

Observable data were given in the description of the release scenario. A recap of the information in the scenario description is given in Table 5-6. For modeling done for planning purposes, the direction that the hole is facing should be assumed to be in the same direction as the wind. This ensures that maximum ground-level impacts of the released material are predicted by the model.

5.3.2 Chemical Data Requirements

The chemical data for pure chlorine are in Appendix B.

5.3.3 Release Class

This section describes the calculations required to determine the release class for this example. The flow diagram in Figure 4-1 is used as a guide. Many of the calculations required to determine the release class are also required for other model input. Rather than presenting all calculations in one section, reference is made to the appropriate section for each calculation.

In this scenario, there are three releases. The first release is the two-phase flow of the liquid escaping the container. The second release is the constant-rate release of the remaining liquid in the container as it vaporizes. The third release is the decreasing-rate, gas-phase release from the container that occurs as the pressure in the container falls to 1 atm. Only the first release is a two-phase flow, so only it will be described in this section. The second and third release classes that occur are gas releases with varying emission rates.

The initial release class was determined by using the flow diagram in Figure 4-1. The chlorine is stored as a liquid. As the flash diagram in

TABLE 5-6. OBSERVABLE DATA SUMMARY FOR THE TWO PHASE PRESSURIZED LIQUID RELEASE EXAMPLE

Release Description

Species: Chlorine
Container: Horizontal cylinder

Diameter:	30 inches (0.762 m)
Length:	81.5 inches (2.07 m)
Volume:	33.34 ft^3 (0.944 m^3)
Total liquid:	500 lbs
Liquid below liquid eductor:	30 lbs
Temperature:	70°F (294.3 °K)
Pressure:	6.86 atm (absolute) (6.95 x 10^5 Pa)

Hole site: Connected tubing

Length:	3.281 ft (1 m)
Outer diameter:	3/8 inch (0.009525 m)
Inner diameter:	0.2770 inch (0.007036 m)
Height of tube:	6.562 ft (2 m)

Nearest boundary: 328.1 ft (100 m)

Meteorology:

Temperature:	70°F (294.3 °K)
Relative Humidity:	50%
Pressure:	1 atm (101325 Pa)
Wind Speed:	10 mph (4.47 m/s)
Wind Direction:	South (180°)
Measurement hgt:	32.81 ft (10 m)
Surface Roughness:	0.01 m
Cloud cover:	4/8
Time:	Mid-morning

Appendix B indicates, when chlorine is stored as a liquid flashing may occur. Therefore, the value of F_{rel} is required to make the final release class decision. But, in order to calculate F_{rel}, the value of T_{rel} is required. This value is obtained by solving the equation described in Section 4.8.2:

$$p_a = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_{rel}}\right)\right] .$$

or, for this example:

$$p_a = 101325\text{Pa} \exp\left[\frac{(2.878\text{x}10^5\text{J/kg})(70.914\text{kg/kmol})}{8314\text{J/kmol°K}} \left(\frac{1}{239.09°\text{K}} - \frac{1}{T_{rel}}\right)\right]$$

Setting p_a to 1 atm (101325 Pa) leads to a T_{rel} of 239.09 °K (the boiling point).

After T_{rel} has been calculated, the value for F_{rel} (see Section 4.9.3) can be obtained by:

$$F_{rel} = \frac{C_{pl}(T_s - T_{rel})}{\lambda}$$

$$= \frac{(927.13\text{J/kg°K})\ (294.3°\text{K} - 239.09°\text{K})}{2.878\text{x}10^5\text{J/kg}}$$

$$= 0.1779$$

Since F_{rel} is between zero and one, according to the flow chart shown in Figure 4-1, this release is two-phase. Now the flow chart shown in Figure 4-2 can be used to determine the model input.

5.3.4 Continuous or Instantaneous Release Categories

In this example, the emission rate is 0.3170 kg/s (from Section 5.3.8). The duration of the two-phase portion of the release is however long it takes for the liquid to escape the container. There are 500 lbs of liquid in the container, but 30 lbs still remain after the liquid has stopped being released. Thus, the duration of the release (t_d) is:

$$t_d = \frac{(500-30)\text{lbs}\left(\frac{0.4536\text{kg}}{\text{lb}}\right)}{0.3170\frac{\text{kg}}{\text{s}}}$$

$$=673\text{s}$$

$$=11.2\text{minutes}$$

For a non-source-term model, the value of t_d must be compared to advection time to a receptor or maximum downwind distance reached by a concentration of interest. Using the formula given in Section 4.4 for t_{trav}, and assuming a wind speed of 10 mph (4.47 m/s) and a distance of 100 meters, the advection time is 44.7 seconds. Since the emission duration is longer than the time it takes the material to reach the downwind point of interest, the release is considered continuous.

For a source-term model, the value of t_d is sufficiently long to treat this release as a continuous release for most receptors.

Note that, initially, it should be assumed that the release is continuous until an emission duration (calculated from the emission rate) can be compared to travel times to the receptors of interest, as described in Section 4.3.

5.3.5 Release-class-specific Calculations

The flow chart of the calculations of input for a two-phase pressurized liquid release is shown in Figures 4-2 and 4-6.

5.3.6 Determination of Choked Flow for Gas Releases

This determination is not required since this is a liquid release.

5.3.7 Emission Rate

As described in Section 4.7.3, to calculate the emission rate, the first task is to compare the ratio of L_p/L_e to 1. In this example, the value of L_p is 1 m and the value of L_e is 0.1 m. Since the ratio is 10, a pipe friction factor (F) must be calculated. This is given by:

$$F^2 = \frac{1}{\left(1 + \frac{4fL_p}{D_p}\right)}$$

$$= \frac{1}{\left(1 + \frac{(4)(0.0015)(1m)}{0.007036m}\right)}$$

$$= 0.5397$$

$$F = 0.7347$$

The emission rate can then be calculated by the equation:

$$E = A_o F \left(\frac{\lambda M p_s}{R T_s^2}\right)\left(\frac{T_s}{C_{pl}}\right)^{\frac{1}{2}}$$

$$E = (3.888\text{x}10^{-5}\text{m}^2)(0.7347)$$

$$\left(\frac{(2.878\text{x}10^5\text{J/kg})(70.91\text{kg/kmol})(6.951\text{x}10^5\text{Pa})}{(8314\text{J/kmol°K})(294.3\text{°K})^2}\right)$$

$$\left(\frac{294.3\text{°K}}{927.13\text{J/kg°K}}\right)^{\frac{1}{2}}$$

$$= 0.3170 \text{ kg/s}$$

5.3.8 Release Temperature

The value of T_{rel} was already calculated in Section 5.3.3 in determining the release class. Its value is 239.09 °K.

5.3.9 Vapor Fraction

The value of F_{rel} was already calculated in Section 5.3.3 in determining the release class. Its value is 0.1779.

5.3.10 Initial Concentration

Since this is a two-phase flow, it is safe to assume that only chlorine is being emitted. Based on this assumption the concentrations (described in Section 4.10) are:

$f_a = 0.0$

$f_w = 0.0$

$f_l = 1.0$

5.3.11 Density

The release starts as chlorine aerosol and vapor. The water vapor molar fraction is assumed to be zero. The density of the water vapor component of the atmosphere is also assumed to be negligible. As explained in Section 4.11, when aerosol is present, the DEGADIS model will require two triplets, one describing pure air and one describing the chlorine aerosol and vapor mixture. For one of the triplets, the density of air at the ambient temperature is required. Assuming that the air behaves as a perfect gas:

$$\rho_a = \frac{p_a M_a}{RT_a}$$

$$= \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol}^\circ\text{K})(294.3^\circ\text{K})}$$

$$= 1.197 \text{ kg/m}^3$$

The water vapor density is given as:

$$\rho_w = \frac{p_a M_w}{RT_a}$$

$$= \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol}^\circ\text{K})(294.3^\circ\text{K})}$$

$$= 0.7462 \text{ kg/m}^3$$

The mole fractions of ambient water vapor (f_w') and air (f_a') are given as:

$$f_w' = \left(\frac{RH}{100}\right) 10^{\left(6.3994 - \frac{2353}{T_a}\right)}$$

$$f_w' = \left(\frac{50}{100}\right) 10^{\left(6.3994 - \frac{2353}{294.3°K}\right)}$$

$$= 0.01268$$

and

$$f_a' = 1 - f_w' = 1 - 0.01268 = 0.9873$$

The apparent molecular weight of the air and water vapor of the ambient atmosphere is:

$$M_T' = f_a' M_a + f_w' M_w$$

$$= (0.9873)(28.9\text{kg/kmol}) + (0.01268)(18.02\text{kg/kmol})$$

$$= 28.76\text{kg/kmol}$$

The ambient density ρ_a' is given as:

$$\rho_a' = \left(\frac{f_a' M_a}{M_T' \rho_a} + \frac{f_w' M_w}{M_T' \rho_w}\right)^{-1}$$

$$= \left(\frac{(0.9873)(28.9\text{kg/kmol})}{(28.76\text{kg/kmol})(1.197\text{kg/m}^3)} + \frac{(0.01268)(18.02\text{kg/kmol})}{(28.76\text{kg/kmol})(0.7462\text{kg/m}^3)}\right)^{-1}$$

$$= 1.191 \text{ kg/m}^3$$

For the second triplet, the density of the chlorine aerosol/vapor mixture at the initial portion of the release is required. To calculate the density of the aerosol/vapor mixture (ρ_i), the densities of the chlorine vapor and liquid must be known. The temperature used in this calculation is the release temperature. In this example, the release temperature is the boiling

point of chlorine. Assuming a perfect gas, the density of the chlorine gas state (ρ_g) is:

$$\rho_g = \frac{p_a M_i}{RT_e}$$

$$= \frac{(101325\text{Pa})(70.914\text{kg/kmol})}{(8314\text{J/kmol}^\circ\text{K})(239.09^\circ\text{K})}$$

$$= 3.615 \text{ kg/m}^3$$

The chlorine liquid density at the boiling point is given in Appendix B as 1562 kg/m^3. Using the formula given in Section 4.11, the overall chlorine density is:

$$\rho_i = \left(\frac{F_{rel}}{\rho_g} + \frac{(1-F_{rel})}{\rho_l}\right)^{-1}$$

$$\rho_i = \left(\frac{0.1779}{3.615\text{kg/m}^3} + \frac{(1-0.1779)}{1562\text{kg/m}^3}\right)^{-1}$$

$$= 20.11\text{kg/m}^3$$

Since the release is of pure chlorine, the release density (ρ_{rel}) is equal to the chlorine density (ρ_i).

5.3.12 Release Diameter or Area

With a hole diameter of 0.2770 inches (0.007936 meters), the hole area is 4.946×10^{-5} m^2. Since the storage phase is liquid, the storage density (ρ_s) is that of the liquid, 1562 kg/m^3 (from Appendix B). The exit velocity can then be estimated (from Section 4.12) as:

$$u = \frac{E}{A\rho_s}$$

$$= \frac{0.3170\text{kg/s}}{(4.964\text{x}10^{-5}\text{m}^2)(1562\text{kg/m}^3)}$$

$$= 4.09\text{m/s}$$

With such a high emission velocity, the release diameter can be calculated using the high momentum formula given in Section 4.12.2, which requires the density inside the vessel.

Using the high momentum formula, the release diameter is:

$$D_{rel} = D_s \sqrt{\frac{\rho_s}{\rho_{rel}}}$$

$$= 0.007036\text{m} \sqrt{\frac{1562\text{kg/m}^3}{20.11\text{kg/m}^3}}$$

$$= 0.06201\text{m}$$

5.3.13 Release Buoyancy

The release buoyancy is used to determine if a dense gas model should be used rather than a neutral or positive buoyancy model. The first step is to compare ρ_{rel} to ρ_a'. If ρ_{rel} is less than or equal to ρ_a', the release should not be treated as a dense gas release. In this case, ρ_{rel} is 20.11 kg/m^3 and ρ_a is 1.191 kg/m^3. Since ρ_{rel} is greater than ρ_a', the next step it to apply the denser-than-air criterion.

Since this is being considered a continuous release (Section 5.3.4), the calculation of the denser-than-air criterion should use the formula given in Section 4.13.1. The criterion (C_ρ) is given by:

$$C_\rho = \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}}$$

$$= (4.47\text{m/s})\left[\frac{(9.806\text{m/s}^2)(0.3170\text{kg/s}/20.11\text{kg/m}^3)}{0.06201\text{m}}\left(\frac{20.11\text{kg/m}^3 - 1.191\text{kg/m}^3}{1.191\text{kg/m}^3}\right)\right]^{-\frac{1}{3}}$$

$$= 1.311$$

Since $C_\rho < 6$, a dense gas model should be used.

5.3.14 Release Height

The tubing that has been severed is 2 meters above the ground. Since the released material immediately flashes and all liquid is assumed to be suspended as an aerosol, the release height is assumed to be the same as the height where the liquid leaves the container system, i.e. 2 meters.

5.3.15 Ground Surface Temperature

No direct information is given on the ground surface temperature. Therefore, the ground surface temperature is assumed to be equal to the ambient temperature, which is 70°F or 294.1 °K.

5.3.16 Averaging Time

The averaging time is specified as 15 minutes, to make the model predicted concentrations comparable to the STEL (Short Term Exposure Limit) concentration.

5.3.17 Meteorology

Wind Speed and Direction

The wind speed and direction either are assumed to be available from on-site meteorological equipment or else represent average conditions at the site. The wind speed is given in this example as 10 mph (4.47 m/s). The wind direction is given as south (180°). The measurement height is given as 10 meters. To determine the greatest specific impact, multiple wind speeds may be required in conjunction with multiple stability classes.

Stability Class

The stability class is not given explicitly; however, a class can be estimated from the information provided. Using the method described in the Workbook, Section 3.1.2. In this example, there is 4/8 cloud coverage, and the release is in the mid-morning, indicating that the insolation is moderate. According to Table 3-3 of the Workbook, the stability class for a wind speed of 4.47 m/s at 10 m during a day with moderate insolation is estimated as "B" or "C." For this simulation, the stability class of "C" will be used.

Surface Roughness Length

In keeping with the value suggested for use in modeling done for planning purposes, the surface roughness is assumed to be 0.01 m.

Wind Speed at 10 m Altitude

Since the wind speed at the 10 meters height is given, it is not necessary to estimate this value estimated using stability class and surface roughness.

Ambient Temperature, Relative Humidity, and Pressure

The ambient temperature, relative humidity, and pressure are all assumed to be available from on-site equipment. See the observable data, Table 5-6.

5.3.18 Output Definition

The appropriate concentration to be specified when generating output is the STEL (Short Term Exposure Limit) concentration given in the chlorine data table in Appendix B. The actual impact values to be predicted are listed in Section 7.0.

5.4 TWO-PHASE REFRIGERATED LIQUID EXAMPLE

In this example, a process hold-up vessel contains liquid sulfur dioxide, which is cooled to a temperature below its saturation pressure. The storage temperature is 122°F (50°C, 323.15 °K) and the storage pressure is 15 atmospheres absolute (1.52×10^6 Pa). Referring to the sulfur dioxide triple point diagram contained in Appendix B, this combination of temperature and pressure place sulfur dioxide in the "liquid only" region of the diagram.

A hole develops in the 2-inch (0.05 m) diameter pipe that transports the subcooled sulfur dioxide from the storage vessel to a process area. The hole is 0.5 inches (1.3×10^{-2} m) in diameter, and is located at a point 6.6 ft (2.0 m) downstream of the vessel. At the time of the release, the vessel contains 14,520 lb (6,586 kg) of liquid sulfur dioxide. The feed to the vessel is isolated at the time of the release, however, the release proceeds until all of the sulfur dioxide originally contained in the vessel is depleted. Since the release is remote from the vessel, the temperature and pressure remain constant within the vessel throughout the release.

The sulfur dioxide is released as a liquid. Since it is subcooled and pressurized, however, it vaporizes very quickly upon the release. The release is therefore treated as a gas release with an emission rate equal to that of

the liquid release rate from the vessel. A schematic of the release configuration is provided in Figure 5-3.

The meteorological information is:

- Northeast wind at 7 mph;
- Temperature at 64.4°F;
- Relative Humidity of 42%;
- Pressure of 1 atm (sea level);
- Stability class assumed to be "E"; and
- Measurement height of 6 m.

The nearest public boundary is 80 meters from the release point.

A summary listing of the model input is provided in Table 5-7. The following sections describe how the input values were developed.

5.4.1 Observable Data

The observable data were provided in the scenario description. Table 5-8 summarizes the information provided in the scenario description. For planning purposes, it should be assumed that the direction that the hole is facing is the same direction in which the wind is blowing. This will ensure that ground level impacts of the released material are maximized.

5.4.2 Chemical Data Requirements

The chemical data for sulfur dioxide are provided in Appendix B.

5.4.3 Release Class

This section describes the calculations required to determine the release class for this example. The flow diagram in Figure 4-1 is used as a guide. Many of the calculations required to determine the release class are also required for other model input. Rather than presenting all calculations

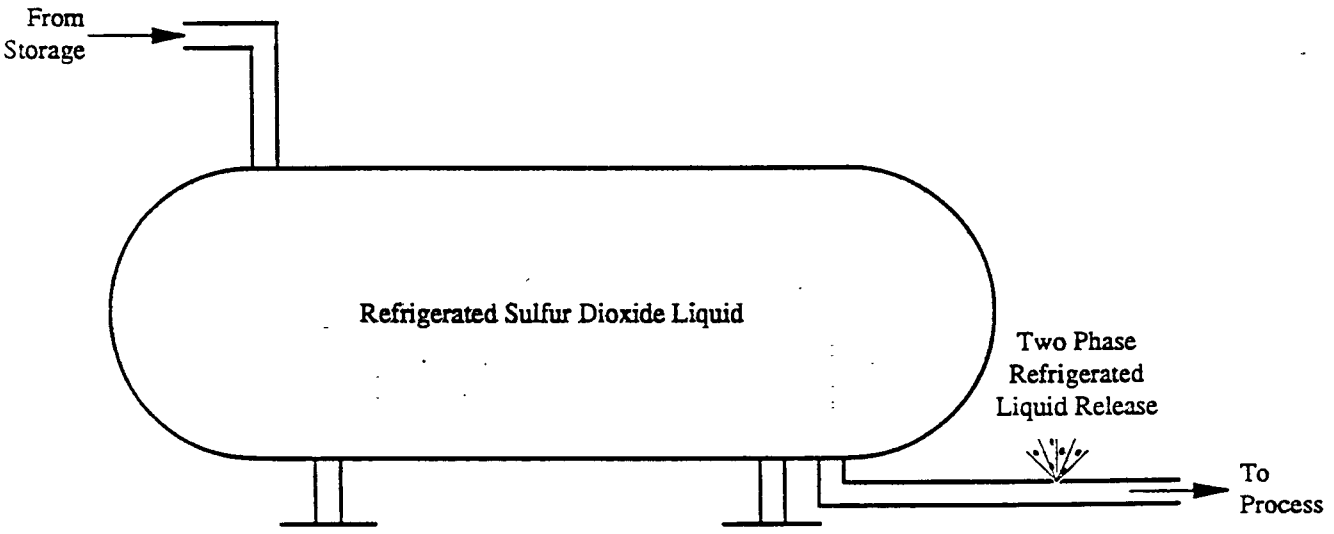


Figure 5-3. Two-Phase Refrigerated Liquid

TABLE 5-7. INPUT SUMMARY FOR THE TWO-PHASE REFRIGERATED LIQUID RELEASE EXAMPLE

Chemical Data (5.4.2)
From Appendix B

Release Type (5.4.3)
Two-phase

Continuous or Instantaneous Release Categories (5.4.4)
Continuous

Emission Rate (5.4.7)
4.154 kg/s

Release Temperature (5.4.8)
263.15 °K (T_b)

Vapor Fraction (5.4.9)
F_{rel} = 0.2140

Initial Concentration (5.4.10)
f_a = 0.0
f_w = 0.0
f_i = 1.0

Density (5.4.11)
ρ_{rel} = 13.76 kg/m^3
ρ_a' = 1.206 kg/m^3 (at ambient temperature)

Release Diameter or Area (5.4.12)
Diameter = 0.1308 m

Release Buoyancy (5.4.13)
C_ρ = 0.5068 < 6 (use dense gas model)

Release Height (5.4.14)
0.3049 m

Ground Surface Temperature (5.4.15)
Same as ambient

Averaging Time (5.4.16)
15 minutes

TABLE 5-7. (CONTINUED)

Meteorology (5.4.17)

Wind Speed and Direction
45° @ 7 mph (3.13 m/s)
Measurement height = 6 m
Speed @ 10 m = 3.72 m/s

Stability Class
E

Surface Roughness Length
Z0 = 0.01 m

Ambient Temperature, Relative Humidity, and Pressure
Temperature = 64.4°F (291.15 °K)
Relative Humidity = 42%
Pressure = 1 atm (101325 Pa)

Output Definition (5.4.18)
STEL
Minimum distance of concern = 80 m

Observable Data (5.4.1)
See Table 5-8

TABLE 5-8. OBSERVABLE DATA SUMMARY FOR THE TWO PHASE PRESSURIZED LIQUID RELEASE EXAMPLE

Release Description

Species: Sulfur dioxide
Container: Horizontal cylinder

Diameter:	4 ft (1.220 m)
Length:	12 ft (3.659 m)
Volume:	150.8 ft^3 (4.277 m^3)
Total SO_2:	14520 lbs (6586 kg)
Temperature:	122°F (323.15 °K)
Pressure:	15 atm (absolute) (1.52 x 10^6 Pa)

Hole site: Connected tubing

Length:	6.562 ft (2 m)
Inner diameter:	0.50 inch (0.0127 m)
Area:	1.267 x 10^{-4} m
Height of tube:	1 ft (0.3049 m)

Nearest boundary: 262.5 ft (80 m)

Meteorology:

Temperature:	64.4°F (291.15 °K)
Relative Humidity:	42%
Pressure:	1 atm (101325 Pa)
Wind Speed:	7 mph (3.13 m/s)
Wind Direction:	NE (45°)
Measurement hgt:	19.68 ft (6 m)
Surface Roughness:	0.01 m
Stability Class:	E

in one section, reference is made to the appropriate section for each calculation.

In this scenario, there are two releases. The first release is the two-phase flow of liquid escaping from the container. The second release is the decreasing-rate gas-phase release from the container that occurs as the pressure in the container falls to 1 atm. All of the liquid escapes from the container. Only the first release is a two-phase flow, so only it is discussed in this section. The second release class is a gas release with a varying emission rate. This second release class needs to be modeled separately.

The initial release class was determined by using the flow diagram shown in Figure 4-1. The value of F_{rel} is required to make the final decision regarding the release class. But in order to calculate F_{rel}, the value of T_{rel} is required. The value for T_{rel} is obtained by solving the equation described in Section 4.8.2:

$$p_a = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_{rel}}\right)\right]$$

or

$$p_a = 101325\text{Pa} \exp\left[\frac{(3.8874\text{x}10^5\text{J/kg})(64.06\text{kg/kmol})}{8314\text{J/kmol°K}}\left(\frac{1}{263.15°\text{K}} - \frac{1}{T_{rel}}\right)\right]$$

Setting p_a to 1 atm (101325 Pa) leads to a T_{rel} of 263.15 °K (the boiling point, T_b).

After T_{rel} has been calculated, the value for F_{rel} (see Section 4.9.3) can be obtained by:

$$F_{rel} = \frac{C_{pl}(T_s - T_{rel})}{\lambda}$$

$$= \frac{(1386.32 J/kg°K)\ (323.15°K - 263.15°K)}{3.8874x10^5 J/kg}$$

$$= 0.2140$$

Since F_{rel} is between zero and one, according to the flow chart in Figure 4-1, this release is two-phase. Now you can use the flow chart in Figure 4-2 to determine the model input.

5.4.4 Continuous or Instantaneous Release Categories

In this example, the emission rate is 4.154 kg/s (from Section 5.4.8). The duration of the two-phase portion of the release is however long it takes for the liquid to escape the container. There are 6586 kg of liquid in the container and all the liquid is lost. Thus, the duration of the release (t_d) is:

$$t_d = \frac{6586 kg}{4.154 \frac{kg}{s}}$$

$$= 1585\ s$$

$$= 26.4\ minutes$$

For a non-source-term model, the value of t_d must be compared to advection time to a receptor or maximum downwind distance reached by a concentration of interest. Using the formula given in Section 4.4 for t_{trav}, and assuming a wind speed of 7 mph (3.13 m/s) and a distance of 80 meters, the advection time is 51.1 seconds. Since the emission duration is longer than the time it takes the material to reach the downwind point of interest, the release is considered continuous.

For a source-term model, the value of t_d is sufficiently long to treat this as a continuous release for most receptors.

5.4.5 Release-class-specific Calculations

The flow chart of the calculations of input for a two-phase refrigerated liquid release is shown in Figures 4-2 and 4-6.

5.4.6 Determination of Choked Flow for Gas Releases

This determination is not required since this is a liquid release.

5.4.7 Emission Rate

As indicated in Section 4.7.4, the parameters p_{sv} and F must be calculated before the emission rate can be estimated. The calculations for these parameters are:

$$p_{sv} = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_s}\right)\right]$$

$$= 101325\text{Pa} \exp\left[\frac{3.8874\text{x}10^5\text{J/kg})(64.06\text{kg/kmol})}{8314\text{J/kmol°K}}\right.$$

$$\left.\left(\frac{1}{263.15°\text{K}} - \frac{1}{323.15°\text{K}}\right)\right]$$

$$= 8.386\text{x}10^5 \text{ Pa}$$

and

$$F^2 = \frac{1}{\left(1 + \frac{4fL_p}{D_p}\right)}$$

$$= \frac{1}{\left(1 + \frac{(4)(0.0015)(2m)}{0.0508}\right)}$$

$$= 0.8089$$

$$F = 0.8994$$

With these parameters, the emission rate can be calculated as:

$$E = A_o\left[2C^2(p_s - p_{sv})\rho_l + \frac{F^2}{C_{pl}T_s}\left(\frac{\lambda M p_s}{RT_s}\right)^2\right]^{\frac{1}{2}}$$

$$= (1.267\text{x}10^{-4}m^2)[(2)(0.6)^2((1.5199\text{x}10^6Pa) - (8.386\text{x}10^5Pa))$$

$$(1460.4kg/m^3) + \frac{(0.8089)}{(1386.32J/kg°K)(323.15°K)}$$

$$\left(\frac{(3.8874\text{x}10^5J/kg)(64.06kg/kmol)(1.5199\text{x}10^6Pa)}{(8314J/kmol°K)(323.15°K)}\right)^2\Bigg]^{\frac{1}{2}}$$

$$= 4.154 \text{ kg/s}$$

5.4.8 Release Temperature

The value of T_{rel} was previously calculated in Section 5.4.3 in determining the release class. Its value is 263.15 °K.

5.4.9 Vapor Fraction

The value of F_{rel} was previously calculated in Section 5.4.3 in determining the release class. Its value is 0.2140.

5.4.10 Initial Concentration

Since this is a two-phase flow, it is safe to assume that all that is being emitted is sulfur dioxide. Based on this assumption the initial concentrations (described in Section 4.10) are:

$f_a = 0.0$

$f_w = 0.0$

$f_i = 1.0$

5.4.11 Density

The release starts as sulfur dioxide aerosol and vapor. The water vapor molar fraction is assumed to be zero. The density of the water vapor component of the atmosphere is also assumed to be negligible. As explained in Section 4.11, when aerosol is present, the DEGADIS model requires two triplets, one describing pure air and one describing the sulfur dioxide aerosol/vapor mixture. The density of air at ambient temperature is required for one of the triplets. Assuming that the air behaves as a perfect gas:

$$\rho_a = \frac{p_a M_a}{R T_a}$$

$$= \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol}^\circ\text{K})(291.15^\circ\text{K})}$$

$$= 1.210 \text{ kg/m}^3$$

Similarly, the water vapor density is given as:

$$\rho_w = \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol°K})(291.15\text{°K})}$$

$$= 0.7543 \text{ kg/m}^3$$

The mole fractions of ambient water vapor (f_w') and air (f_a') are given as:

$$f_w' = \left(\frac{RH}{100}\right) 10^{\left(6.3994 - \frac{2353}{T_a}\right)}$$

$$= \left(\frac{42}{100}\right) 10^{\left(6.3994 - \frac{2353}{291.15\text{°K}}\right)}$$

$$= 0.00873$$

$$f_a' = 1 - f_w' = 1 - 0.00873 = 0.9913$$

The apparent molecular weight of the air and water vapor of the ambient atmosphere is:

$$M_T' = f_a'M_a + f_w'M_w$$

$$= (0.9913)(28.9\text{kg/kmol}) + (0.00873)(18.02\text{kg/kmol})$$

$$= 28.81 \text{ kg/kmol}$$

Finally, the ambient density ρ_a' is given as:

$$\rho_a' = \left(\frac{f_a'M_a}{M_T'\rho_a} + \frac{f_w'M_w}{M_T'\rho_w}\right)^{-1}$$

$$= \left(\frac{(0.9913)(28.9\text{kg/kmol})}{(28.81\text{kg/kmol})(1.210\text{kg/m}^3)} + \frac{(0.00873)(18.02\text{kg/kmc}}{(28.81\text{kg/kmol})(0.7543\text{kg}}\right.$$

$$= 1.206\text{kg/m}^3$$

The density of the sulfur dioxide aerosol/vapor mixture at the initial portion of the release is required for the second triplet. To calculate the density of the aerosol/vapor mixture (ρ_i), the densities of the sulfur dioxide vapor and liquid must be known. The temperature used in this calculation is the release temperature. In this example, the release temperature is the boiling point of sulfur dioxide. Assuming a perfect gas, the density of the sulfur dioxide gas state (ρ_g) is:

$$\rho_g = \frac{p_a M_i}{RT_{rel}}$$

$$= \frac{(101325\text{Pa})(64.06\text{kg/kmol})}{(8314\text{J/kmol°K})(263.15\text{°K})}$$

$$= 2.9668 \text{ kg/m}^3$$

The sulfur dioxide liquid density at the boiling point is given in Appendix B as 1460.4 kg/m^3. The overall sulfur dioxide density is:

$$\rho_i = \left(\frac{F_{rel}}{\rho_g} + \frac{(1-F_{rel})}{\rho_l}\right)^{-1}$$

or

$$\rho_i = \left(\frac{0.2140}{2.9668\text{kg/m}^3} + \frac{(1-0.2140)}{1460.4\text{kg/m}^3}\right)^{-1}$$

$$= 13.761 \text{ kg/m}^3$$

Since the release is of pure sulfur dioxide, the release density (ρ_{rel}) is equal to the sulfur dioxide density (ρ_i).

5.4.12 Release Diameter or Area

Since the storage phase is liquid, the storage density (ρ_s) is that of the liquid, or 1460.4 kg/m^3 (from Appendix B). The exit velocity can then be estimated, as discussed in Section 4.12, as:

$$u = \frac{E}{A\rho_s}$$

$$= \frac{4.154 \text{kg/s}}{(1.267\text{x}10^{-4}\text{m}^2)(1460.4\text{kg/m}^3)}$$

$$= 22.5 \text{m/s}$$

With such a high emission velocity, the release diameter can be calculated using the high momentum formula given in Section 4.12.2. This formula requires that you know the density inside the vessel.

Using the high momentum formula, the release diameter is:

$$D_{rel} = D_s \sqrt{\frac{\rho_s}{\rho_{rel}}}$$

$$D_{rel} = 0.0127 \text{ m} \sqrt{\frac{1460.4 \text{ kg/m}^3}{13.761 \text{ kg/m}^3}}$$

$$= 0.1308 \text{ m}$$

5.4.13 Release Buoyancy

The release buoyancy is used to determine if a dense gas model should be used rather than a neutral or positive buoyancy model. The first step is to compare ρ_{rel} to ρ_a'. If ρ_{rel} is less than or equal to ρ_a', the release should

not be treated as a dense gas release. In this example, ρ_{rel} is 13.76 kg/m^3 and ρ_a' is 1.206 kg/m^3. Since ρ_{rel} is greater than ρ_a', the next step is to apply the denser-than-air criterion.

Since this is being considered a continuous release (Section 5.4.4), the calculation of the denser-than-air criterion should use the formula given in Section 4.13.1, . The criterion (C_ρ) is given by:

$$C_\rho = \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}}$$

$$= (3.13\text{m/s})\left[\frac{(9.806\text{m/s}^2)(4.154\text{kg/s}/13.76\text{kg/m}^3)}{0.1308\text{m}}\left(\frac{13.76\text{kg/m}^3 - 1.206\text{kg/m}^3}{1.206\text{kg/m}^3}\right)\right]^{-\frac{1}{3}}$$

$$= 0.5068$$

Since $C_\rho < 6$, a dense gas model should be used.

5.4.14 Release Height

The tubing that has been severed is 1 foot (0.3049 m) above the ground. Since the released material immediately flashes and all liquid is assumed to be suspended as an aerosol, the release height is assumed to be the same as the height where the liquid leaves the container system, i.e. 0.3049 meter.

5.4.15 Ground Surface Temperature

No direct information is given on the ground surface temperature. Therefore, the ground surface temperature is assumed to be equal to the ambient temperature, which is 291.15 °K.

5.4.16 Averaging Time

The averaging time is specified as 15 minutes. This is to make the model predicted concentrations comparable to the STEL (Short Term Exposure Limit) concentration.

5.4.17 Meteorology

Wind Speed and Direction

The wind speed and direction either are assumed to be available from on-site meteorological equipment or else represent average conditions at the site. The wind speed is given in this example as 7 mph (3.13 m/s). The wind direction is given as northeast (45°). The measurement height is given as 6 meters. To determine the greatest specific impact, multiple wind speeds may be required in conjunction with multiple stability classes.

Stability Class

It is assumed that this simulation is for planning purposes. Thus, the stability class is set to "E".

Surface Roughness Length

In keeping with the value suggested for use in modeling done for planning purposes, the surface roughness is assumed to be 0.01 m.

Wind Speed at 10 m Altitude

With the surface roughness, stability class, and wind speed at 6 meters, the wind speed at 10 meters can be estimated. Using the formula given in

Section 4.17.3 and assuming a stability class of "E," the predicted wind speed at 10 meters (u) is:

$$u = u_1\left(\frac{h}{z_1}\right)^p$$

$$= (3.13\text{m/s})\left(\frac{10\text{m}}{6\text{m}}\right)^{0.34}$$

$$= 3.72\text{m/s}$$

Ambient Temperature, Relative Humidity, and Pressure

The ambient temperature, relative humidity, and pressure are all assumed to be available from on-site equipment. See the observable data, Table 5-8.

5.4.18 Output Definition

The appropriate concentration to be specified when generating output is the STEL (Short Term Exposure Limit) concentration given in the sulfur dioxide data table in Appendix B. The actual impact values to be predicted are listed in Section 7.0.

5.5 SINGLE-PHASE GAS RELEASE (CHOKED) EXAMPLE

In this example, an anhydrous hydrogen fluoride storage vessel contains liquid- and vapor-phase hydrogen fluoride. The vessel is being filled from a rail car through a flexible transfer line when an overpressure/overtemperature condition develops within the vessel, resulting in the actuation of a rupture disk within the vapor space of the vessel. The rupture disk is then piped to a remote area through 13.1 ft (4 m) of pipe with 2.5 inches inside diameter.

At the time of the release, the hydrogen fluoride within the vessel is at the rupture disk set pressure, which is well above the saturation pressure of hydrogen fluoride. Immediately upon actuation of the rupture disk, the

pressure within the vessel drops to its release pressure, which [illegible].01 atmospheres absolute (2.04×10^5 Pa), and the liquid within the vessel remains subcooled at 165°F (347.0 °K). The vessel temperature and pressure conditions remain constant throughout the release. However, the pipe is heated to increase the loft of the effluent. The temperature inside the pipe is 365 °K, which is the temperature of the release into the air. The release is isolated 45 seconds from the time of the rupture disk actuation. During the release, hydrogen fluoride is emitted as a vapor only, with the vapor flow at critical (choked) conditions within the pipe. Figure 5-4 provides a schematic of the release.

The meteorological conditions at the time of the release are:

- Northwest wind at 14 mph;
- Temperature at 71.6°F;
- Relative Humidity of 45%;
- Pressure of 1 atm (sea level);
- 7/8 cloud cover;
- Early-evening release; and
- Measurement height of 20 ft.

The nearest public boundary is 200 meters from the release point. Table 5-9 summarizes the model input. The following sections describe how these input values were developed.

5.5.1 Observable Data

The observable data were discussed in the scenario description, and are summarized in Table 5-10. For modeling that is done for planning purposes, it should be assumed that the direction the hole is facing is the same direction in which the wind is blowing. Most relief valves point vertically, but assuming a horizontal position will ensure maximum ground level impacts of the released material.

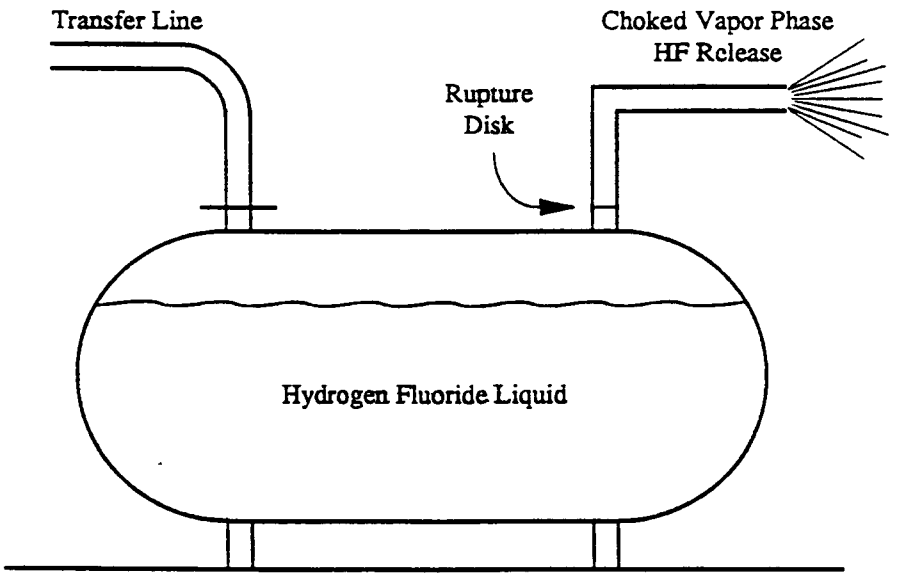


Figure 5-4. Single-Phase Gas Release (Choked)

TABLE 5-9. INPUT SUMMARY FOR THE SINGLE PHASE CHOKED GAS RELEASE EXAMPLE

Chemical Data (5.5.2)
From Appendix B

Release Type (5.5.3)
Single Phase Choked

Continuous or Instantaneous Release Categories (5.5.4)
Instantaneous

Emission Rate (5.5.7)
0.8513 kg/s

Release Temperature (5.5.8)
313.6 °K

Vapor Fraction (5.5.9)
F_{rel} = 1.00 (no flash, but all mass emitted as vapor)

Initial Concentration (5.5.10)
f_a = 0.0
f_w = 0.0
f_i = 1.0

Density (5.5.11)
ρ_{rel} = 1.3602 kg/m^3
ρ_a = 1.188 kg/m^3 (at ambient temperature)

Release Diameter or Area (5.5.12)
Diameter = 4.155 m (instantaneous)
Diameter = 0.06649 m (continuous, choke conditions)
Diameter = 0.0635 m (continuous, expanded)

Release Buoyancy (5.5.13)
C_ρ = 0.332 > 0.2 (use dense gas model) (instantaneous)
C_ρ = 2.638 < 6.0 (use dense gas model) (continuous)

Release Height (5.5.14)
12 ft (3.66 m)

Ground Surface Temperature (5.5.15)
Same as ambient

Averaging Time (5.5.16)
15 minutes

TABLE 5-9. (CONTINUED)

Meteorology (5.5.17)

Wind Speed and Direction
315° @ 14 mph (6.26 m/s)
Measurement height = 20 ft (6.1 m)
Speed @ 10 m = 6.64 m/s

Stability Class
D

Surface Roughness Length
Z0 = 0.01 m

Ambient Temperature, Relative Humidity, and Pressure
Temperature = 22°C (295.15 °K)
Relative Humidity = 45%
Pressure = 1 atm (101325 Pa)

Output Definition (5.5.18)
STEL
Minimum distance of concern = 200 m

Observable Data (5.5.1)
See Table 5-10

TABLE 5-10. OBSERVABLE DATA SUMMARY FOR THE SINGLE PHASE CHOKED GAS RELEASE EXAMPLE

Release Description

Species: Hydrogen Fluoride
Container: Horizontal cylinder

Diameter:	4.9 ft (1.5 m)
Length:	16.4 ft (5 m) Tangent to Tangent
Volume:	187.0 ft^3 (5.30 m^3)
Total HF:	500 lbs (2268 kg)
Temperature:	347 °K
Pressure:	2.01 atm (absolute) (2.0397 x 10^5 Pa)

Hole site: Connected tubing

Length:	13.1 ft (4 m)
Inner diameter:	2.5 inches (0.0635 m)
Area:	3.167×10^{-3} m^2
Height of tube:	12 ft (3.66 m)
Temperature:	365 °K

Nearest boundary: 200 m

Meteorology:

Temperature:	71.6°F (295.15 °K)
Relative Humidity:	45%
Pressure:	1 atm (101325 Pa)
Wind Speed:	14 mph (6.26 m/s)
Wind Direction:	Northwest (315°)
Measurement hgt:	20.0 ft (6.10 m)
Cloud cover:	7/8
Surface Roughness:	0.01 m
Time:	Early evening

5.5.2 Chemical Data Requirements

The data for pure HF is in Appendix B.

5.5.3 Release Class

This section describes the calculations required to determine the release class for this example. The flow diagram in Figure 4-1 is used as a guide. Note that some of the assumptions made in the process of determining the release class conflict with the description of the release scenario. Also, many of the calculations required to determine the release class are also required for other model input. Rather than presenting all calculations in one section, reference is made to the appropriate section for each calculation.

The release is a pure gas release. It must be determined whether the release is choked or unchoked. As shown in Section 5.5.6, it can be determined that the pressure at the exit (p_*) is greater than the ambient pressure, which implies that the release is choked. To determine the release class, it first must be assumed made that the release is single phase. The calculations will be checked at the end to ensure that this assumption is valid. The storage temperature just before the release is 365 °K. This value is assumed to be the storage temperature (T_s).

The value of T_* can then be estimated by the equation:

$$T_* = T_s \left[\frac{2}{\gamma + 1}\right]$$

$$= (365.0°K)\left[\frac{2}{1.3976 + 1}\right]$$

$$= 304.5°K$$

The value of T_* is less than the critical temperature of hydrogen fluoride, which is given in Appendix B. So the vapor pressure at T_* must now be

compared to p_*. Using the vapor pressure equation in the Appendix, at temperature T_*=304.5° K, the vapor pressure is 1.524×10^5 Pa. According to the flow chart in Figure 4-1, since this vapor pressure is greater than p_*, this release class is a single-phase gas release. The flow chart in Figure 4-3 can now be used to determine the model input.

5.5.4 Continuous or Instantaneous Release Categories

The duration of the release (t_d) is given as only lasting 45 seconds.

For a non-source-term model, the value of t_d must be compared either to advection time to a receptor or to the time it takes a concentration of interest to reach a maximum downwind distance. Using the formula in Section 4.4 for t_{trav}, and assuming a wind speed of 14 mph (6.26 m/s) and a distance of 200 meters, the advection time is calculated to be 63.9 seconds. This emission duration is shorter than the time required to reach the downwind point of interest. Therefore, the release should be considered either instantaneous or of finite duration.

For a source-term model, the value of t_d is short enough to treat this as an instantaneous or finite duration release for most receptors.

5.5.5 Release-class-specific Calculations

The flow chart showing the calculations of input for a choked single-phase gas release is presented in Figures 4-3 and 4-6.

5.5.6 Determination of Choked Flow for Gas Releases

Section 4.6 explains how to determine whether a release is choked or unchoked. The pressure at the exit point of the gas (p_*) is given by:

$$p_* = p_s\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{(\gamma-1)}}$$

$$= 2.0397\text{x}10^5\text{Pa}\left(\frac{2}{1.3976+1}\right)^{\frac{1.3976}{(1.3976-1)}}$$

$$= 1.0784\text{x}10^5\text{Pa}$$

where: $\gamma = C_p / C_v$ = 1455.57 J/kg °K / 1041.49 J/kg °K = 1.3976.

Since $p_* \geq p_a$ = 101325 Pa, the flow in this release is choked.

5.5.7 Emission Rate

Knowing that the release is classified as a single-phase choked gas release, we can determine its emission rate, using the information provided in Section 4.7.5.

$$E = CA_o\left[p_s\rho_s\gamma\left(\frac{2}{\gamma + 1}\right)^{\frac{(\gamma+1)}{(\gamma-1)}}\right]^{\frac{1}{2}}$$

and

$$\rho_s = \frac{p_s M}{RT_s}$$

$$= \frac{(2.0397\text{x}10^5\text{Pa})(20.006\text{kg/kmol})}{(8314\text{J/kmol°K})(365\text{°K})}$$

$$= 1.3447\ \text{kg/m}^3$$

So,

$$E = (0.75)(3.167\text{x}10^{-3}\text{m}^2)$$

$$\left[(2.0397\text{x}10^5\text{Pa})(1.3447\text{kg/m}^3)1.3976\left(\frac{2}{1.3976+1}\right)^{\frac{(1.3976+1)}{(1.3976-1)}}\right]^{\frac{1}{2}}$$

$$= 0.8513\text{kg/s}$$

5.5.8 Release Temperature

We can determine the release temperature based on the information provided in Section 4.8.5.

$$T_{rel} = T_s\left[1 - 0.85\left(\frac{\gamma - 1}{\gamma + 1}\right)\right]$$

$$= (365°\text{K})\left[1 - 0.85\left(\frac{1.3976 - 1}{1.3976 + 1}\right)\right]$$

$$= 313.6°\text{K}$$

5.5.9 Vapor Fraction

This is a single-phase release; therefore, all of the emission is in the gas phase.

5.5.10 Initial Concentration

Since this is a single-phase release of pure HF, the initial concentrations (described in Section 4.10) are:

$f_a = 0.0$

$f_w = 0.0$

$f_1 = 1.0$

5.5.11 Density

As discussed in Section 4.11, hydrogen fluoride can associate into oligomers at high concentrations and temperatures lower than about 50°C[17]. Inside the vessel, this was not a problem because the temperature was kept at about 92°C. However, when released, the temperature is 313.6 °K (40°C), so self association can be important. The self association can be considered in the density calculation by treating the hydrogen fluoride as having an apparent molecular weight (M_i'). Pure HF at 313.6 °K would have an apparent molecular weight of about 25.3 kg/kmol[17]. Since the apparent molecular weight increases rapidly with decreasing temperature and a rapid temperature reduction would be expected immediately upon release, a higher molecular weight will be assumed by using the value at a temperature about 10 °C lower than the storage temperature. This gives an apparent molecular weight of about 35 kg/kmol. The temperature and, therefore, the apparent molecular weight, is about what it was at choked flow conditions, T_*. This value of the apparent molecular weight, 35 kg/kmol, should be used in calculating density effects. Since the apparent molecular weight changes as the release is dispersed, the DEGADIS model should be supplied a pair of triplets created using ρ_{rel} and ρ_a (calculated below).

The release is entirely in the gas phase of a pure component. The release density (ρ_{rel}) is equal to the density of the component (ρ_{rel}) in the gas phase. The density is then:

$$\rho_{rel} = \rho_g = \frac{p_a M_i'}{RT_{rel}}$$

$$= \frac{(101325\text{Pa})(35\text{kg/kmol})}{(8314\text{J/kmol°K})(313.6\text{°K})}$$

$$= 1.3602\text{kg/m}^3$$

The ambient air density is also required for buoyancy effects. The dry air component of the atmosphere is given by the perfect gas law as:

$$\rho_a = \frac{p_a M_a}{RT_a}$$

$$= \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol}^\circ\text{K})(295.15^\circ\text{K})}$$

$$= 1.193\text{kg/m}^3$$

Similarly, the water vapor density is given as:

$$\rho_w = \frac{p_a M_w}{RT_a}$$

$$= \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol}^\circ\text{K})(295.15^\circ\text{K})}$$

$$= 0.7441\text{kg/m}^3$$

The mole fractions of ambient water vapor (f_w') and air (f_a') are given as:

$$f_w' = \left(\frac{RH}{100}\right) 10^{\left(6.3994 - \frac{2353}{T_a}\right)}$$

$$= \left(\frac{45}{100}\right) 10^{\left(6.3994 - \frac{2353}{295.15^\circ\text{K}}\right)}$$

$$= 0.0120$$

$$f_a' = 1 - f_w' = 1 - 0.0120 = 0.9880$$

The apparent molecular weight of the air and water vapor of the ambient atmosphere is:

$$M_T' = f_a' M_a + f_w' M_w$$

$$= (0.9880)(28.9\text{kg/kmol}) + (0.00120)(18.02\text{kg/kmol})$$

$$= 28.77\text{kg/kmol}$$

Finally, the ambient density (ρ_a') is given as:

$$\rho_a' = \left(\frac{f_a' M_a}{M_T' \rho_a} + \frac{f_w' M_w}{M_T' \rho_w} \right)^{-1}$$

$$= \left(\frac{(0.9880)(28.9\text{kg/kmol})}{(28.77\text{kg/kmol})(1.193\text{kg/m}^3)} + \frac{(0.0120)(18.02\text{kg/kmol})}{(28.77\text{kg/kmol})(0.7441\text{kg/m}^3)} \right)^{-1}$$

$$= 1.188\text{kg/m}^3$$

5.5.12 Release Diameter or Area

Since the emission is assumed to be instantaneous, the size of the release can be estimated from the volume required to hold the emitted mass at ρ_{rel}. The amount of mass released (E_t) can be calculated from the emission rate (E) and duration of the release as:

$$E_t = E\ \Delta t$$

$$= (0.8513\text{kg/s})(45\text{s})$$

$$= 38.31\ \text{kg}$$

The volume required (V) is then:

$$V = \frac{E_t}{\rho_{rel}}$$

$$= \frac{38.31\text{kg}}{1.3602\text{kg/m}^3}$$

$$= 28.16 \text{ m}^3$$

Assuming that the cloud is in the form of a cylinder with a radius equal to the cloud depth, the diameter can be calculated as:

$$D_{rel} = 2\left(\frac{V}{\pi}\right)^{\frac{1}{3}}$$

$$= 2\left(\frac{28.16\text{m}^3}{\pi}\right)^{\frac{1}{3}}$$

$$= 4.155 \text{ m}$$

If it is assumed that the release is not instantaneous, the pseudo hole diameter needs to be calculated. Since this release is choked, there are two release diameters to be considered. The one that is to be used depends on the model being used. The first release diameter to consider is that which represents the choke condition. This diameter replaces the actual hole size in those models that require hole size. If the actual hole size were used, the calculated exit velocity would be greater than sonic. The choke point release diameter from the high momentum formula is then:

$$D_{rel} = D_s \sqrt{\frac{\rho_*}{\rho_{rel}}}$$

$$D_{rel} = 0.0635m \sqrt{\frac{1.491kg/m^3}{1.360kg/m^3}}$$

$$= 0.06649m$$

where ρ_* is the density at the choked conditions and is given by:

$$\rho_* = \frac{p_* M_i}{RT_*} = \frac{(1.0784x10^5 Pa)(35kg/kmol)}{(8314J/kmol°K)(304.5°K)}$$

$$= 1.491 \ kg/m^3$$

The second release diameter is calculated using the storage density (ρ_s) rather than the choke density. This diameter is used in those models that require the after-expansion size of a release. However, because of the difference in molecular weight of the material in the storage state (20.006) from when it is released (35), the release density (ρ_{rel}) is larger than ρ_s. This would lead to a diameter smaller than the actual diameter. Therefore, in this case, the actual diameter should be used.

5.5.13 Release Buoyancy

From the information provided in Section 4.13.2, the criterion for determining whether an instantaneous release should be considered denser-than-air is if:

$$C_\rho = \left[\frac{g(E_t/\rho_{rel})^{1/3}}{U_r^2} \left(\frac{\rho_{rel} - \rho_a'}{\rho_a'} \right) \right]^{\frac{1}{2}} > 0.2 \quad .$$

The value of E_t must be calculated from the emission rate (E) and the duration of the release such that:

$$E_t = E\ \Delta t$$

$$= (0.8513 kg/s)(45s)$$

$$= 38.31\ kg$$

The buoyancy criterion is then:

$$C_\rho = \left[\frac{9.806 m/s^2 (38.31 kg/1.3602 kg/m^3)^{1/3}}{(6.26 m/s)^2} \left(\frac{1.3602 kg/m^3 - 1.188 kg/m^3)}{(1.188 kg/m^3)}\right)\right]^{\frac{1}{2}}$$

$$= 0.332$$

Since $C_\rho > 0.2$, a dense gas model should be used for this example.

If it is assumed that the release is not instantaneous, the buoyancy criterion would be given by:

$$C_\rho = \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}}$$

$$= (6.26 m/s)\left[\frac{(9.806 m/s^2)(0.8513 kg/s/1.360 kg/m^3)}{0.06649 m} \left(\frac{1.360 kg/m^3 - 1.188 kg/m^3}{1.188 kg/m^3}\right)\right]^{-\frac{1}{3}}$$

$$= 2.638$$

Since $C_\rho < 6$, a dense gas model should be used.

5.5.14 Release Height

The rupture disk is located at the top of the vessel at a height of 12 ft (3.66 m).

5.5.15 Ground Surface Temperature

No direct information was given on the ground surface temperature. Therefore, the ground surface temperature is assumed to be equal to the ambient temperature, which is 22°C (295.15 °K).

5.5.16 Averaging Time

The averaging time is specified as 15 minutes in order to make the model-predicted concentrations comparable to the STEL (Short Term Exposure Limit) concentrations.

5.5.17 Meteorology

Wind Speed and Direction

The wind speed and direction are assumed either to be available from on-site meteorological equipment or else are representative of average conditions at the site. The wind speed in this example is 14 mph (6.26 m/s). The wind direction is northwest (315°). The measurement height is given as 20 ft (6.10 m). To determine the greatest specific impact, multiple wind speeds may be required in conjunction with multiple stability classes.

Stability Class

The stability class is not given explicitly. However, a class can be estimated from the information provided using the method described in the Workbook, Section 3.1.2. In this example, there is 7/8 cloud coverage and the release is in the mid-morning, indicating that the insolation is slight.

Based on Table 3-2 of the Workbook, the stability class for a wind speed of 6.26 m/s during the day with slight insolation would be "D."

Surface Roughness Length

In keeping with the value suggested for modeling done for planning purposes, the surface roughness is assumed to be 0.01 meters.

Wind Speed at 10 m Altitude

With the surface roughness, stability class, and wind speed at 6.1 meters, the wind speed at 10 meters can be estimated. Using the formula in Section 4.17.3 and assuming a stability class of "D," the predicted wind speed at 10 meters (u) is:

$$u = u_1\left(\frac{h}{z_1}\right)^p$$

$$= (6.26\text{m/s})\left(\frac{10\text{m}}{6.1\text{m}}\right)^{0.12}$$

$$= 6.64\text{m/s}$$

which falls within the wind speed limits for "D" stability.

Ambient Temperature, Relative Humidity, and Pressure

The ambient temperature, relative humidity, and pressure are all assumed to be available from on-site equipment. See the observable data, Table 5-10.

5.5.18 Output Definition

The appropriate concentration level to be used for generating output is the STEL (Short Term Exposure Limit) concentration given in the hydrogen

fluoride data table in Appendix B. The actual impact values to be predicted are listed in Section 7.0.

5.6 SINGLE-PHASE GAS RELEASE (UNCHOKED) EXAMPLE

In this example, an absorption tower is employed to recover hydrogen chloride vapor from a waste gas stream in a process facility. Vapor phase hydrogen chloride and air are fed to the tower, which uses water as an absorption media to remove all of the hydrogen chloride during normal operations. A pump failure in the water supply system to the tower results in a temporary decrease in the capacity of the water supply to the tower. The resulting decrease in absorption efficiency results in the release of 4,250 actual cfm (2.01 m^3/s) of a mixture of hydrogen chloride, water vapor, and air for twelve minutes before shut off.

The stack temperature (at the point of release) is 120°F (322.0 °K). At this temperature, the emission is saturated with water vapor (12.4% water). The volume (molar) percentages of hydrogen chloride and air are 72.9% and 14.7%, respectively. A mist eliminator removes all of the entrained liquid phase materials at the top of the stack, and only vapor is released to the atmosphere. The stack is 34 inches (0.86 m) in diameter and 28 ft (8.54 m) tall. A schematic of the release is provided in Figure 5-5.

The meteorological conditions at the time of release are:

- East wind at 2.2 mph;
- Temperature of 64°F;
- Relative Humidity of 36%;
- Pressure of 1 atm (sea level);
- 3/8 cloud cover;
- Early-morning release; and
- Measurement height of 10 m.

The nearest public boundary is 525 ft from the release point.

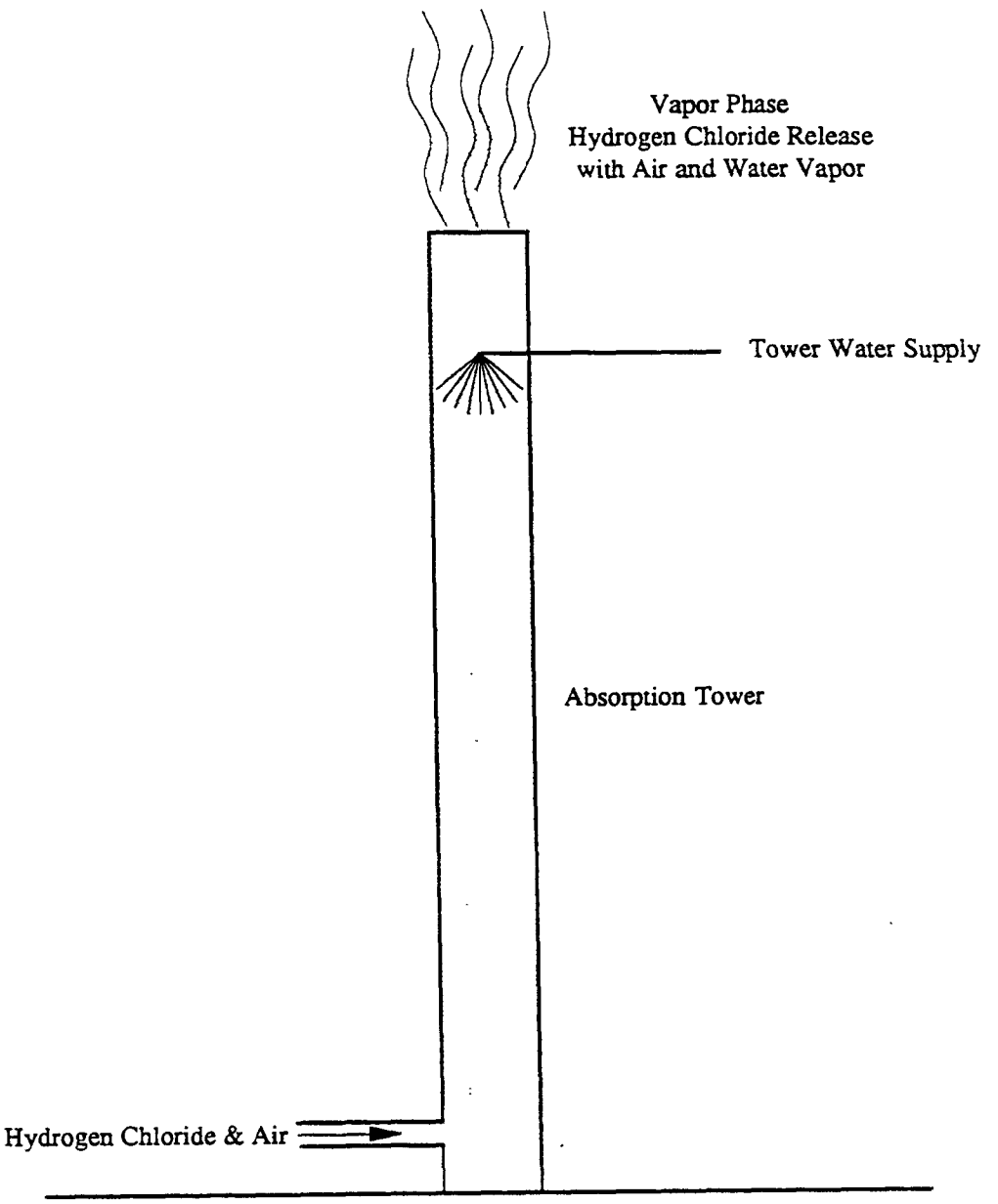


Figure 5-5. Single-Phase Gas Release (Unchoked)

Table 5-11 summarizes the model input for this example. The following sections describe how the input values were developed.

5.6.1 Observable Data

Observable data were presented in the scenario description and are summarized in Table 5-12.

5.6.2 Chemical Data Requirements

The data for pure hydrogen chloride are in Appendix B. However, this emission is a mixture of hydrogen chloride, water, and air, all in the gas phase. Therefore, the emission may be treated as a pseudo chemical consisting of this mixture. Some models can handle the mixture internally by specifying the initial concentrations of each of the components. These initial concentrations are calculated in Section 5.6.10. In other models, it is assumed that the emission is always of a pure chemical and so the emission must be of the pseudo chemical.

Since this release contains only the gas phase, the only parameters required to describe the pseudo chemical are the apparent molecular weight and the gas-phase specific heat. The method for calculation of the parameters for a pseudo chemical is given in Section 4.2.

The apparent molecular weight is calculated in Section 5.6.11 using the molar fractions of the components, which are given in Section 5.6.10. The specific heats are given in units of J/kg °K, which are mass units, so the calculation needs mass fractions. The relationship between mass fraction and molar fraction is given by:

$$w_i M = f_i M_i$$

TABLE 5-11. INPUT SUMMARY FOR THE SINGLE PHASE UNCHOKED GAS RELEASE EXAMPLE

Chemical Data (5.6.2)
From Appendix B

Release Type (5.6.3)
Single Phase Unchoked

Continuous or Instantaneous Release Categories (5.6.4)
Continuous

Emission Rate (5.6.7)
2.5151 kg/s

Release Temperature (5.6.8)
322.04 °K

Vapor Fraction (5.6.9)
F_{rel} = 1.00 (no flash, but all mass emitted as vapor)

Initial Concentration (5.6.10)
f_a = 0.1467
f_w = 0.1238
f_i = 0.7295

Density (5.6.11)
ρ_{rel} = 1.2513 kg/m^3
ρ_a = 1.208 kg/m^3 (at ambient temperature)

Release Diameter or Area (5.6.12)
Diameter = 0.8636 m

Release Buoyancy (5.6.13)
C_ρ = 1.048 < 6 (use dense gas model)

Release Height (5.6.14)
8.54 m

Ground Surface Temperature (5.6.15)
Same as ambient

Averaging Time (5.6.16)
30 minutes

TABLE 5-11. (CONTINUED)

Meteorology (5.6.17)

Wind Speed and Direction
90° @ 2.2 mph (0.98 m/s)
Measurement height = 10 m
Speed @ 10 m = 0.98 m/s

Stability Class
B

Surface Roughness Length
Z0 = 0.01 m

Ambient Temperature, Relative Humidity, and Pressure
Temperature = 64°F (290.9 °K)
Relative Humidity = 36%
Pressure = 1 atm (101325 Pa)

Output Definition (5.6.18)
IDLH
Minimum distance of concern = 525 ft (160.1 m)

Observable Data (5.6.1)
See Table 5-12

TABLE 5-12. OBSERVABLE DATA SUMMARY FOR THE SINGLE PHASE UNCHOKED GAS RELEASE EXAMPLE

Release Description

Species: Hydrogen chloride
Container: Stack

Diameter:	34 in (0.8636 m)
Height:	28 ft (8.54 m)
Volume rate:	4250 ft^3/min (2.01 m^3/s)
Temperature:	120°F (322.04 °K)

Nearest boundary: 525 ft (160.1 m)

Meteorology:

Temperature:	64°F (290.9 °K)
Relative Humidity:	36%
Pressure:	1 atm (101325 Pa)
Wind Speed:	2.2 mph (0.98 m/s)
Wind Direction:	East (90°)
Measurement hgt:	32.81 ft (10 m)
Surface Roughness:	0.01 m
Cloud cover:	3/8
Time:	Early morning

so, for this example,

$$w_a = \frac{f_a M_a}{M}$$

$$= \frac{(0.1467)(28.9\text{kg/kmol})}{(33.07\text{kg/kmol})}$$

$$= 0.1282$$

$$w_w = \frac{f_w M_w}{M}$$

$$= \frac{(0.1238)(18.02\text{kg/kmol})}{(33.07\text{kg/kmol})}$$

$$= 0.06746$$

$$w_{HCl} = \frac{z_{HCl} M_{HCl}}{M}$$

$$= \frac{(0.7295)(36.46\text{kg/kmol})}{(33.07\text{kg/kmol})}$$

$$= 0.8043$$

The specific heat is then calculated as:

$$C_p = \sum w_i C_{pi}$$

$$C_p = w_a C_{pa} + w_w C_{pw} + w_{HCl} C_{pHCl}$$
$$= (0.1282)(1004 J/kg°K)$$
$$+ (0.06746)(4180 J/kg°K)$$
$$+ (0.8043)(799.81 J/kg°K)$$
$$= 1054 J/kg°K$$

5.6.3 Release Class

The release class is determined following the flow chart in Figure 4-1. First, since this is a stored gas, we must determine whether the release is choked or unchoked. In Section 5.6.6, it is determined that the exit velocity is much smaller than sonic velocity. Since choke flow only occurs at or near sonic velocity, the flow in this release is unchoked.

The next step in determining if the release is two phase or not is to compare the vapor pressure of the HCl at the release temperature to the release pressure. The release pressure is 1 atm. The release temperature is given as 322 °K. The boiling point of pure HCl is 188.1 °K, which means the vapor pressure should be well in excess of 1 atm at 322 °K. According to the flow chart shown in Figure 4-1, since the HCl vapor pressure is greater than the release pressure, the release is single phase. Thus, it is concluded that this release scenario should be treated as an unchoked single-phase gas release. The flow chart in Figure 4-3 should be used to determine the model input.

5.6.4 Continuous or Instantaneous Release Categories

The duration of the release (t_d) is given as 12 minutes.

For a non-source-term model, the value of t_d must be compared either to the advection time to a receptor or to the time it takes a concentration of interest to reach maximum downwind distance. Using the formula in Section 4.4

for t_{trav}, and assuming a wind speed of 2.2 mph (0.98 m/s) and a distance of 525 ft (160.1 m), the advection time is calculated as 327 seconds. Since the emission duration is longer than the time to reach the downwind point of interest, the release is considered continuous.

For a source-term model, the value of t_d is also sufficiently long to treat this as a continuous release for most receptors.

5.6.5 Release-class-specific Calculations

The flow chart showing the calculations of input for an unchoked single-phase gas release is given in Figures 4-3 and 4-6.

5.6.6 Determination of Choked Flow for Gas Releases

We can determine whether or not the flow is choked by calculating the exit velocity. Since this release is a stack release, the formula using pressure cannot be used. However, the exit velocity (v_e) may be calculated from the stack area (A_0) and the volumetric release rate (V_f). So,

$$v_e = \frac{V_f}{A_0}$$

$$= \frac{2.01 m^3/s}{0.586 m^2}$$

$$= 3.43 \text{ m/s}$$

Since v_e is very much less than sonic velocity, we can consider the stack emission to be unchoked; choked flow occurs when the exit velocity is at or near sonic velocity.

5.6.7 Emission Rate

The total mass emission can be calculated from the specified volumetric release rate (V_f) and the release density (ρ_{rel}). Therefore,

$$E = V_f \rho_{rel}$$

$$= (2.01 m^3/s)(1.2513 kg/m^3)$$

$$= 2.5151 \text{ kg/s}$$

5.6.8 Release Temperature

The release temperature (T_{rel}) at the stack exit is specified as 120°F (322.04 °K). It is a measured value for this example.

5.6.9 Vapor Fraction

The emission is completely in the vapor phase.

5.6.10 Initial Concentration

From Section 4.10, the water vapor fraction can be estimated if the temperature is known. Since the release temperature (T_{rel}) is 322.04 °K, the saturated molar fraction of the water vapor (e_s) at 1 atm of pressure is:

$$e_s = 10^{\left(6.3994 - \frac{2353}{T_{rel}}\right)}$$

$$= 10^{\left(6.3994 - \frac{2353}{322.04°K}\right)}$$

$$= 0.1238$$

$$= f_w$$

The fractions of HCl and air emitted during the release are specified as $f_i = 0.7295$ and $f_a = 0.1467$, respectively.

5.6.11 Density

The densities are calculated using the formulas presented in Section 4.11. Since this release is completely in vapor phase, the release density can be calculated assuming an ideal gas.

$$\rho_i = \frac{p_a M_i}{RT_{rel}}$$

$$\rho_w = \frac{p_a M_w}{RT_{rel}}$$

$$\rho_a = \frac{p_a M_a}{RT_{rel}}$$

T_{rel} = 322.04 °K

M_i = 36.46 kg/kmol

M_w = 18.02 kg/kmol

M_a = 28.9 kg/kmol

Therefore,

$$\rho_i = \frac{(101325\text{Pa})(36.46\text{kg/kmol})}{(8314\text{J/kmol°K})(322.04\text{°K})}$$

$$= 1.3798 \text{ kg/m}^3$$

$$\rho_w = \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol}^\circ\text{K})(322.04^\circ\text{K})}$$

$$= 0.6819 \text{ kg/m}^3$$

$$\rho_a = \frac{(101325\text{Pa})\ (28.9\text{kg/kmol})}{(8314\text{J/kmol}^\circ\text{K})\ (322.04^\circ\text{K})}$$

$$= 1.0937 \text{ kg/m}^3$$

The density at release (ρ_{rel}) can be calculated by:

$$\rho_{rel} = \left[\frac{f_{aM_a}}{M_T\rho_a} + \frac{f_{wM_w}}{M_T\rho_w} + \frac{f_{iM_i}}{M_T\rho_i}\right]^{-1}$$

where:

$$M_T = f_aM_a + f_wM_w + f_iM_i$$

$$= (0.1467)(28.9\text{kg/kmol}) + (0.1238)(18.02\text{kg/kmol})$$

$$+ (0.7295)(36.46\text{kg/kmol})$$

$$= 33.07 \text{ kg/kmol}$$

Therefore,

$$\rho_{rel} = \left[\frac{(0.1467)(28.9\text{kg/kmol})}{(33.07\text{kg/kmol})(1.0937\text{kg/m}^3)} + \frac{(0.1238)(18.02\text{kg/kmol})}{(33.07\text{kg/kmol})(0.6810\text{kg/m}^3)} + \frac{(0.7295)(36.46\text{kg/kmol})}{(33.07\text{kg/kmol})(1.3798\text{kg/m}^3)}\right]^{-1}$$

$$\rho_{rel} = 1.2513 \text{ kg/m}^3$$

The density of the ambient air also needs to calculated so that buoyancy can be determined. The ambient air density can be derived from the perfect gas law at the ambient temperature, 290.9 °K:

$$\rho_a = \frac{p_a M_a}{RT_a}$$

$$= \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol°K})(290.9\text{°K})}$$

$$= 1.211\text{kg/m}^3$$

$$f_a = 1 - f_w = 1 - 0.00736 = 0.9926$$

Similarly, the water vapor density is given as:

$$\rho_w = \frac{p_a M_w}{RT_a}$$

$$= \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol°K})(290.9\text{°K})}$$

$$= 0.7549\text{kg/m}^3$$

The mole fractions of ambient water vapor (f_w') and air (f_a') are given as:

$$f_w' = \left(\frac{RH}{100}\right) 10^{\left(6.3994 - \frac{2353}{T_a}\right)}$$

$$= \left(\frac{36}{100}\right) 10^{\left(6.3994 - \frac{2353}{290.9\text{°K}}\right)}$$

$$= 0.00736$$

The apparent molecular weight of the air and water vapor of the ambient atmosphere is:

$$M_T' = f_a'M_a + f_w'M_w$$

$$= (0.9926)(28.9\text{kg/kmol}) + (0.00736)(18.02\text{kg/kmol})$$

$$= 28.82 \text{ kg/kmol}$$

Finally, the ambient density ρ_a' is given as:

$$\rho_a' = \left(\frac{f_a'M_a}{M_T'\rho_a} + \frac{f_w'M_w}{M_T'\rho_w}\right)^{-1}$$

$$= \left(\frac{(0.9926)(28.9\text{kg/kmol})}{(28.82\text{kg/kmol})(1.211\text{kg/m}^3)} + \frac{(0.00736)(18.02\text{kg/kmol})}{(28.82\text{kg/kmol})(0.7549\text{kg/m}^3)}\right)^{-1}$$

$$= 1.208\text{kg/m}^3$$

5.6.12 Release Diameter or Area

The temperature inside the stack is the same as the temperature at the exit. The pressure is atmospheric both inside and outside the stack. Because this is an unchoked stack release of a gas, the density can be calculated from the perfect gas law. Since the in-stack and at-exit temperatures are the same, the density inside the stack (ρ_s) is the same as the density of the release (ρ_{rel}).

The exit velocity is calculated in Section 5.6.6 as 3.43 m/s. With such a high emission velocity, the release diameter can be calculated using the high momentum formula in Section 4.12.2. However, the formula modifies the actual hole size by the square root of the ratio of the release density inside the stack to the release density outside the stack. Since these two densities are equal, the release diameter (D_{rel}) is equal to the actual diameter (D_s). The formula for the release diameter requires the density inside the vessel.

The area of interest is the stack, which has a diameter of 34 inches (0.8636 m).

5.6.13 Release Buoyancy

The release buoyancy is used to determine if a dense gas model should be used rather than a neutral or positive buoyancy model. The first step is to compare ρ_{rel} to ρ_a'. If ρ_{rel} is less than or equal to ρ_a', the release is not to be treated as a dense gas release. In this case, ρ_{rel} is 1.2513 kg/m^3 and ρ_a' is 1.208 kg/m^3. Since ρ_{rel} is greater than ρ_a', the next step is to calculate the denser-than-air criterion to determine whether this release should be treated as a dense release gas or not.

The calculation of the denser-than-air criterion should use the formula in Section 4.13.1, since this is being considered a continuous release (Section 5.6.4). The criterion (C_ρ) is given by:

$$C_\rho = \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}}$$

$$= (0.98\text{m/s})\left[\frac{(9.806\text{m/s}^2)(2.5151\text{kg/s}/1.2513\text{kg/m}^3)}{0.8636\text{m}}\left(\frac{1.2513\text{kg/m}^3 - 1.208\text{kg/m}^3}{1.208\text{kg/m}^3}\right)\right]^{-\frac{1}{3}}$$

$$= 1.048$$

Since $C_\rho < 6$, a dense gas model should be used.

5.6.14 Release Height

The stack height is 28 ft (8.54 m), which is where the emission enters the atmosphere.

5.6.15 Ground Surface Temperature

No direct information is directly given on the ground surface temperature. Therefore, the ground surface temperature is assumed to be equal to the ambient temperature, which is 64°F (290.9 °K).

5.6.16 Averaging Time

The averaging time is specified as 30 minutes to make the model predicted concentrations comparable to the IDLH (Immediately Dangerous to Life and Health) concentration.

5.6.17 Meteorology

Wind Speed and Direction

The wind speed and direction either are assumed to be available from on-site meteorological equipment or else represent average conditions at the site. In this example, the wind speed is 2.2 mph (0.98 m/s). The wind direction is east (90°). The measurement height is given as 32.81 ft, or 10 m. To determine the greatest specific impact, multiple wind speeds may be required in conjunction with multiple stability classes.

Stability Class

The stability class is not explicitly given. However, the stability class can be estimated from the information provided using the method described in the Workbook, Section 3.1.2. In this example, there is 3/8 cloud coverage and the release takes place in the early morning, indicating that insolation is slight. Based on Table 3-2 in the Workbook, the stability class estimated for a wind speed to be 0.98 m/s at 10 m during the day with slight insolation would be "B."

Surface Roughness Length

In keeping with the value suggested for modeling done for planning purposes, the surface roughness is assumed to be 0.01 m.

Wind Speed at 10 m Altitude

Since the wind speed at 10 meters height is given, it does not need to be estimated using stability class and surface roughness.

Ambient Temperature, Relative Humidity, and Pressure

The ambient temperature, relative humidity, and pressure are all assumed to be available from on-site equipment. See the observable data, Table 5-12.

5.6.18 Output Definition

The appropriate concentration level to use to generate output should be the STEL (Short Term Exposure Limit) concentration given in the hydrogen chloride data table in Appendix B. The actual impact values to be predicted are listed in Section 7.0.

5.7 SINGLE-PHASE LIQUID RELEASE (HIGH VOLATILITY) EXAMPLE

In this example, ethylene oxide is stored in its liquid phase within a vessel by maintaining the ethylene oxide at a temperature just below its boiling temperature. A 0.25 inch hole develops near the bottom of the tank. At the time of the release, the ambient pressure is 1 atm, and the ethylene oxide within the vessel is at its saturation pressure of 1 atm and is also at its normal boiling temperature of 51.3°F (283.85 °K). The liquid level within the 3.5 meter diameter tank is 9.2 ft (2.8 m) above grade level. The hole is located 0.15 ft (0.5 m) above grade level.

Liquid ethylene oxide is released under the column head pressure of vessel contents until the liquid level reaches that of the hole. The ambient temperature at the time of the release is 82.4°F (301.15 °K). Since the boiling point of ethylene oxide (equal to the release temperature of 283.85 °K) is below the ambient temperature, the liquid vaporizes very rapidly as it leaves the vessel. The release is therefore treated as a vapor phase release at a rate equaling the liquid release rate from the vessel. A schematic of the release is provide in Figure 5-6.

The meteorological conditions at the time of release are:

- North wind at 2.0 m/s;
- Temperature at 28°C;
- Relative Humidity of 50%;
- Pressure of 1 atm (sea level);
- Stability class assumed to be "E"; and
- Measurement height of 10 m.

The nearest public boundary is 100 meters from the release point.

Table 5-13 summarizes the model input for this example. The following sections describe how the input values were developed.

5.7.1 Observable Data

The observable data was given in the scenario description. Table 5-14 summarizes this information. For modeling done for planning purposes, the direction that the hole is facing should be assumed to be in the same direction in which the wind is blowing. This will ensure maximum transport of the released material.

5.7.2 Chemical Data Requirements

The chemical data for pure ethylene oxide is given in Appendix B.

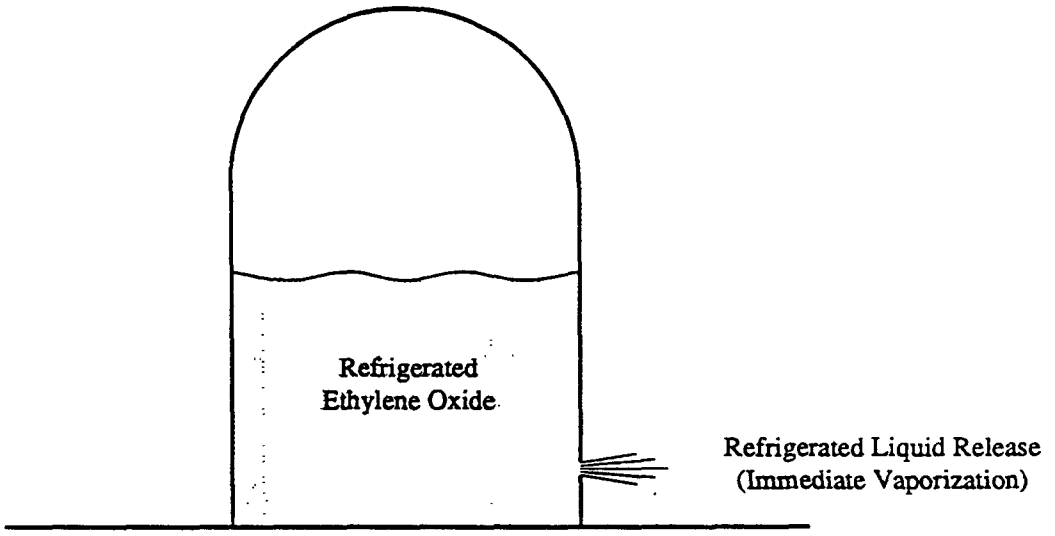


Figure 5-6. Single-Phase Liquid Release (High Volatility)

TABLE 5-13. INPUT SUMMARY FOR THE HIGH-VOLATILITY, SINGLE PHASE LIQUID RELEASE EXAMPLE

Chemical Data (5.7.2)
From Appendix B

Release Type (5.7.3)
Two-phase

Continuous or Instantaneous Release Categories (5.7.4)
Continuous

Emission Rate (5.7.7)
0.1220 kg/s

Release Temperature (5.7.8)
283.85 °K (T_b)

Vapor Fraction (5.7.9)
F_{rel} = 0.0 (from flash, but assumed to boil/evaporate immediately)

Initial Concentration (5.7.10)
f_a = 0.0
f_w = 0.0
f_i = 1.0

Density (5.7.11)
ρ_{rel} = 1.891 kg/m^3
ρ_a = 1.162 kg/m^3 (at ambient temperature)

Release Diameter or Area (5.7.12)
Diameter = 0.1372 m

Release Buoyancy (5.7.13)
C_ρ = 1.403 < 6 (use dense gas model)

Release Height (5.7.14)
0.5 m

Ground Surface Temperature (5.7.15)
Same as ambient

Averaging Time (5.7.16)
30 minutes

TABLE 5-13. (CONTINUED)

Meteorology (5.7.17)

Wind Speed and Direction
0° @ 2 m/s
Measurement height = 10 m
Speed @ 10 m = 2 m/s

Stability Class
E

Surface Roughness Length
Z0 = 0.01 m

Ambient Temperature, Relative Humidity, and Pressure
Temperature = 301 °K
Relative Humidity = 50%
Pressure = 1 atm (101325 Pa)

Output Definition (5.7.18)
IDLH
Minimum distance of concern = 100 m

Observable Data (5.7.1)
See Table 5-14

TABLE 5-14. OBSERVABLE DATA SUMMARY FOR THE HIGH-VOLATILITY, SINGLE PHASE LIQUID RELEASE EXAMPLE

Release Description

Species: Ethylene oxide
Container: Vertical cylinder

Diameter:	3.5 m
Height:	
Volume:	
Total EO:	23780 kg
Temperature:	283.85 °K (T_b)
Pressure:	1 atm (absolute) (101325 Pa)

Hole site: In vessel

Liquid above hole:	2.3 m
Inner diameter:	0.25 inch (6.35×10^{-3} m)
Area:	3.167×10^{-5} m
Height of hole:	0.5 m

Nearest boundary: 328.1 ft (100 m)

Meteorology:

Temperature:	28°C (301 °K)
Relative Humidity:	50%
Pressure:	1 atm (101325 Pa)
Wind Speed:	2 m/s
Wind Direction:	North (0°)
Measurement hgt:	10 m
Surface Roughness:	0.01 m
Stability Class:	E

5.7.3 Release Class

In this scenario, only one release occurs. The liquid pours out of the container until the liquid level is at the hole level. Since the liquid is stored at its boiling point, the gas pressure inside the container is at one atmosphere. No significant gas release would be expected since the inside and outside pressures are the same, unless the refrigeration stopped. In that case, the remaining liquid may boil and the resulting vapor would escape.

The release class is determined using the flow diagram in Figure 4-1. The ethylene oxide is stored as a liquid. The flash diagram in Appendix B indicates that flashing will not occur since the storage temperature is equal to the boiling point and the flash diagram curve begins its upward branch just at the boiling point.

Since no flash will occur, the next step is to decide if the boiling point is above or below the ambient temperature. The boiling point is 283.85 °K. The ambient temperature is 301 °K. Since the boiling point is below the ambient temperature, the material released will boil/evaporate as soon as it reaches the atmosphere. From the flow chart in Figure 4-1, this scenario is defined as a high-volatility liquid release. The flow chart in Figure 4-5 should be used to determine the model input.

5.7.4 Continuous or Instantaneous Release Categories

In this example, the emission rate is 0.1220 kg/s (from Section 5.7.8). The duration of the release is how long it takes for the liquid to escape the container. There is 23,780 kg liquid in the container at a depth of 2.8 m. The hole is at a height of 0.5 m above the container bottom. This means that the fraction of the liquid that remains in the container after the liquid stops being released is 0.5/2.8. The duration of the release (t_d) is then calculated as:

$$t_d = \frac{(1 - (0.5m/2.8m)))23780kg}{0.1220\frac{kg}{s}}$$

$$t_d = 160111s$$

$$= 44.5 \text{ hours}$$

For a non-source-term model, the value of t_d must be compared either to the advection time to a receptor or to the time it takes the concentration of interest to reach the maximum downwind distance. Using the formula in Section 4.4 for t_{trav}, and assuming a wind speed of 2 m/s and a distance of 100 meters, the advection time is calculated to be 327 seconds. Since the emission duration is longer than the time required to reach the downwind point of interest, the release is considered continuous.

For a source-term model, the value of t_d is also sufficiently long to treat this as a continuous release for most receptors.

5.7.5 Release-class-specific Calculations

The flow chart showing the calculations of input for a single-phase high volatility liquid release is presented in Figures 4-4 and 4-6.

5.7.6 Determination of Choked Flow for Gas Releases

This determination is not required since this scenario involves a high volatility liquid release.

5.7.7 Emission Rate

From Section 4.7.7, to calculate the emission rate, the pressure at the exit hole first must be calculated. This is done by the equation:

$$P_h = \max(p_a, p_{sv}) + \rho_s g H_l$$

or, in this example,

$$P_h = 1.01325\text{x}10^5\text{Pa} + (882.70\text{kg/m}^3)(9.806\text{m/s}^2)(2.3\text{m})$$

$$= 1.212\text{x}10^5\text{Pa}$$

Since the storage pressure (p_{sv}) is the same as the ambient pressure (p_a), 1 atm, the maximum is also 1 atm.

The term β (as defined in Section 4.7.6) approaches zero in this release from a tank since the area of the hole is very much smaller than the area of the tank. This means that K is equal to C (0.65). The equation in Section 4.7.7 can then be written as;

$$E = CA_o[2\rho_s(p_h - p_a)]^{\frac{1}{2}}$$

or

$$E = (0.65)(3.167\text{x}10^{-5}\text{m}^2)$$

$$[2(882.70\text{kg/m}^3)((1.2123\text{x}10^5\text{Pa}) - (1.01325\text{x}10^5\text{Pa}))]^{\frac{1}{2}}$$

$$= 0.1220 \text{ kg/s}$$

5.7.8 Release Temperature

For this release class, it is assumed that, as soon as the liquid leaves the container, it vaporizes. Therefore, the release temperature can be assumed to be the normal boiling point of the chemical.

5.7.9 Vapor Fraction

The value of F_{rel} was previously determined to be zero in the determination of the release class (Section 5.7.3). However, it is also assumed that, after the liquid gets into the atmosphere, it will boil/evaporate immediately without forming a pool or liquid droplets, since the boiling point is lower than the ambient temperature and storage pressure is near ambient pressure.

5.7.10 Initial Concentration

Since this is a high volatility flow, it is safe to assume that only ethylene oxide is being emitted. Based on this assumption the initial concentrations (described in Section 4.10) are:

$f_a = 0.0$
$f_w = 0.0$
$f_i = 1.0$

5.7.11 Density

The densities required can be calculated using the formulas discussed in Section 4.11. The release starts as pure ethylene oxide gas. The water vapor molar fraction is assumed to be zero. The density of the water vapor component of the atmosphere is also assumed to be negligible. The density of air at the ambient temperature is required in order to calculate density effects. Assuming that the air behaves as a perfect gas:

$$\rho_a = \frac{p_a M_a}{R T_a}$$

$$\rho_a = \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol°K})(301.15\text{°K})}$$

$$= 1.170\text{kg/m}^3$$

Similarly, the water vapor density is given as:

$$\rho_w = \frac{p_a M_w}{RT_a}$$

$$= \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol°K})(301.15\text{°K})}$$

$$= 0.7293\text{kg/m}^3$$

The mole fractions of ambient water vapor (f_w') and air (f_a') are given as:

$$f_w' = \left(\frac{RH}{100}\right) 10^{\left(6.3994 - \frac{2353}{T_a}\right)}$$

$$= \left(\frac{50}{100}\right) 10^{\left(6.3994 - \frac{2353}{301.15\text{°K}}\right)}$$

$$= 0.01927$$

$$f_a' = 1 - f_w'$$

$$= 1 - 0.01927$$

$$= 0.9807$$

The apparent molecular weight of the air and water vapor of the ambient atmosphere is:

$$M_T' = f_a'M_a + f_w'M_w$$

$$= (0.9807)(28.9\text{kg/kmol}) + (0.01927)(18.02\text{kg/kmol})$$

$$= 28.69\text{kg/kmol}$$

Finally, the ambient density ρ_a' is given as:

$$\rho_a' = \left(\frac{f_a'M_a}{M_T'\rho_a} + \frac{f_w'M_w}{M_T'\rho_w}\right)^{-1}$$

$$= \left(\frac{(0.9807)(28.9\text{kg/kmol})}{(28.69\text{kg/kmol})(1.170\text{kg/m}^3)} + \frac{(0.01927)(18.02\text{kg/kmol})}{(28.69\text{kg/kmol})(0.7293\text{kg/m}^3)}\right)^{-1}$$

$$= 1.162\text{kg/m}^3$$

Because the ethylene oxide is assumed to vaporize instantaneously upon release, the release density can be calculated using the perfect gas law:

$$\rho_{rel} = \frac{p_a M}{RT_{rel}}$$

$$= \frac{(101325\text{Pa})(44.053\text{kg/kmol})}{(8314\text{J/kmol°K})(283.85\text{°K})}$$

$$= 1.8914\text{kg/m}^3$$

5.7.12 <u>Release Diameter or Area</u>

With a hole diameter of 0.2770 in (0.007936 m), the hole area is $3.167\text{x}10^{-5}$ m^2. Since the storage phase is liquid, the storage density (ρ_s) is the same as that of the liquid, or 883 kg/m^3 (from Appendix B). The exit velocity (from Section 4.12) can then be estimated as:

$$u = \frac{E}{A\rho_s}$$

$$u = \frac{0.1220\text{kg/s}}{(3.167\text{x}10^{-5}\text{m}^2)(883\text{kg/m}^3)}$$

$$= 4.363\text{m/s}$$

With such a high emission velocity, the release diameter can be calculated using the high momentum formula given in Section 4.12.2. The release diameter calculated using the high momentum formula is:

$$D_{rel} = D_s \sqrt{\frac{\rho_s}{\rho_{rel}}}$$

$$= 0.00635\text{m} \sqrt{\frac{883\text{kg/m}^3}{1.8914\text{kg/m}^3}}$$

$$= 0.1372\text{m}$$

5.7.13 Release Buoyancy

The release buoyancy is used to determine if a dense gas model should be used rather than a neutral or positive buoyancy model. The first step is to compare ρ_{rel} to ρ_a'. If ρ_{rel} is less than or equal to ρ_a', the release should not be treated as a dense gas release. In this case, ρ_{rel} is 1.8914 kg/m^3 and ρ_a' is 1.162 kg/m^3. Since ρ_{rel} is greater than ρ_a', the next step is to apply the denser-than-air criterion.

The calculation of the denser-than-air criterion should be based on the formula given in Section 4.13.1, since this is being considered a continuous release (Section 5.7.4). The criterion (C_ρ) is given by:

$$C_\rho = \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}}$$

$$= (2.0\text{m/s}) \left[\frac{(9.806\text{m/s}^2)(0.1220\text{kg/s}/1.8914\text{kg/m}^3)}{0.1372\text{m}} \left(\frac{1.8914\text{kg/m}^3 - 1.162\text{kg/m}^3}{1.162\text{kg/m}^3}\right)\right]^{-\frac{1}{3}}$$

$$= 1.403$$

Since $C_\rho < 6$, a dense gas model should be used.

5.7.14 Release Height

The hole in the tank is 0.5 meters above the ground. Since the released liquid is assumed to vaporize immediately upon release, the release height is assumed to be the same as the height where the liquid leaves the container system, or 0.5 meters above the ground.

5.7.15 Ground Surface Temperature

No information on the ground surface temperature is given. Therefore, the ground surface temperature is assumed to be equal to the ambient temperature, 301.15 °K.

5.7.16 Averaging Time

The averaging time is specified as 30 minutes to make the model-predicted concentrations comparable to the IDLH (Immediately Dangerous to Life and Health) concentrations.

5.7.17 Meteorology

Wind Speed and Direction

The wind speed and direction are assumed either to be available from on-site meteorological equipment or representative of average conditions at the site. In this example, the wind speed is given as 2 m/s. The wind direction is north (0°). The measurement height is given as 10 meters. To determine the greatest specific impact, multiple wind speeds may be required in conjunction with multiple stability classes.

Stability Class

It is assumed that this simulation is for planning purposes. Therefore, the stability class is set to "E".

Surface Roughness Length

In keeping with the value suggested for modeling done for planning purposes, the surface roughness is assumed to be 0.01 m.

Wind Speed at 10 m Altitude

Since the wind speed at 10 meters height is given, it does not have to be estimated using stability class and surface roughness.

Ambient Temperature, Relative Humidity, and Pressure

The ambient temperature, relative humidity, and pressure are all assumed to be available from on-site equipment. See the observable data, Table 5-14.

5.7.18 Output Definition

The appropriate concentrations to be specified when generating output are the three ERPG (Emergency Response Planning Guideline) concentrations given in the ethylene oxide data table in Appendix B. The actual impact values to be predicted are listed in Section 7.0.

5.8 SINGLE-PHASE LIQUID RELEASE (LOW VOLATILITY) EXAMPLE

In this example, an ambient temperature vessel is used to store 30% weight hydrochloric acid in its liquid phase. The vessel is a 12-foot diameter tank with the liquid level 9 feet (2.7 m) above grade. A 0.75-inch tank glass connection is broken at the vessel wall near the bottom of the vessel, 1 foot (0.3 m) above grade level. The resulting hole is 0.75 inches (0.0191 m) in diameter. The storage temperature is equal to the ambient temperature, which is 65°F (291.5 °K). The tank is located within a 576 ft^2 (53.54 m^2) diked area. The dike is designed to contain the entire contents of the vessel when full.

The 30% weight hydrochloric acid is released as a liquid under its column head pressure within the vessel. Since the boiling point of the bulk liquid hydrochloric acid (370.2 °K) is above ambient temperature (291.5 °K), the liquid forms a pool within the dike from which evaporation occurs. Figure 5-7 provides a schematic of the release.

The meteorological conditions at the time of the release are:

- Northeast wind at 5 mph;
- Temperature at 65°F;
- Relative Humidity of 58%;
- Pressure of 1 atm (sea level);
- 3/8 cloud cover;
- Late-afternoon release; and
- Measurement height of 35 ft.

The nearest public boundary is 450 feet from the release point.

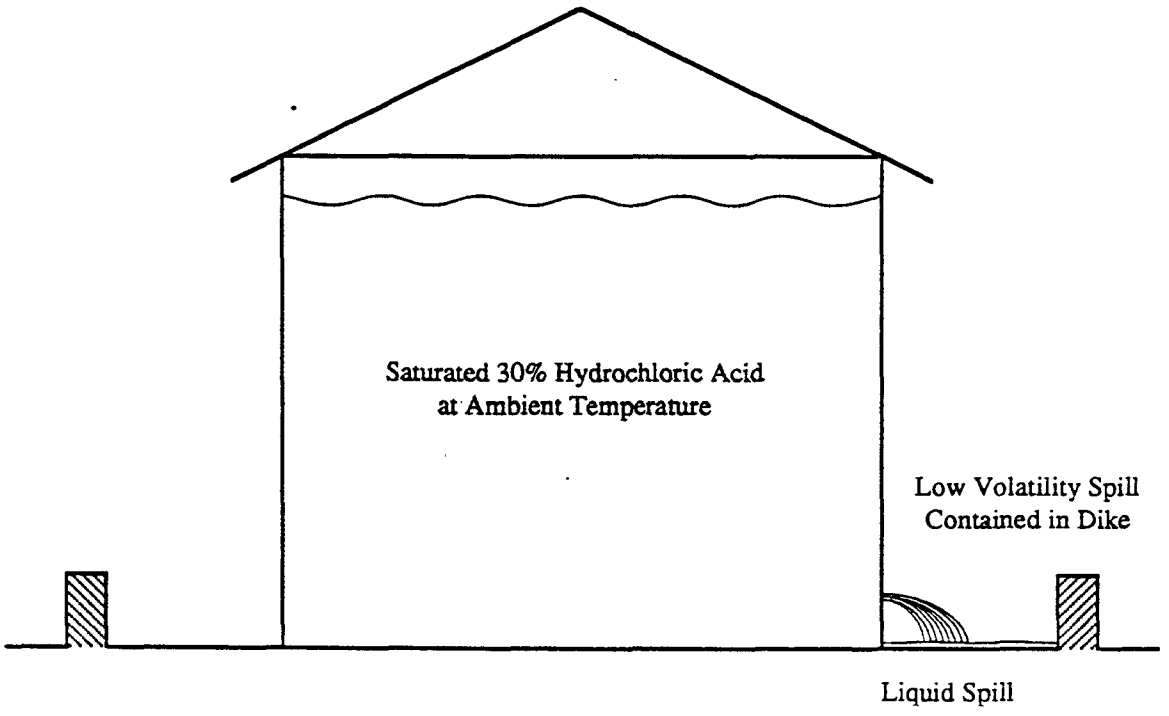


Figure 5-7. Single-Phase Liquid Release (Low Volatility)

Table 5-15 summarizes the model input for this example. The following sections describe how the input values were developed.

5.8.1 Observable Data

The observable data were presented in the scenario description. Table 5-16 summarizes these data.

5.8.2 Chemical Data Requirements

The chemical data for a 30% weight hydrochloric acid solution is given in Appendix B.

5.8.3 Release Class

In this scenario, only one release occurs. The liquid pours out of the container until the liquid level is at the hole level. The release class is determined using the flow diagram in Figure 4-1.

The hydrochloric acid solution is stored as a liquid. The flash diagram in Appendix B indicates that flashing will not occur since the storage temperature is below the boiling point and the flash diagram curve begins its upward branch just at the boiling point.

Since no flash will occur, the next step is to decide if the boiling point is above or below the ambient temperature. In this example, the boiling point is 370.2 °K. The ambient temperature is 291.48 °K. Thus, the boiling point is higher than the ambient temperature. According to the flow chart in Figure 4-1, this scenario fits the definition of a low volatility liquid release. Since the boiling point is above the ambient temperature, the material will evaporate but will not boil. The evaporation rate will be temperature- and wind-speed-controlled. Use the flow chart in Figure 4-5 to determine the model input.

TABLE 5-15. INPUT SUMMARY FOR THE LOW-VOLATILITY LIQUID RELEASE EXAMPLE

Chemical Data (5.8.2)
From Appendix B

Release Type (5.8.3)
low volatility liquid

Continuous or Instantaneous Release Categories (5.8.4)
Continuous

Emission Rate (5.8.7)
0.005365 kg/s (total), 0.004272 kg/s (hydrogen chloride)

Release Temperature (5.8.8)
291.48 °K

Vapor Fraction (5.8.9)
F_{rel} = 0 (flash) All emission is in vapor state

Initial Concentration (5.8.10)
f_a = 0.9689
f_w = 0.0185
f_i = 0.01258

Density (5.8.11)
ρ_{rel} = 1.204 kg/m^3
ρ_a' = 1.203 kg/m^3

Release Diameter or Area (5.8.12)
Diameter = 8.256 m

Release Buoyancy (5.8.13)
C_ρ = 136.7 > 6 (do not use dense gas model)

Release Height (5.8.14)
0.0 m

Ground Surface Temperature (5.8.15)
Same as ambient

Averaging Time (5.8.16)
One hour

TABLE 5-15. (CONTINUED)

Meteorology (5.8.17)

Wind Speed and Direction
45° @ 5 mph (2.24 m/s)
Measurement height = 10.7 m
Speed @ 10 m = 2.23 m/s

Stability Class
C

Surface Roughness Length
Z0 = 0.01 m

Ambient Temperature, Relative Humidity, and Pressure
Temperature = 65°F (291.48 °K)
Relative Humidity = 58%
Pressure = 1 atm (101325 Pa)

Output Definition (5.8.18)
ERPG concentrations
Minimum distance of concern = 450 ft (137.2 m)

Observable Data (5.8.1)
See Table 5-16

TABLE 5-16. OBSERVABLE DATA SUMMARY FOR THE LOW-VOLATILITY LIQUID RELEASE EXAMPLE

Release Description

Species: Hydrogen chloride 30% wt solution
Container: Vertical cylinder

Diameter:	12 ft (3.66 m)
Height of liquid:	9 ft (2.74 m)
Total liquid:	63126 lb (28634 kg)
Temperature:	65°F (291.48 °K)
Pressure:	1 atm (absolute) (1.01325×10^5 Pa)
Bounding dike:	24 x 24 ft, 576 ft^2 (53.54 m^2)

Hole site:

Inner diameter:	0.75 inch (0.0191 m)
Area:	3.0680×10^{-3} ft^2 (2.85×10^{-4} m^2)
Height of hole:	1 ft (0.30 m)

Nearest boundary: 450 ft (137.2 m)

Meteorology:

Temperature:	65°F (291.48 °K)
Relative Humidity:	58%
Pressure:	1 atm (101325 Pa)
Wind Speed:	5 mph (2.24 m/s)
Wind Direction:	Northeast (45°)
Measurement hgt:	35 ft (10.7 m)
Surface Roughness:	0.01 m
Cloud cover:	3/8
Time:	Late-afternoon

5.8.4 Continuous or Instantaneous Release Categories

In this example, the emission rate into the atmosphere is 0.005365 kg/s (from Section 5.8.8). The duration of the release is how long it takes for the liquid to escape the container. There is 28634 kg liquid in the containerat a depth of 2.74 meters. The hole is at a height of 0.3 meters above the container bottom. This means that the fraction of liquid that remains in the container after the liquid stops being released is 0.3/2.74. The duration of the release (t_d) then is:

$$t_d = \frac{(1 - (0.3m/2.74m)))28634kg}{0.005365\frac{kg}{s}}$$

$$= 4752822s$$

$$= 1320 \text{ hours}$$

There is, however, another emission rate, that of the liquid coming from the container. Its duration is calculated as:

$$t_d = \frac{(1 - (0.3m/2.74m)))28634kg}{1.273\frac{kg}{s}}$$

$$= 20031 \text{ s}$$

$$= 5.56 \text{ hours}$$

For a non-source-term model, the value of t_d must be compared either to the advection time to a receptor or to the time it takes a concentration of interest to reach the maximum downwind distance. Using the formula in Section 4.4 for t_{trav}, and assuming a wind speed of 5 mph (2.24 m/s) and a distance of 450 ft (137.2 m), the advection time is calculated at 122 seconds. Since both emission durations are longer than the time required to reach the downwind point of interest, the release is considered continuous.

For a source-term model, the two values of t_d also are sufficiently long to treat this as a continuous release for most receptors.

5.8.5 Release-class-specific Calculations

The flow chart showing the calculations of input for a single-phase low volatility liquid release is presented n Figures 4-5 and 4-6.

5.8.6 Determination of Choked Flow for Gas Releases

This determination is not required since it is a low volatility liquid release.

5.8.7 Emission Rate

There are two emission rates of importance in a low volatility liquid release. The first is the emission rate of the liquid as it releases from the container. The second is the evaporation rate from the pool that forms. These two emission rates must be compared to determine which one is the limiting emission.

To calculate the emission rate from the container, the same technique is followed as for a high volatility spill (Section 4.7.7). First, the storage pressure (p_{sv}) must be calculated using:

$$p_{sv} = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_s}\right)\right]$$

$$p_{sv} = 101325\text{Pa} \exp\left[\frac{(2.3549\text{x}10^6\text{J/kg})(21.24\text{kg/kmol})}{(8314\text{J/kmol°K})}\left(\frac{1}{370.2\text{°K}} - \frac{1}{291.48\text{°K}}\right)\right]$$

$$= 1.2579\text{x}10^3\text{Pa}$$

Next, the pressure at the exit hole must be calculated. This is done by the equation:

$$P_h = \max(p_a, p_{sv}) + \rho_s g H_l$$

or, in this example,

$$P_h = 1.01325\text{x}10^5\text{Pa} + (993.30\text{kg/m}^3)(9.806\text{m/s}^2)(2.44\text{m})$$

$$= 1.2509\text{x}10^5\text{Pa}$$

Since the storage pressure (p_{sv}) is less than the ambient pressure (p_a), the maximum is taken as 1 atm. Also note that the stored liquid density is assumed to be that at the normal boiling point, rather than at the storage temperature. This assumption was made as a matter of convenience instead of approximating through extrapolation of the actual liquid density using assumed temperature dependencies. The error is probably minimal in comparison to other assumptions in the emission rate calculation.

The term β (as defined in Section 4.7.7) approaches zero in this release from a tank since the area of the hole is very much smaller than the area of the tank. This means that K is equal to C (0.65). The equation in Section 4.7.7 can then be written as:

$$E = CA_o\left[2\rho_s(p_h - p_a)\right]^{\frac{1}{2}}$$

and

$$E = (0.65)(2.85\text{x}10^{-4}\text{m}^2)$$

$$[2(993.30\text{kg/m}^3)((1.2509\text{x}10^5\text{Pa}) - (1.01325\text{x}10^5\text{Pa}))]^{\frac{1}{2}}$$

$$= 1.273 \text{ kg/s}$$

Finally, the maximum pool evaporation rate must be calculated and compared to the container emission rate. Whichever emission rate is the smaller is the limiting emission rate. The pool evaporation rate (E_{pool} in Section 4.7.8) is calculated from:

$$E_{pool} = 6.94\text{x}10^{-7}(1 + 0.0043(T_{rel} - 273.15)^{*2})U_r^{0.75}A_pM\frac{p_v}{p_{vh}}$$

Before E_{pool} can be calculated, three parameters must be known. One of the parameters, release temperature (T_{rel}), is determined in Section 5.8.8 as 291.48 °K. The other two, p_v and p_{vh}, need to be calculated here. As discussed in Section 4.7.8, the emission E_{pool} should be calculated at both T_{rel} and T_a; the larger value of E_{pool} should then be used. In this example, however, T_{rel} and T_a are the same, so only one calculation is required.

The parameter p_v is the vapor pressure of the entire hydrochloric acid solution. It is the sum of the partial pressures of the water vapor and the anhydrous hydrogen chloride over the solution. The pool emission rate must be compared to the liquid emission rate from the container. Since the liquid is made up of both water and hydrogen chloride, the pool emission rate should take into account both species. From the data base, at T_{rel}:

$$p_v(HCl) = 1274.2\text{Pa}$$
$$p_v(H_2O) = 655.8\text{Pa}$$
$$p_v = 1930.0\text{Pa}$$

If this were not a mixture, the parameter p_v is calculated from the equation:

$$p_v = 101325\text{Pa} \exp\left[\frac{\lambda M}{R}\left(\frac{1}{T_b} - \frac{1}{T_{rel}}\right)\right]$$

The parameter p_{vh} is the vapor pressure of hydrazine at T_{rel}. It can be calculated from:

$$p_{vh} = \exp\left[76.8580 - \frac{7245.2}{T_{rel}} - 8.22\ln(T_{rel}) + 0.0061557T_{rel}\right]$$

$$= \exp\left[76.8580 - \frac{7245.2}{291.48°K} - 8.22\ln(291.48°K)\right.$$

$$\left. + 0.0061557(291.48°K)\right]$$

$$= 1270.8\text{Pa}$$

This makes the value of E_{pool}:

$$E_{pool} = 6.94\text{x}10^{-7}(1 + 0.0043(291.48°K - 273.15°K)^{*2})(2.24\text{m/s})^{0.75}$$
$$(53.54\text{m}^2)(21.24\text{kg/kmol})\frac{1930.0\text{Pa}}{1270.8\text{Pa}}$$

which gives a value of 0.005365 kg/s. Thus, E_{pool} is less than E. The pool size is at its maximum of 53.54 m^2. An important point about the emission rate is that it includes the emissions of both water vapor and hydrogen chloride. The actual emission rate used in a model should be for the hydrogen chloride alone. The emission rates of the water and hydrogen chloride vapors are in the same ratio as their weight per cent ratio. This means that the hydrogen chloride emission rate (E_{HCl}) can be calculated using:

$$E_{HCl} = \left(\frac{p_v(HCl)}{p_v}\right)\left(\frac{M_{HCl}}{M_T}\right)E_{pool}$$

$$E_{HCl} = \left(\frac{1274.2Pa}{1930.0Pa}\right)\left(\frac{36.461kg/kmol}{30.23kg/kmol}\right)(0.005365kg/s)$$

$$= 0.004272kg/s$$

where: M_{HCl} = molecular weight of hydrogen chloride (36.46 kg/kmol); and

M_T = average molecular weight of the water vapor and hydrogen chloride mixture.

$$M_T = \left(\frac{p_v(HCl)}{p_v}\right)M_{HCl} + \left(\frac{p_v(H_2O)}{p_v}\right)M_{H_2O}$$

$$= \left(\frac{1274.2Pa}{1930.0Pa}\right)(36.46kg/kmol) + \left(\frac{655.8Pa}{1930.0Pa}\right)(18.02kg/kmol)$$

$$= 30.19kg/kmol$$

5.8.8 Release Temperature

The liquid is released at its storage temperature. For a conservative approach, the release temperature should be assumed to be either the storage or ambient temperature, whichever is higher. Both of these temperatures are the same in this example, so the release temperature (T_a) is assumed to be 291.48 °K.

5.8.9 Vapor Fraction

The value of F_{rel} was determined to be zero in the process of determining the release class (Section 5.8.3). That is, no flashing occurred.

5.8.10 Initial Concentration

The method for calculating initial concentration is given in Section 4.10.2. The release in the current example has all three components

allowed: air, water vapor, and chemical of interest. The molar fractions of each of these components must be determined. The f_i parameter is the ratio of the vapor pressure of the hydrogen chloride to the ambient pressure. The partitioning of the emission is of particular importance because, in the air, the chemical of interest is hydrogen chloride, not water vapor. Therefore, only the hydrogen chloride vapor pressure is used in determining the initial concentration of the chemical of interest. This gives:

$$f_i = \frac{p_v(HCl)}{p_a}$$

$$= \frac{1274.2Pa}{101325Pa}$$

$$= 0.01258$$

The remaining components are just the air and water vapor. Water vapor comes from both the ambient atmosphere and the source. The easiest approach is to solve for the molar fraction of air and then determine the water vapor fraction by subtracting the sum of f_i and f_a from 1.

The molar fraction in the atmosphere that is not taken up from the emission species is $(1 - f_i')$ where f_i' is the molar fraction due to the water vapor and hydrogen chloride being emitted from the source. The value of f_i' is calculated just as f_i was calculated, namely:

$$f_i' = \frac{p_v(HCl) + p_v(H_2O)}{p_a}$$

$$= \frac{1930.0Pa}{101325Pa}$$

$$= 0.01905$$

The molar fractions in the ambient air of air and water vapor also need to be calculated. The water vapor fraction is a function of the temperature and

relative humidity. The water vapor molar fraction in the ambient air (f_w') is:

$$f_w = \left(\frac{RH}{100}\right) e_s$$

where: e_s is calculated from:

$$\log_{10} e_s = 6.3994 - \frac{2353}{T}$$

$$= 6.3994 - \frac{2353}{291.48°K}$$

which leads to a value of e_s of 0.0212. With a relative humidity of 58%, this leads to a value of f_w' of 0.0123. The value of molar air fraction in the atmosphere (f_a') is the complement of f_w', or 0.9877. The molar fraction of air in the emission is:

$$f_a = f_a'(1 - f_i')$$

$$= 0.9877(1 - 0.01905)$$

$$= 0.9689$$

and the molar fraction of water vapor is:

$$f_w = 1 - (f_i + f_a)$$

$$= 1 - (0.01258 + 0.9689)$$

$$= 0.0185$$

In summary:

f_a = 0.9689
f_w = 0.0185
f_i = 0.01258

5.8.11 Density

The density input parameters required are calculated using the formulas given in Section 4.11. Since the emission has the three components (air, water vapor, and hydrogen chloride), each component contributes to the density of the emission. The first step in calculating the overall density is to calculate the individual densities of the three components. Since only the gas phase of hydrogen chloride is being emitted, ρ_i is equal to ρ_g. The densities of the three components, if they were the only components in the release, would be given by:

$$\rho_i = \rho_g$$

$$= \frac{p_a M_i}{RT_{rel}}$$

$$= \frac{(101325\text{Pa})(36.47\text{kg/kmol})}{(8314\text{J/kmol°K})(291.48\text{°K})}$$

$$= 1.525\text{kg/m}^3$$

$$\rho_a = \frac{p_a M_a}{RT_{rel}}$$

$$= \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol°K})(291.48\text{°K})}$$

$$= 1.208\text{kg/m}^3$$

and finally,

$$\rho_w = \frac{p_a M_w}{RT_{rel}}$$

$$= \frac{(101325\text{Pa})(18.02\text{kg/kmol})}{(8314\text{J/kmol°K})(291.48\text{°K})}$$

$$= 0.7534\text{kg/m}^3$$

Note that the molecular weight for pure hydrogen chloride gas was used rather than the mixture molecular weight. The mixture molecular weight is for the liquid phase. Only the gas phase emissions into the atmosphere are being considered here. The release density (ρ_{rel}) is then given by as described in Section 4.11):

$$\rho_{rel} = \left(\frac{f_a M_a}{M_T \rho_a} + \frac{f_w M_w}{M_T \rho_w} + \frac{f_i M_i}{M_T \rho_i}\right)^{-1}$$

where:

$$M_T = f_a M_a + f_w M_w + f_i M_i$$

In this case:

$$M_T = (0.9689)(28.9\text{kg/m}^3) + (0.0185)(18.02\text{kg/m}^3)$$

$$+ (0.01258)(36.47\text{kg/m}^3)$$

$$= 28.79\text{kg/m}^3$$

and so,

$$\rho_{rel} = \left(\frac{(0.9689)(28.9\text{kg/kmol})}{(28.79\text{kg/kmol})(1.208\text{kg/m}^3)} + \frac{(0.0185)(18.02\text{kg/kmol})}{(28.79\text{kg/kmol})(0.7534\text{kg/m}^3)} + \frac{(0.01258)(36.47\text{kg/kmol}}{(28.79\text{kg/kmol})(1.525\text{kg/m}^3)} \right)^{-1}$$

$$= 1.204\text{kg/m}^3$$

The fact that the release comprises three components also complicates the calculation of the actual ambient air density. In the above calculation, a value was calculated for ρ_a, but that value was for dry air only. The ambient air density needs to be calculated in the same manner as the release density, except that the f_a' and f_w' are used instead of f_a and f_w. First, the apparent molecular weight of the air is given by:

$$M_a' = f_a' M_a + f_w' M_w$$

$$= (0.9877)(28.9\text{kg/kmol}) + (0.0123)(18.02\text{kg/kmol})$$

$$= 28.77\text{kg/kmol}$$

Then the ambient air density is given by the equation:

$$\rho_a' = \left(\frac{f_a' M_a}{M_a' \rho_a} + \frac{f_w' M_w}{M_a' \rho_w} \right)^{-1}$$

$$= \left(\frac{(0.9877)(28.9\text{kg/kmol})}{(28.77\text{kg/kmol})(1.208\text{kg/m}^3)} + \frac{(0.0123)(18.02\text{kg/kmol})}{(28.77\text{kg/kmol})(0.7534\text{kg/m}^3)} \right)^{-1}$$

$$= 1.203\text{kg/m}^3$$

5.8.12 Release Diameter or Area

Part of this release is from an evaporating pool. The exit velocity of evaporation is negligible. The release diameter is simply the diameter of the pool. Assuming that the pool is circular, this leads to:

$$D_{rel} = \sqrt{\frac{4}{\pi}A_0}$$

$$= \sqrt{\frac{4}{\pi}(53.54m^2)}$$

$$= 8.256m$$

5.8.13 Release Buoyancy

The release buoyancy is used to determine if a dense gas model should be used, rather than a neutral or positive buoyancy model. The first step is to compare ρ_{rel} to ρ_a'. If ρ_{rel} is less than or equal to ρ_a, the release is not to be treated as a dense gas release. In this example, ρ_{rel} is 1.204 kg/m^3 and ρ_a is 1.203 kg/m^3. The value for ρ_a is actually the value of ρ_a', which was calculated in Section 5.8.11 and represents the moist ambient density. Since ρ_{rel} is greater than ρ_a, the next step is to apply the denser-than-air criterion.

The calculation of the denser-than-air criterion is based on the formula in Section 4.13.1, since this release is classified as a continuous release (Section 5.8.4). The criterion (C_ρ) is given by:

$$C_\rho = \frac{U_r}{\left[\frac{g(E/\rho_{rel})}{D_{rel}}\left(\frac{\rho_{rel} - \rho_a}{\rho_a}\right)\right]^{\frac{1}{3}}}$$

$$C_\rho = (2.24\text{m/s})\left[\frac{(9.806\text{m/s}^2)(0.005365\text{kg/s}/1.204\text{kg/m}^3)}{8.256\text{m}}\left(\frac{1.204\text{kg/m}^3 - 1.203\text{kg/m}^3}{1.203\text{kg/m}^3}\right)\right]^{-\frac{1}{3}}$$

$$= 136.7$$

Since $C_\rho > 6$, a dense gas model should not be used. In most low volatility spills, this will be the case. In the process of arriving at this point, however, most of the input for a non-dense gas model has also been developed.

5.8.14 Release Height

The hole in the tank is 0.3 meters above the ground. The liquid spills out of the hole onto the ground and evaporates. The gas phase of the release enters the atmosphere at the pool level, which is at ground level. Therefore, the release height is zero.

5.8.15 Ground Surface Temperature

No information is given on the ground surface temperature. Therefore, the ground surface temperature is assumed to be equal to the ambient temperature, or 291.48 °K.

5.8.16 Averaging Time

The averaging time is specified as 1 hour to make the model-predicted concentrations comparable to the ERPG (Emergency Response Planning Guideline) concentrations.

5.8.17 Meteorology

Wind Speed and Direction

The wind speed and direction are assumed either to be available from on-site meteorological equipment or are representative of average conditions at the site. The wind speed in this example is given as 5 mph (2.24 m/s). The wind direction is northeast (45°). The measurement height is given as 10.7 meters. To determine the greatest specific impact, multiple wind speeds may be required in conjunction with multiple stability classes.

Stability Class

The stability class is not given explicitly. However, a class can be estimated from the information provided using the method described in the Workbook, Section 3.1.2. In this example, there is 3/8 cloud coverage, and the release is in the late-afternoon, which indicates that the insolation is slight. As shown in Table 3-2 of the Workbook, the stability class estimated for a wind speed of 2.24 m/s at 10 meters during a day with slight insolation is "C."

Surface Roughness Length

In keeping with the value suggested for modeling done for planning purposes, the surface roughness is assumed to be 0.01 meters.

Wind Speed at 10 m Altitude

With the surface roughness, stability class, and wind speed at 10.7 meters, the wind speed at 10 meters can be estimated. Using the equation in 4.17.3:

$$u = u_1\left(\frac{z}{z_1}\right)^p$$
$$= 2.24\text{m/s}\left(\frac{10.0\text{m}}{10.7\text{m}}\right)^{0.06}$$
$$= 2.23\text{m/s}$$

This wind speed at 10 meters altitude still indicates a "C" stability class.

Ambient Temperature, Relative Humidity, and Pressure

The ambient temperature, relative humidity, and pressure are all assumed to be available from on-site equipment. See the observable data, Table 5-16.

5.8.18 Output Definition

The concentration levels to specify when generating output should be the three ERPG (Emergency Response Planning Guideline) concentrations given in the hydrogen chloride data table in Appendix B. The actual impact values to be predicted are listed in Section 7.0.

SECTION 6

MODEL INPUT USED

This section describes the input used by each model for each release class. Any differences between input derived in Section 5 for a given release class and that required by a specific model are noted. Example output from each of the models is provided in Section 7, as well as how to find impact estimates.

The computer models discussed in this document operate in one of two ways. "Batch type" models accept input by reading a file containing the numerical values of required parameters. "Interactive type" models, accept input as the user enters parameter values through input screens presented by the program.

In a batch model, the input must be created before the model is run. The input is simply a list of numbers arranged in a set order. In an interactive model, the input is entered while the program is running by "filling in the blanks" on input screens. Interactive models often allow the user to enter the input in any order. In this section, the input used by the batch models is given as lists to resemble what the input would need to look like for the model to run. The input for the interactive models is listed in a more descriptive table.

Of the models considered in this document, ADAM and HGSYSTEM require the most discussion. In the case of ADAM, there are some outside calculations that may be required for a simulation. The outside calculations are unique to ADAM and not provided in Sections 4 or 5. The outside calculations are described in this section. In the case of HGSYSTEM, since it is made up of a number of models run in series, there can be more than one input stream per

simulation. Normally, the output from one HGSYSTEM model, which becomes the input for another HGSYSTEM model, does not require user interaction. However, since the input may be varied by the user during a specific simulation, all intermediate input files (called "link" files) are shown.

6.1 ADAM

The ADAM model is an interactive model. The input is entered in a screen-by-screen method. The input for each scenario modeled by ADAM is given in Tables 6-1 through 6-6. Only six of the scenarios were simulated. The Single-Phase Gas Release (Unchoked) was not modeled because ADAM cannot model stack releases and does not account for non-anhydrous chemical releases. The Single-Phase Liquid Release (Low Volatility) was not modeled because ADAM only simulates heavier-than-air releases. Even if the Single-Phase Liquid Release (Low Volatility) scenario resulted in a heavier-than-air release it still would not have been modeled because ADAM does not account for non-anhydrous chemical releases.

Since ADAM was designed and developed specifically to satisfy the needs of the Air Force, the capabilities of the model are very specific regarding the scenarios that can be modeled. Certain technical details about the ADAM model that need to be taken into account when preparing input are:

- All releases are assumed to occur at ground level. Elevated releases are not accounted for.
- In the case of liquids and liquified gases, storage tanks are assumed to be cylinders full of liquid with axes normal to the ground. The bottom of the tank is assumed to be at ground level.
- Tank storage pressure and temperature are assumed to remain constant throughout a release. Tank blow-down is not accounted for.
- The physical and thermodynamic state of a chemical is calculated by ADAM and fixed by specifying the storage temperature and pressure.

TABLE 6-1. INPUT PARAMETERS FOR THE TWO-PHASE ETHYLENE OXIDE GAS RELEASE (CHOKED) (Reference Table 5-2)

Chemical Name:	Ethylene Oxide (C_2H_4O)
Run Title:	EOX1
Data File:	EOX1.DAT
Plot File:	EOX1.PLT
Release:	Hole in Pipe
Release Type:	Continuous
Calculate Source Terms?	Yes
Pipe Diameter:	0.0762 m (3 in.)
Fluid Velocity in Pipe:	Arbitrary for gas flow
Hole diameter:	0.01347 m (.53 in.)
Storage Temperature:	306.67 °K (92.2 °F)
Storage Pressure:	2.02×10^5 Pa (2.0 atm abs)
Meteorology:	
Temperature:	287.52 °K (57.2 °F)
Relative Humidity:	62 %
Pressure:	101325 Pa (1 atm abs)
Wind Speed:	5.37 m/s (12.0 mph)
Measurement Height:	4.57 m (15.0 ft)
Wind Direction:	Northeast (45°)
Surface Roughness:	0.01 m
By-pass Atmospheric calculation?	Yes
Wind Speed @ 10 meters:	6.04 m/s (13.5 mph)
Stability Class:	C (2.5 index)
Concentration Contour:	800 ppm IDLH[1]
Averaging Time:	30 minutes
Include Variable Wind Effects:	No
Minimum Distance of Interest:	200 m (656.2 ft)
Time & Location Parameters:	N/A
Scaling:	Automatic

[1]Because of the currently set up distance step sizes in ADAM distances calculated to LEL & UEL tend to be inaccurate

TABLE 6-2. INPUT PARAMETERS FOR THE TWO-PHASE ETHYLENE OXIDE GAS RELEASE (UN-CHOKED) (Reference Table 5-4)

Chemical Name:	Ethylene Oxide (C_2H_4O)
Run Title:	EOX2
Data File:	EOX2.DAT
Plot File:	EOX2.PLT
Release:	Hole in Pipe
Release Type:	Continuous
Calculate Source Terms?	Yes
Pipe Diameter:	0.0762 m (3 in.)
Fluid Velocity in Pipe:	Arbitrary for gas flow
Hole diameter:	0.0127 m (.5 in.)
Storage Temperature:	298.16 °K (76.9 °F)
Storage Pressure:	151990. Pa (1.5 atm abs)
Meteorology:	
Temperature:	296.5 °K (74.0 °F)
Relative Humidity:	37 %
Pressure:	101325 Pa (1 atm abs)
Wind Speed:	2.68 m/s (6.0 mph)
Measurement Height:	6.09 m (20.0 ft)
Wind Direction:	Southwest (225°)
Surface Roughness:	0.01 m
By-pass Atmospheric calculation?	Yes
Wind Speed @ 10 meters:	2.89 m/s (6.47 mph)
Stability Class:	C (2.5 index)
Concentration Contour:	800 ppm IDLH[2]
Averaging Time:	30 minutes
Include Variable Wind Effects:	No
Minimum Distance of Interest:	300 m (984.3 ft)
Time & Location Parameters:	N/A
Scaling:	Automatic

[2]Because of the currently set up distance step sizes in ADAM distances calculated to LEL & UEL tend to be inaccurate

TABLE 6-3. INPUT PARAMETERS FOR THE TWO-PHASE PRESSURIZED LIQUID CHLORINE RELEASE (Reference Table 5-6)

Chemical Name:	Chlorine (Cl_2)
Run Title:	CLX1
Data File:	CLX1.DAT
Plot File:	CLX1.PLT
Release:	Tank
Release Type:	Instantaneous
Calculate Source Terms?	Yes
Tank Diameter:	0.762 m (30.0 in.)
Volume of Chemical:	0.152 m^3
Storage Temperature:	294.3 °K (70.0 °F)
Storage Pressure:	6.95×10^5 Pa (6.86 atm abs)
Meteorology:	
Temperature:	294.3 °K (70.0 °F)
Relative Humidity:	50 %
Pressure:	101325 Pa (1 atm abs)
Wind Speed:	4.47 m/s (10.0 mph)
Measurement Height:	10 m (32.81 ft)
Wind Direction:	South (180°)
Surface Roughness:	0.01 m
By-pass Atmospheric calculation?	Yes
Wind Speed @ 10 meters:	4.47 m/s (10.0 mph)
Stability Class:	C (2.5 index)
Concentration Contour:	1 ppm (STEL)
Averaging Time:	15 minutes
Include Variable Wind Effects:	No
Minimum Distance of Interest:	100 m (328.1 ft)
Time & Location Parameters:	N/A
Scaling:	Automatic

TABLE 6-4. INPUT PARAMETERS FOR THE TWO-PHASE PRESSURIZED LIQUID SULFUR DIOXIDE RELEASE (Reference Table 5-8)

Chemical Name:	Sulfur Dioxide (SO_2)
Run Title:	SFD1
Data File:	SFD1.DAT
Plot File:	SFD1.PLT
Release:	Hole in Pipe
Release Type:	Continuous
Calculate Source Terms?	Yes
Pipe Diameter:	0.05 m (2 in.)
Hole diameter:	0.0127 m (.5 in.)
Fluid Velocity:	28.0 m/s (91.9 ft/s)
Storage Temperature:	323.15 °K (122 °F)
Storage Pressure:	1.52×10^6 Pa (15 atm abs)
Meteorology:	
Temperature:	291.15 °K (64.4 °F)
Relative Humidity:	42 %
Pressure:	101325 Pa (1 atm abs)
Wind Speed:	3.13 m/s (7.0 mph)
Measurement Height:	6 m (19.7 ft)
Wind Direction:	Northeast (45°)
Surface Roughness:	0.01 m
By-pass Atmospheric calculation?	Yes
Wind Speed @ 10 meters:	3.38 m/s (7.56 mph)
Stability Class:	E (4.5 index)
Concentration Contour:	5 ppm (STEL)
Averaging Time:	15 minutes
Include Variable Wind Effects:	No
Minimum Distance of Interest:	80 m (262.5 ft)
Time & Location Parameters:	N/A
Scaling:	Automatic

TABLE 6-5. INPUT PARAMETERS FOR THE SINGLE-PHASE ANHYDROUS HYDROGEN FLUORIDE GAS RELEASE (CHOKED) (Reference Table 5-10)

Chemical Name:	Hydrogen Fluoride (HF)
Run Title:	HFX1
Data File:	HFX1.DAT
Plot File:	HFX1.PLT
Release:	Severed Pipe
Release Type:	Continuous
Calculate Source Terms?	Yes
Pipe Inner Diameter:	0.0635 m
Fluid Velocity in Pipe:	Arbitrary for gas flow
Storage Temperature:	365.0 °K (197.0 °F)
Storage Pressure:	2.0397×10^5 Pa (2.01 atm abs)
Meteorology:	
Temperature:	295.15 °K (71.6 °F)
Relative Humidity:	45 %
Pressure:	101325 Pa (1 atm abs)
Wind Speed:	6.26 m/s (14.0 mph)
Measurement Height:	6.096 m (20.0 ft)
Wind Direction:	Northwest (315°)
Surface Roughness:	0.01 m
By-pass Atmospheric calculation?	Yes
Wind Speed @ 10 meters:	6.74 m/s (15.1 mph)
Stability Class:	D (3.5 index)
Concentration Contour:	6 ppm (STEL)
Averaging Time:	15 minutes
Include Variable Wind Effects:	No
Minimum Distance of Interest:	76.2 m (250 ft)
Time & Location Parameters:	N/A
Scaling:	Automatic

TABLE 6-6. INPUT PARAMETERS FOR THE SINGLE-PHASE LIQUIFIED ETHYLENE OXIDE RELEASE (Reference Table 5-14)

Chemical Name:	Ethylene Oxide (C_2H_4O)
Run Title:	EOX3
Data File:	EOX3.DAT
Plot File:	EOX3.PLT
Release:	Tank Release
Release Type:	Continuous
Calculate Source Terms?	Yes
Container:	Vertical Axis Cylinder
Diameter:	3.5 m (11.4 ft)
Volume of Liquid:	26.9 m^3 (950.0 ft^3)
Height of Hole:	0.5 m (1.64 ft)
Hole diameter:	0.00635 m (0.25 in)
Storage Temperature:	283.85 °K (51.3 °F)
Storage Pressure:	1.01×10^5 Pa (1.0 atm abs)
Meteorology:	
Temperature:	301.15 °K (82.4 °F)
Relative Humidity:	50 %
Pressure:	101325 Pa (1 atm abs)
Wind Speed:	2.0 m/s (4.47 mph)
Measurement Height:	10 m (32.81 ft)
Wind Direction:	North (0°)
Surface Roughness:	0.01 m
By-pass Atmospheric calculation?	Yes
Wind Speed @ 10 meters:	2.0 m/s (4.47 mph)
Stability Class:	E (4.5 index)
Concentration Contour:	800 ppm IDLH[3]
Averaging Time:	30 minutes
Include Variable Wind Effects:	No
Minimum Distance of Interest:	100 m (328.1 ft)
Time & Location Parameters:	N/A
Scaling:	Automatic

[3]ERPG limits are not available

- Mechanical losses and two-phase flows in pipes are not accounted for.

  The mass flow rate throughout a release is assumed to be constant and equal to the initial flow rate. All releases occur in the direction of the wind and chemical dispersion continues until the concentration of interest is reached. Limited duration releases are not accounted for, i.e., continuous releases of finite quantities (in the tank) are not modeled exactly.

- Dispersion of chemicals not in the ADAM list of chemicals is modeled as a non-reactive chemical release, provided the thermodynamic property data are included in standard database format.

Presently, there are eight anhydrous chemicals in the model. Materials not appearing in the standard ADAM chemical selection may be modeled if:

1) the material is anhydrous (pure, non-aqueous);

2) the vapors produced after the release of the chemical into the atmosphere are heavier than air;

3) the material is non-reactive upon release, i.e., it does not polymerize, undergo spontaneous dissociation, or combine with ambient moisture to form other species, and;

4) physical and thermodynamic properties of the material are available and are similar to those of chlorine.

If the above conditions are met, a database of physical properties of the chemical to be modeled must be compiled, the name of which is assigned the file name for chlorine (CLXPORP.DAT). The actual chlorine properties file must then be moved from the ADAM directory and saved by the user, and the new chemical file substituted for it. It is important that the original CLXPROP.DAT file be saved so that it can replace the new chemical file in case chlorine is to be modeled in the future. Modeling the new material simply requires choosing the chemical "Chlorine" from the ADAM chemicals list. This method was implemented for the ethylene oxide releases.

Although the method of modeling alternate materials is rather simplistic, the format of the properties data base is extremely structured and

specific. Deviation from the file format will cause unpredictable model operation and results. If the modeling of alternate materials is desired, the providers of ADAM should be consulted for assistance.

ADAM has the capability to calculate dispersion model input parameters (source-term mode) based on observable data (storage and atmospheric conditions) or to provide for the input of these values calculated by other means (non-source-term mode). To run ADAM in the non-source-term mode requires that the following parameters be provided:

- Width and depth of the released plume;
- Heat rate to source plume; and
- Mass rate of air entrained initially.

The methods for calculating these parameters have not been provided in this document. Since these parameters are internally calculated by ADAM from obsevable data, all the release classes were simulated using the ADAM source-term mode of operation.

In the title of each of the tables listing the ADAM input is a reference table. This reference table refers to the table in Section 5 from which the input was derived. Since all the simulations were done with the source-term mode of operation, all the tables refered to are the observable data tables rather than the calculated input tables.

Extra Calculations

Some calculations are needed to create input outside the ADAM model either because the input is unique to ADAM or because the ADAM model developer suggests a method of calculation different from that presented in Section 4. Since these calculations or methods affect more than one release class, they are presented here as general calculations for ADAM. The input given in Tables 6-1 through 6-6 is only that which is used after a decision has been made as to whether the release should be treated as instantaneous or

continuous. As discussed below, it is suggested that ADAM be run assuming both conditions and then selecting the appropriate simulation. In the discussion of each release class, all input requiring calculation for both the instantaneous and continuous cases is presented.

Stability Class

In most cases it is desirable to over-ride atmospheric calculations and simply supply to the model the atmospheric stability category from which dispersion parameters are determined. The stability class can be determined from cloud cover and insolation information by following the guidance provided in the EPA Workbook, Section 3.1.2. Instead of the letter classification (A through F), ADAM uses a numerical index for stability. Stability class "A" is represented by an index between 0 and 1. Stability class "B" is represented by an index between 1 and 2, etc.

When over-riding atmospheric calculations, it is also necessary to input the wind speed at the standard meteorological reference height of 10 meters. In some cases, the wind speed may be listed in the scenario description at a height other than 10 meters. The method described here is what is used internally in ADAM, which is different from that described in Section 4.17.3. Assuming a logarithmic velocity distribution, the wind velocity at 10 meters (U_{10}) may be calculated by:

$$U_{10} = U_z \times \frac{\ln \frac{10}{z_0}}{\ln \frac{z}{z_0}}$$

where: U_z = wind speed at height z (m/s);

Z_0 = surface roughness (m); and

Z = height at which velocity U_z is measurement (m).

The Effect of the Vertical Axis Tank Assumption on Liquid and Liquified Gases

In ADAM, it is assumed that all tank releases are from cylindrical containers with their bases on the ground. That is, the cylinder's axis is vertical. If the tank has liquid in it, it is assumed to be full. Tanks that have horizontal axes must be simulated as if they were vertical. For a continuous liquid release from a tank, the rate at which the liquid escapes is determined by the pressure inside the tank and the column pressure due to the depth of liquid. To simulate in ADAM the rate at which a liquid releases from a horizontal cylinder, the depth of liquid in the horizontal cylinder must be equal to the depth of liquid in a vertical cylinder. This is done by specifying a vertical tank height equal to the depth of liquid (h_ℓ) in the cylinder.

Calculating the depth of liquid in a partially full horizontal cylinder is not trivial. If the volume of liquid in the horizontal cylinder is known, h_ℓ can be calculated iteratively from:

$$\frac{V_\ell}{L} = \frac{d^2}{4} \operatorname{Cos}^{-1}\left(\frac{d - 2h_\ell}{d}\right) - \left(\frac{d}{2} - h_\ell\right)\sqrt{dh_\ell - h_\ell^2}$$

where: V_ℓ = volume of liquid in tank (m^3);
L = tank length (m); and
d = tank diameter (m).

The only unknown value in the equation is h_ℓ. Therefore, the equation can be solved iteratively by solving for one of the h_ℓs values in the equation. To do this, assume a value of h_ℓ (for example, one half of d) and solve for a new value of h_ℓ. Use the new value to calculate another h_ℓ. Continue solving for new values of h_ℓ until two consecutive values of h_ℓ do not differ

significantly (perhaps one percent of $\dot{d}$). If the mass of liquid m_ℓ (kg) is known, the volume of liquid, V_ℓ (m^3), may be calculated by:

$$V_\ell = \frac{m_\ell}{\rho_\ell},$$

where the liquid density, ρ_ℓ (kg/m^3), is obtained from the chemical data in Appendix B.

The discussion above describes the calculation required for a continuous liquid release. For a continuous gas release, to simulate a horizontal cylinder under ADAM, it is only necessary that the vertical cylinder assumed in the model be of the same volume as the horizontal cylinder. When simulating an instantaneous release, the volume of liquid or gas released is required. For instantaneous releases of liquid or liquified gas from a tank, only the volume of material in the tank is significant. If an instantaneous release of compressed gas is being modeled, the volume of material specified should be the volume of gas at atmospheric pressure and the temperature of the gas released. Because only the volume is required for an instantaneous release, the shape of the container is not assumed in ADAM.

Pipe Flow Velocity

When using the pipe release option for liquids or liquified gases, the velocity of fluid in the pipe (which is assumed to be unaffected by friction) is a necessary input parameter. This variable is unique to ADAM and is not required by any of the other models in this document. If the mass flow rate is available for a given release, the liquid velocity, U_ℓ, may be determined by:

$$U_\ell = \frac{M_{flow}}{(\rho_\ell)(A_{pipe})}$$

where: M_{flow} = mass flow rate in pipe (kg/s);

ρ_ℓ = liquid density at chemical temperature (kg/m^3); and

A_{pipe} = inner cross sectional area of pipe (m^2).

In the case of a storage tank supplying a liquid or liquified gas pipe flow, the velocity in the pipe can be set equal to the fluid exit velocity at the tank/pipe connection. In this case, the tank liquid exit velocity, can be determined by:

$$U_\ell = (C_C)(C_V)\sqrt{2\left(\frac{P_{stor}-P_{atm}}{\rho_\ell} + g(h_\ell - h_h)\right)}$$

where:

C_C = contraction loss coefficient (.61);

C_V = velocity loss coefficient (.98);

P_{stor} = storage pressure (Pa);

P_{atm} = atmospheric pressure (Pa);

ρ_ℓ = liquid density at the storage temperature (kg/m^3);

h_ℓ = liquid height in tank (m); and

h_h = height of hole above ground level (bottom of tank) (m).

For a partially-full horizontal cylinder tank, the height of liquid, h_ℓ, should be set equal to a tank height that is calculated based on the tank diameter and volume of material modeled. This calculation is described in the preceding section on the "Vertical Axis Tank Assumption."

For gas pipe flows, the velocity of the gas at any point in the flowing stream is calculated based on the pressure, density, and ratio of specific heats at constant pressure and constant volume. Although the velocity parameter is available as input for gas flows in pipes, the value entered can be anything. ADAM ignores whatever is entered and internally calculates the velocity.

Instantaneous vs. Continuous Release

As suggested in Section 4.4, to determine whether a given release should be modeled as instantaneous or continuous, the release duration needs to be compared to the dispersion duration based on a continuous release. If the resulting dispersion duration is less than the release duration, the release should be treated as continuous. Conversely, if the dispersion duration is greater than the release duration, the release should be treated as instantaneous.

An alternative method of determining the release type is to compare the dispersion distance for both instantaneous and continuous cases. If the dispersion distance to the concentration of interest is greater for a continuous release than that for an instantaneous release, the release should be modeled as instantaneous; otherwise the release is continuous. This method requires running ADAM twice for each release. The volume of material released is required for each simulation.

In summary, to determine whether a release is continuous or instantaneous for a given scenario:

1) Model the scenario as a continuous release, recording the dispersion distance;

2) Model the scenario as an instantaneous release, recording the dispersion distance;

3) If the dispersion distance for the continuous case is less than that for the instantaneous case, the release can be treated as continuous; otherwise, it is instantaneous.

Two-phase Gas Release (Choked) Example

This scenario may be modeled utilizing the continuous release hole-in-a-pipe option. Since the scenario description assumes a pipe length of zero, the assumption of frictionless pipe flow in the ADAM source model is valid. In

using the pipe option, it is necessary to provide as input the pipe diameter and the fluid velocity. However, for gas flows, the velocity entered is arbitrary because it is internally calculated by the model.

ADAM assumes, by default, that at the chemical temperature of 303.67 °K (86.9 °F) and pressure of 202650 Pa (2.0 atm abs), the ethylene oxide exists in the pipe as a saturated liquid (ADAM assumes that all materials are in the liquid phase at the saturation temperature and pressure). To model the material as a saturated vapor, it is necessary to specify chemical temperature approximately 3 degrees higher than the saturation temperature. Therefore, in modeling the scenario as a continuous release, the temperature of the material must be specified as 306.67 °K.

For an instantaneous release, ADAM assumes that the temperature of the ethylene oxide gas in the atmosphere (right after release) is equal to the ambient temperature of 287.2 °K. The volume of ethylene oxide at atmospheric conditions is determined and modeled as equivalent to the instantaneous volume.

Since ADAM models only ground level releases, it is assumed that the pipe height relative to the ground is zero (i.e., the height of 12 feet cannot be accounted for in ADAM). Also, since fixed duration continuous releases are not accounted for, the plume is assumed to exist for the entire duration over which the contour of the specified concentration is achieved.

For the given release conditions and a specified concentration of interest of 30,000 ppm LEL, the mode of output from ADAM suggests that the source concentration upon mixing with entrained air is at least lower than the 30,000 ppm limit of interest. In this case, dispersion calculations were aborted and the predicted dispersion distance was output as zero meters. These results indicate that for a 30,000 ppm concentration (and any concentration higher), a toxic vapor cloud hazard does not exist. To illustrate the method by which this scenario is modeled, the IDLH limit of 800 ppm is used.

- Wind speed at 10 meters. Based on a wind speed of 5.37 m/s (12.0 mph) at 4.57 m (15.0 ft), a surface roughness of .01 meters, and a logarithmic wind velocity profile, the wind speed at 10 meters is:

$$U_{10m} = 5.37 \text{ m/s} \times \frac{\ln \frac{10 \text{ m}}{.01 \text{ m}}}{\ln \frac{4.57 \text{ m}}{.01 \text{ m}}} = 6.06 \text{ m/s.}$$

- Instantaneously released volume. Assuming ideal gas behavior and that the temperature of the gas is equal to that ambient temperature, the in air volume of material that would be instantaneously released, based on 8 minutes and the flow rate calculated in Section 5.1.7 is:

$$V = \frac{(0.0634 \text{kg/s})(480 \text{s}) \left(\frac{8314 \text{J}}{\text{kmol}^\circ\text{K}}\right) (287.7^\circ\text{K})}{\left(\frac{44.053 \text{ kg}}{\text{kmol}}\right) (101325 \text{ Pa})} = 16.3 \text{ m}^3$$

This value would be used in modeling the release as instantaneous.

- Instantaneous or continuous release. The results of the simulation for this release indicate that the maximum downwind distance for a continuous and instantaneous release is 9 m and 248 meters, respectively. Based on the methodology described above, the release should be modeled as continuous.

Two-phase Gas Release (Unchoked) Example

With the exception of meteorological conditions, chemical temperature and pressure, and chocked flow, this scenario is essentially identical to the pipe release in the first release class example. In light of this, the discussion presented for the two-phase gas release (choked) example is also applicable here.

As in the two-phase gas release (choked) example, the temperature of the material must be specified at least 3 degrees higher than the saturation temperature (298.16 °K instead of 295.16 °K) in order for it to be modeled as a release of saturated vapor. Also, as in the previous scenario, the UEL and LEL limits were higher than the concentration at the source because of the chemical release and air entrainment. Likewise, for this scenario, dispersion calculations were aborted and the predicted dispersion distance was set to

zero. To illustrate the method of modeling this release, the IDLH limit of 800 ppm will be used.

- Wind speed at 10 meters. Based on a wind speed of 2.68 m/s (6.0 mph) at 6.09 m (20.0 ft), a surface roughness of .01 meters, and a logarithmic wind velocity profile, the wind speed at 10 meters is:

$$U_{10m} = 2.68 \text{ m/s} \times \frac{\ln \frac{10 \text{ m}}{.01 \text{ m}}}{\ln \frac{6.09 \text{ m}}{.01 \text{ m}}} = 2.89 \text{ m/s.}$$

- Instantaneous or continuous release. Assuming that the flow rate through the pipe hole would not be substantially less than that of the choked flow in the first release class example, and the fact that the continuous dispersion distance for this release is minimal (9 meters), the release in this scenario will be modeled as continuous.

Two-Phase Pressurized Liquid Example

This release scenario (as described in Section 5)involves mechanical losses and two-phase flow through a tube, which is not a release class that is within the capabilities of ADAM. However, if these phenomena are neglected (equivalent to assuming the pipe length is zero) the scenario can be modeled as a continuous release based on the severed pipe. In order to use this option correctly, the pipe diameter specified in ADAM must be set equal to the severed tube diameter described in the scenario. Since the severed pipe option requires the input of the liquid velocity in the pipe, the flow rate from the one-ton container must be calculated and the velocity determined from the resulting value. ADAM assumes the height of the pipe relative to ground is zero.

To model the release as instantaneous, it is necessary to input the tank diameter and volume of material released. The calculations are:

- Chemical density at 293.4 °K. Using the correlation[4] A+T*(B+T*C) where A=2170.0, B=-2.6, and C=0.0, the storage density is:

$$\rho_l\ (293.4°K) = 2170.0 + 294.3 \times (-2.6) = 1405.0\ \frac{kg}{m^3}.$$

- Initial volume of chemical. At the storage temperature of 293.4 °K, the total volume of chlorine is:

$$V_{ch} = \frac{226.8\ kg}{1405\ kg/m^3} = 0.161\ m^3.$$

Similarly, the volume of liquid remaining after the liquid level falls below the eductor is:

$$ch = \frac{13.6\ kg}{1405\ kg/m^3} = 0.009\ m^3$$

Therefore, the volume of liquid released is 0.152 m^3.

- Height of liquid in one ton container. For the one-ton container described in the scenario description, the liquid height based on 500 lbs of liquid ethylene oxide (0.161 m^3) is 0.145 meters. Similarly, the height at which 30 lbs (13.6 m^3) of liquid remain in the container is 0.0234 meters.

- Liquid velocity in tube. Disregarding mechanical losses and transition to two-phase flow and assuming that the velocity through the tube is equal to the velocity at the tank/eductor connection, the velocity is:

$$U_\ell = (.61)(.98)\sqrt{2(\frac{695090\ Pa - 101325\ Pa}{1405\ kg/m^3} + 9.81\ \frac{m}{s^2}(.145\ m - .0234\ m))}$$

$$= 17.43\ m/s$$

- Instantaneous or continuous release. The results of the simulation indicate that the maximum downwind distance for a continuous and an instantaneous release is, respectively, 4159 m and 2984 m. Based on the methodology described above, the release should be modeled as instantaneous (the instantaneous release is based on 470 lbs of liquid chlorine).

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[4]Correlation and coefficients obtained from the United States Coast Guard Hazard Assessment Computer Systems (HACS). This correlation is used in ADAM.

Two-phase Refrigerated Liquid Example

To model this scenario as a continuous release, it must be assumed that there are negligible losses along the length of pipe through which the liquid sulfur dioxide flows. If this assumption is made, then the "hole-in-a-pipe" option may be used to model the scenario. To use this option, it is necessary to determine the liquid velocity in the pipe and specify it as an input to the model. To calculate the liquid velocity, it is assumed that the pipe connection occurs at the bottom of the tank and that the tank is liquid full. The velocity at the pipe/tank location is then calculated and the fluid velocity in the pipe set equal to the resulting value. ADAM, by default, assumes that the height of the pipe relative to the ground is zero.

For an instantaneous release, the volume of material is determined based on the mass of sulfur dioxide released (6586 kg). The calculations are:

- Chemical liquid density at 323.15 °K. Using the ADAM liquid sulfur dioxide density correlation[5] A+T*(B+T*C), where A=2085.6, B=-2.4, and C=0.0, the liquid storage density is:

$$\rho_l\ (323.15°K) = 2085.6 + 323.15 \times (-2.40) = 1310\ \frac{kg}{m^3}.$$

- Initial volume of chemical. At the storage temperature of 332.15 °K, the volume of chemical is:

$$V = \frac{6586\ kg}{1310\ kg/m^3} = 5.03\ m^3.$$

Note: although the scenario description specifies the tank volume as 4.277 m^3 (calculated from the specified diameter and length), the difference between 4.277 m^3 and the calculated chemical volume of 5.03 m^3 is probably made up in the semi-spherical ends of the tank.

[5]Correlation and coefficients obtained from the United States Coast Guard Hazard Assessment Computer Systems (HACS). This correlation is used in ADAM.

- Fluid velocity in the pipe. Assuming that the tank is liquid full (depth of liquid = tank diameter) and the pipe is connected to the bottom of the tank, the fluid velocity in the pipe is:

$$U_\ell = (.61)(.98)\sqrt{2\left(\frac{1519875\ \text{Pa} - 101325\ \text{Pa}}{1310\ \text{kg/m}^3} + 9.81\ \frac{\text{m}}{\text{s}^2}(1.22\ \text{m} - 0.0\ \text{m})\right)}$$

$$= 28.0\ \text{m/s}$$

- Wind speed at 10 meters. The wind speed at 10 meters must be obtained from the given meteorological conditions. Based on a wind speed of 3.13 m/s (7.0 mph) at 6 m (19.7 ft), a surface roughness of .01 meters, and a logarithmic wind velocity profile, the wind speed at 10 meters is:

$$U_{10m} = 3.13\ \text{m/s} \times \frac{\ln\frac{10\ \text{m}}{.01\ \text{m}}}{\ln\frac{6\ \text{m}}{.01\ \text{m}}} = 3.38\ \text{m/s}.$$

- Instantaneous or continuous release. For the scenario being modeled, the maximum downwind distance for a continuous and instantaneous release is 16972 meters and 24032 meters, respectively. Therefore, the release should be modeled as continuous.

Single-phase Gas Release (Choked) Example

If the effects of friction are neglected, the release may be modeled using the severed pipe, continuous release option. This option requires the user to enter the pipe's inner diameter and the fluid velocity. However, for gas flows in pipe, the fluid velocity is arbitrary. Since ADAM has a specific algorithm for handling severed pipes the release diameter at choked conditions at the hole (0.06962 m) will not be used. Only the pipe's inner diameter will be used.

In the case of an instantaneous release, the volume of gaseous hydrogen fluoride released into the atmosphere must be determined at the release temperature and ambient pressure. To be consistent with ADAM calculations, the

release temperature is assumed to be equal to the ambient temperature of 295.2 °K. The calculations are:

- Wind speed at 10 meters. For a wind speed of 6.26 m/s at 6.10 meters, a surface roughness of .01 meters, and a logarithmic wind velocity profile, the wind speed at 10 meters is:

$$U_{10m} = 6.26 \text{ m/s} \times \frac{\ln \frac{10 \text{ m}}{.01 \text{ m}}}{\ln \frac{6.096 \text{ m}}{.01 \text{ m}}} = 6.74 \text{ m/s.}$$

- Instantaneous release volume. For 226.8 kg of hydrogen fluoride, the volume of gas at the release temperature and ambient pressure, assuming ideal behavior, is:

$$V = \frac{(226.8 \text{ kg})\ (8314 \text{ J/kmol°K})\ (295.2\text{°K})}{(68.1 \text{ kg/kmol})\ (101325 \text{ Pa})} = 80.7 \text{ m}^3.$$

  Note: 68.1 kg/kmol is the apparent molecular weight of pure hydrogen fluoride at 295.2 °K as calculated internally by ADAM based on the equation (156.67-.3*T) where T is the ambient temperature for this scenario.

- Instantaneous or continuous release. For a concentration of 6 ppm, the maximum downwind distance for a continuous and instantaneous release is 1407 meters and 4951 meters, respectively. Based on the methodology described above, the release should be treated as continuous.

Single-phase Liquid Release (High Volatility) Example

No modifications to the scenario description are necessary. The tank volume specified in ADAM was determined based on the total mass of ethylene oxide and the liquid density at the material's normal boiling point (882.67 kg/m3).

Because the ethylene oxide is stored at its normal boiling point, the material is released as a single phase liquid (flash fraction is 0.0 at the normal boiling point of 283.85 °K). Also, since the flash fraction is only 0.05 at the ambient temperature of 301.15° K, ADAM models the release as a high volatility liquid that forms a pool on the ground which subsequently

boils and evaporates. It is assumed that the release from the tank occurs in the liquid phase, i.e., the release of ethylene oxide vapor is not accounted for. The calculations are:

- Initial volume of chemical. At the storage temperature of 283.35° K, the volume of liquid ethylene oxide is:

$$V = \frac{23780 \text{ kg}}{882.67 \text{ kg/m}^3} = 26.9 \text{ m}^3.$$

- Instantaneous or continuous release. For the scenario being modeled, the evaporation rate from a slowly forming pool resulting from the continuous release of ethylene oxide is much less than that resulting from an instantaneous release and the formation of a pool of a volume equal to the total volume of material in the tank (executing the source-term model for both continuous and instantaneous releases resulted in evaporation rates [chemical ejection rate to the atmosphere] of 0.020 kg/s and 0.813 kg/s, respectively).

In light of the reduced evaporation rate of the continuous release, it is reasonable to assume that the dispersion distance for the continuous release would also be less than that for an instantaneous release. Based on this assumption, the release should be treated as continuous. In fact, executing the instantaneous release model for decreasing evaporation rates (characteristic of a smaller size pool) results in decreasing dispersion distances.

6.2 ALOHA

The ALOHA model falls into the interactive model category. When the model is run, a summary of the input is provided to the user. Parts of the text summary are duplicated here to indicate the input used. The input is given in Tables 6-7 through 6-14. The input is entered into the model through a series of input screens and menus from which the user selects options and enters numerical and text values. The input used for each release example comes from the tables cited in the title for each of the Tables 6-7 through 6-14.

TABLE 6-7. TEXT SUMMARY FOR TWO-PHASE GAS RELEASE (CHOKED)
(Reference Table 5-2)

SITE DATA INFORMATION:

Location: Newport Beach, California
Building Air Exchanges Per Hour: 0.01 (User Specified)
Date & Time: Using computer's internal clock

CHEMICAL INFORMATION:

Chemical Name: ETHYLENE OXIDE Molecular Weight: 44.05 kg/kmol
TLV-TWA: 1.00 ppm IDLH: 800.00 ppm
Note: Potential or confirmed human carcinogen
Footprint Level of Concern: 800 ppm
Boiling Point: 10.70 °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: 12 mph from NE No Inversion Height
Stability Class: C Air Temperature: 57.2 °F
Relative Humidity: 62% Ground Roughness: 1 centimeter
Cloud Cover: 4 tenths

SOURCE STRENGTH INFORMATION:

Gas leak from hole in spherical tank selected
Tank Diameter: 2.3 meters
Tank Volume: 6.37 cubic meters
Internal Temperature: 86.9 °F Internal Press: 2 atmospheres
Chemical Mass in Tank: 23.3 kilograms
Circular Opening Diameter: 0.5 inches
Release Duration: 8 minutes
Max Computed Release Rate: 2.59 kilograms/min
Max Average Sustained Release Rate: 2.45 kilograms/min
(averaged over a minute or more)
Total Amount Released: 11.2 kilograms

TABLE 6-8. TEXT SUMMARY FOR TWO-PHASE GAS RELEASE (UNCHOKED)
(Reference Table 5-4)

SITE DATA INFORMATION:

Location: Newport Beach, California
Building Air Exchanges Per Hour: 0.01 (User Specified)
Date & Time: Fixed at November 7, 1992 & 0600 hours

CHEMICAL INFORMATION:

Chemical Name: ETHYLENE OXIDE Molecular Weight: 44.05 kg/kmol
TLV-TWA: 1.00 ppm IDLH: 800.00 ppm
Note: Potential or confirmed human carcinogen
Footprint Level of Concern: 800 ppm
Boiling Point: 10.70 °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: 6 mph from SW No Inversion Height
Stability Class: C Air Temperature: 57.2 °F
Relative Humidity: 37% Ground Roughness: 1 centimeter
Cloud Cover: 6 tenths

SOURCE STRENGTH INFORMATION:

Gas leak from hole in spherical tank selected
Tank Diameter: 2.4 meters
Tank Volume: 7.24 cubic meters
Internal Temperature: 71.6 °F Internal Press: 1.48 atmospheres
Chemical Mass in Tank: 20.0 kilograms
Circular Opening Diameter: 0.5 inches
Release Duration: 8 minutes
Max Computed Release Rate: 1.88 kilograms/min
Max Average Sustained Release Rate: 1.75 kilograms/min
(averaged over a minute or more)
Total Amount Released: 6.27 kilograms

TABLE 6-9. TEXT SUMMARY FOR TWO-PHASE PRESSURIZED LIQUID (Reference Table 5-6)

SITE DATA INFORMATION:

Location: Newport Beach, California
Building Air Exchanges Per Hour: 0.01 (User Specified)
Date & Time: Fixed at September 25, 1992 & 1100 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: 10 mph from S No Inversion Height
Stability Class: C Air Temperature: 70.0 °F
Relative Humidity: 50% Ground Roughness: 1 centimeter
Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:

Liquid leak from short pipe or valve in horizontal cylindrical tank selected
Tank Diameter: 0.762 meters Tank Length: 2.07 meters
Tank Volume: 0.94 cubic meters
Internal Temperature: 70 °F
Chemical Mass in Tank: 500.0 lbs Tank is 16% full
Circular Opening Diameter: 0.277 inches
Opening is 0 meters from tank bottom
Release Duration: ALOHA limited the duration to 1 hour
Max Computed Release Rate: 22.7 kilograms/min
Max Average Sustained Release Rate: 12.9 kilograms/min
(averaged over a minute or more)
Total Amount Released: 193 kilograms
Note: The release was a two phase flow.

TABLE 6-10. TEXT SUMMARY FOR TWO-PHASE REFRIGERATED LIQUID
(Reference Tables 5-7 and 5-8)

SITE DATA INFORMATION:
Location: MOBILE, ALABAMA
Building Air Exchanges Per Hour: 0.01 (User Specified)
Date & Time: Fixed at October 27, 1992 & 0600 hours

CHEMICAL INFORMATION:
Chemical Name: SULFUR DIOXIDE Molecular Weight: 64.07 kg/kmol
TLV-TWA: 2.00 ppm IDLH: 100.00 ppm
Footprint Level of Concern: 100 ppm
Boiling Point: -10.02 °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: 7 mph from NE No Inversion Height
Stability Class: E Air Temperature: 64.4 °F
Relative Humidity: 42% Ground Roughness: 1 centimeter
Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
Direct Source: 4.15 kilograms/sec Source Height: 0 m
Release Duration: ALOHA limited the duration to 1 hour
Release Rate: 249 kilograms/min
Total Amount Released: 14954 kilograms
Note: This chemical may flash boil and/or result in two phase flow.

TABLE 6-11. TEXT SUMMARY FOR SINGLE-PHASE GAS RELEASE (CHOKED)
(Reference Tables 5-9 and 5-10)

SITE DATA INFORMATION:
Location: NEWPORT BEACH, CALIFORNIA
Building Air Exchanges Per Hour: 0.01 (User Specified)
Date & Time: Fixed at June 1, 1992 & 1700 hours

CHEMICAL INFORMATION:
Chemical Name: HYDROGEN FLUORIDE
Apparent Molecular Weight: 35.00 kg/kmol
TLV-TWA: 3.00 ppm IDLH: 30.00 ppm
Footprint Level of Concern: 30 ppm
Boiling Point: 19.52 °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: 14 mph from NW No Inversion Height
Stability Class: D Air Temperature: 71.6 °F
Relative Humidity: 45% Ground Roughness: 1 centimeter
Cloud Cover: 3 tenths

SOURCE STRENGTH INFORMATION:
Direct Source: 51 kilograms Source Height: 0 m
Release Duration: 1 minute
Release Rate: 851 grams/sec
Total Amount Released: 51.1 kilograms
Note: This chemical may flash boil and/or result in two phase flow.

TABLE 6-12. TEXT SUMMARY FOR SINGLE-PHASE GAS RELEASE (UNCHOKED)
(Reference Tables 5-11 and 5-12)

SITE DATA INFORMATION:
Location: NEWPORT, CALIFORNIA
Building Air Exchanges Per Hour: 0.01 (User Specified)
Date & Time: Fixed at November 2, 1992 & 0737 hours

CHEMICAL INFORMATION:
Chemical Name: HYDROCHLORIC ACID ANHYDROUS
Molecular Weight: 36.46 kg/kmol
TLV-TWA: 5.00 ppm IDLH: 100.00 ppm
Footprint Level of Concern: 100 ppm
Boiling Point: -121.00 °F
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: 2.2 mph from E No Inversion Height
Stability Class: B Air Temperature: 64 °F
Relative Humidity: 36% Ground Roughness: 1 centimeter
Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
Direct Source: 4250 cubic feet/min Source Height: 28 m
Source State: Gas
Source Temperature: 120 °F
Source Pressure: equal to ambient
Release Duration: ALOHA limited the duration to 1 hour
Release Rate: 367 pounds/min
Total Amount Released: 22,046 kilograms
Note: This chemical may flash boil and/or result in two phase flow.

TABLE 6-13. TEXT SUMMARY FOR SINGLE-PHASE LIQUID RELEASE (HIGH VOLATILITY)
(Reference Tables 5-13 and 5-14)

SITE DATA INFORMATION:
Location: MOBILE, ALABAMA
Building Air Exchanges Per Hour: 0.01 (User Specified)
Date & Time: Fixed at June 26, 1992 & 0600 hours

CHEMICAL INFORMATION:
Chemical Name: ETHYLENE OXIDE Molecular Weight: 44.05 kg/kmol
TLV-TWA: 1.00 ppm IDLH: 800.00 ppm
Footprint Level of Concern: 800 ppm
Boiling Point: 10.70 °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: E Air Temperature: 28 °C
Relative Humidity: 50% Ground Roughness: 1 centimeter
Cloud Cover: 5 tenths

SOURCE STRENGTH INFORMATION:
Liquid leak from hole in vertical cylindrical tank selected
Direct Source: 3.5 meters Tank Length: 6 meters
Tank Volume: 57.7 cubic meters
Internal Temperature: 51.3 °F
Chemical Mass in Tank: 23,852 kilograms
Tank is 47% full
Circular Opening Diameter: 0.25 inches
Opening is 0.5 meters from tank bottom
Release Duration: ALOHA limited the duration to 1 hour
Max Computed Release Rate: 6.88 kilograms/min
Max Average Sustained Release Rate: 6.53 kilograms/min
(averaged over a minute or more)
Total Amount Released: 392 kilograms
Note: The release was a two phase flow.

TABLE 6-14. TEXT SUMMARY FOR SINGLE-PHASE LIQUID RELEASE (LOW VOLATILITY)
(Reference Tables 5-15 and 5-16)

SITE DATA INFORMATION:
Location: NEWPORT, CALIFORNIA
Building Air Exchanges Per Hour: 0.01 (User Specified)
Date & Time: Fixed at November 3, 1992 & 1600 hours

CHEMICAL INFORMATION:
Chemical Name: HYDROCHLORIC ACID, ANHYDROUS
Molecular Weight: 36.46 kg/kmol
TLV-TWA: 5.00 ppm IDLH: 100.00 ppm
Footprint Level of Concern: 100 ppm
Boiling Point: -85.00 °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: 5 mph from NE No Inversion Height
Stability Class: C Air Temperature: 65 °F
Relative Humidity: 58% Ground Roughness: 1 centimeter
Cloud Cover: 4 tenths

SOURCE STRENGTH INFORMATION:
Direct Source: 0.005365 kilograms/sec Source Height: 0 m
Release Duration: ALOHA limited the duration to 1 hour
Release Rate: 322 grams/min
Total Amount Released: 19.3 kilograms
Note: This chemical may flash boil and/or result in two phase flow.

ALOHA has source-term models for puddles, tanks, and pipes. In those cases the observable data can be supplied to the model and it will internally compute emission rates, temperatures, etc. The model also allows direct input of emission rate, etc., if the release is not covered by one of the source term sub-models. Variations between the supplied input and those used in the ALOHA simulations are discussed below.

Two-phase Gas Release (Choked and Unchoked) Examples

ALOHA does not treat the case of a step-function emission. The size of the tank must be assumed to be large enough to supply a steady discharge of gas for 8 minutes. Larger tanks are immaterial as far as the source strength is concerned. However, large tanks will overestimate doses because of an increase in exposure time.

By trial and error, a tank having a 2.3-meter diameter was found to produce an 8-minute discharge. The volume contained in a 3-inch pipe, limited to a 200-to-1 length-to-diameter ratio by ALOHA, is much too small to supply an 8-minute discharge.

The assumption of a steady-state emission rate would be more conservative than simulating an 8-minute step function using a 2.3-meter diameter tank. However, the difference between a 2.3-meter diameter tank and a 10-meter diameter tank was about 15 percent. Considering the fact that the original pipe's length had already been set to zero, the above error is probably in the model noise level.

In the unchoked release example, ALOHA warned that the supplied storage pressure was too high for vapor-liquid equilibrium at the supplied temperature. This is probably due to differences in the vapor pressure curve data used in ALOHA and the data given in this document.

Single-phase Gas Release (Choked) Example

ALOHA does not account for the varying molecular weight of HF as its temperature and concentration levels change. Because of this fact, when ALOHA is being used to model HF releases, it must be clearly understood that the results are only an estimation of what may occur and these may be a larger error than when simulating other compounds.

Single-phase Gas Release (Unchoked) and
Single-phase Liquid Release (Low Volatility) Examples

These examples were modeled as pure hydrogen chloride releases, although the emissions were actually mixtures. Therefore, in ADAM, the concentrations reported should be modified by the factor f_i, which has value of 0.7295 for the gas release example and 0.01258 for the liquid release example. ALOHA does not allow specifying an initial concentration. The initial concentration is assumed to be 100%. It may be more correct to add new pseudo chemicals to the database. Apparent molecular weights for the gas phase were calculated in Sections 5.6.11 and 5.8.7. For the gas release example, an apparent gas phase specific heat was calculated in Section 5.6.2. The gas-phase specific heat is already supplied in the database in Appendix B for the 30 weight% hydrogen chloride mixture.

ALOHA can not simulate an elevated release of a heavier-than-air release. Therefore the standard ALOHA model was used, rather than the ALOHA-DEGADIS model even though indications are that the release is heavier-than-air.

6.3 DEGADIS

Table 6-15 lists the specific input required by the DEGADIS model and gives a brief description of each input. It includes information on the physical property information on the material released; release rate, height

TABLE 6-15. DEGADIS MODEL INPUT PARAMETERS

Input Parameter Name	Description of Input Parameter	Comments
U0	ambient wind speed (m/s) at height Z0	4.17.1
Z0	reference height (m) of wind speed U0	4.17.1
ZR	surface roughness (m)	4.17.3
INDVEL	Wind velocity profile and Monin-Obukhov calculation flag	1 = DEGADIS will calculate Monin-Obukhov length. This was used in all cases.
ISTAB	Pasquill-Gifford stability category	1 = A, 2 = B, etc.
RML	Monin-Obukhov length (m)	Set to 0.0 for all cases since INDVEL set to 1
TAMB	ambient temperature (°K)	4.17.5
PAMB	ambient pressure (atm)	4.17.5
RELHUM	relative humidity (%)	4.17.5
TSURF	ground surface temperature (°K)	4.15
GASNAM	three letter designation of contaminant	
GASMW	contaminant molecular weight (kg/kmol)	4.2
AVTIME	averaging time (s)	4.16
TEMJET	temperature of the released contaminant (°K)	4.8
GASUL	higher concentration for determining extent (mole fraction)	4.18
GASLL	lower concentration for determining extent (mole fraction)	4.18
Input Parameter Name	Description of Input Parameter	Comments

TABLE 6-15. (CON'T.)

Input Parameter Name	Description of Input Parameter	Comments
ZLL	receptor elevation (m)	4.18
INDHT	switch to indicate if atmosphere heat transfer is to be included	If 0, no calculation to be done. In all cases here it is set to 0.
CPK	contaminant heat capacity constant (J/kg °K)	Since INDHT is 0, this value is ignored
CPP	contaminant heat capacity power	Since INDHT is 0, this value is ignored
NDEN	number of density triplets	Set to 2 for all cases with aerosol or HF with changing molecular weight. Otherwise 0.
F, C, RHO	density triplet of contaminant mole fraction (F), contaminant concentration (C, kg/m^3), and mixture density (RHO, kg/m^3)	4.11 0, 0, ρ_a (triplet 1) 0, ρ_{rel}, ρ_{rel} (triplet 2) Only required if aerosol present or release is of HF
ERATE	emission rate (kg/s)	4.8
ELEJET	jet elevation (m)	4.14
DIAJET	jet diameter (m)	4.12
TEND	duration of release (s)	0.0 indicates continuous release
DISTMX	distance between output points (m)	

(jet), and duration; emission densities; concentration averaging time; maximum downwind distance between output points; meteorological information; and site roughness characteristics. In the comments column for many of the input parameters of Table 6-15 the subsection in Section 4 is given which discusses how that parameter is calculated.

Table 6-16 shows the value of each input parameter used for the first seven release class examples. The eighth example was not simulated due to the fact that the release is not heavier-than-air. Standard passive atmospheric dispersion methods should apply. In the column header for each release class (RC) example, the table in Section 5 from which the input was taken is referenced. The tables in Section 5, in turn, each reference the section in which the calculation was done.

The release class examples are:

Release Class (RC)	Title
1	Two-Phase Gas Release (Choked)
2	Two-Phase Gas Release (Unchoked)
3	Two-Phase Pressurized Liquid
4	Two-Phase Refrigerated Liquid
5	Single-Phase Gas Release (Choked)
6	Single-Phase Gas Release (Unchoked)
7	Single-Phase Liquid Release (High Volatility)
8	Single-Phase Liquid Release (Low Volatility)

Averaging time was taken as the lesser of the release duration or time requested for averaging. When the averaging time used is less than the requested averaging time, the output must be converted to represent the requested averaging time. See Section 7.3 for further discussion on the output conversion technique.

TABLE 6-16. DEGADIS INPUT. A () INDICATES REFERENCE TABLE OF INPUT DATA.

Input Parameter Name	Input Values RC 1 (5-1)	Input Values RC 2 (5-2)	Input Values RC 3 (5-3)	Input Values RC 4 (5-4)	Input Values RC 5 (5-5)	Input Values RC 6 (5-6)	Input Values RC 7 (5-7)
UO	5.37	2.68	4.47	3.13	6.26	0.98	2.0
ZO	4.57	6.1	10	6	6.1	10	10
ZR	0.01	0.01	0.01	0.01	0.01	0.01	0.01
INDVEL	1	1	1	1	1	1	1
ISTAB	3	3	3	5	4	2	5
RML	0.0	0.0	0.0	0.0	0.0	0.0	0.0
TAMB	287.5	296.5	294.3	291.15	295.15	290.9	301.0
PAMB	1.0	1.0	1.0	1.0	1.0	1.0	1.0
RELHUM	62	37	50	42	45	36	50
TSURF	287.5	296.5	294.3	291.15	295.15	290.9	301.0
GASNAM	EOX	ETO	CL2	SO2	HF	HCL	ETO
GASMW	44.05	44.05	70.91	64.06	20.0	33.1	44.05
AVTIME	0.0	0.0	678.0	900.0	45.0	720.0	1800.0
TEMJET	283.85	283.85	239.1	263.13	313.6	322.0	283.85
GASUL	1.0	1.0	1.0×10^{-5}	1.0×10^{-5}	1.2×10^{-5}	2.74×10^{-4}	1.60×10^{-3}
GASLL	0.03	0.03	1.0×10^{-6}	5.0×10^{-6}	6.0×10^{-6}	1.37×10^{-4}	8.00×10^{-4}
ZLL	0.0	0.0	0.0	0.0	0.0	0.0	0.0
INDHT	0	0	0	0	0	0	0
CPK	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CPP	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NDEN	2	2	2	2	2	0	0
F, C, RHO	0, 0, 1.220	0, 0, 1.183	0, 0, 1.191	0, 0, 1.206	0, 0, 1.188		
F, C, RHO	1, 1.916, 1.916	1, 1.934, 1.934	1, 20.11, 20.11	1, 13.76, 13.76	1, 1.360, 1.360		
ERATE	0.0634	0.0503	0.3170	4.154	0.8513	2.515	0.1220
ELEJET	3.66	3.66	2.0	0.3049	3.66	8.54	0.5
DIAJET	0.01347	0.0127	0.00704	0.0127	0.06649	0.86	0.1372
TEND	0.0	0.0	0.0	0.0	0.0	0.0	0.0
DISTMX	0.1	0.1	50.0	50.0	50.0	50.0	50.0

In all cases, the release is initially modeled as a vertically pointing jet. The simulation of a vertical jet should represent the lower bound of predicted concentrations since such a release represents maximum dilution. All other jet orientations should result in either the same amount of mixing or less as long as the jet is not directed into the wind. It is suggested that an upper limit of the concentration impacts be determined by also simulating the release as a low-momentum, ground-level source. The source diameter would need to be estimated by using the low-momentum formula given in Section 4.12.1.

In all cases, it was initially assumed that the release was continuous (TEND was set to 0.0). After each simulation, the travel time to the distance of interest was estimated. If the travel time was longer than the release duration, a transient simulation was performed. A transient simulation is made by changing the TEND parameter in the DEGADIS input file to the release duration. If the simulation can be assumed to be continuous rather than transient, the interpretation of the output is made simpler. See Section 7.3 for further discussion on the interpretation of the output.

Two-phase Gas Release (Choked and Unchoked) Examples

The concentrations of concern are so high and the dispersion is so rapid that the jet sub-model needed to be run twice. The first time the distance between outputs was too large (50 m) to see the distance downwind of a 3% concentration. Therefore, the model had to be rerun with a step decrease of 0.1 meters.

6.4 HGSYSTEM

Table 6-17 presents a summary of the models that were used in analyzing the eight release class examples. The rationale for model selection and implementation is presented in the following sub-sections. It should be noted that there may be equally valid alternative methods for modeling the

TABLE 6-17. SUMMARY OF THE HGSYSTEM MODELS USED

Release Class	Chemical	Release Conditions	HGSYSTEM Models Used: Near Field	Far Field	Post Processing
1	Ethylene Oxide	Two-Phase Gas Release (Choked)	HEGADASS	HEGADASS	HSPOST-GET2COL
2	Ethylene Oxide	Two-Phase Gas Release (Unchoked)	HEGADASS	HEGADASS	HSPOST-GET2COL
3	Chlorine	Two-Phase Pressurized Liquid	HEGADASS	HEGADASS	HSPOST
4	Sulfur Dioxide	Two-Phase Refrigerated Liquid	PLUME	PGPLUME	
5	Hydrogen Fluoride	Single-Phase Gas (Choked)	HEGADAST	HEGADAST	HTPOST
6	Hydrogen Chloride	Single-Phase Gas (Unchoked)	PLUME	PGPLUME	
7	Ethylene Oxide	Single-Phase Liquid Release (High Volatility)	PLUME	HEGADASS	GET2COL
8	30% Hydrochloric Acid	Single-Phase Liquid (Low Volatility)	HEGADASS	HEGADASS	

consequences of these scenarios other than the ones presented in this analysis.

Averaging Time Issues

HGSYSTEM allows for finite duration releases. Accordingly, the averaging time selection may affect the accuracy of the model, especially if the averaging time is larger than the release duration. For scenarios for which this is true, HGSYSTEM models were applied in the following manner. The averaging time for σ_y (AVTIMC) was set equal to the release duration. Thus the amount of plume meander was restricted to the length of time that a plume actually existed. That is, if the duration of a release was 5 minutes and we are interested in a 15-minute average, it is not appropriate to use a σ_y averaging time that is longer than the duration of the release (5-minutes not 15-minutes). This approach is taken because there is a 10-minute period in which the plume does not exist and, therefore, will not undergo any meander. For situations where the model predicts that a gas blanket (i.e., a situation in which the cloud is not advected downwind because of density differences) exists for a period longer than the actual release duration, the length of time that the gas blanket persisted should be used to establish the σ_y averaging time to determine the period over which the gas blanket remained (this would require iterative model runs).

There is a second aspect to calculating the average concentration for this situation. It is related to the integration of the plume in the along-wind (x axis). At a given downwind distance, the plume concentrations must be integrated to account for the variations in concentration as a function of time. To illustrate, consider a case in which the plume would persist at a given location for a period of approximately 5 minutes (the HEGADAST model will calculate this time precisely) and during the remaining 10-minutes, of the 15-minute period, no plume would be present. In order to compute an accurate average concentration, this integration of the time-varying concentrations needs to be included in the model predictions. This can be accomplished by using the σ_x averaging option in the HTPOST post processor

program for HEGADAST. Thus, in the example given above where the averaging time is 15-minutes, the σ_x processing would be calculated for a 15-minute average. See the HGSYSTEM user's manual for more information on setting the σ_x parameter.

In summary, the average concentration is based on a σ_y average that is equal to the release duration and a σ_x averaging time equivalent to the averaging time of the level of concern (LOC). This is the approach that was generally taken for all EPA examples where the release duration is less than the averaging time.

This approach for simulating average concentrations is important for situations where the release duration is less than the averaging time of concern, and becomes important if one is attempting to simulate a release where the emissions vary as a function of time.

Two-phase Gas Release (Choked) Example

This case described a two-phase release of ethylene oxide under choked conditions. The purpose of modeling this case was to identify flammability issues related to this hypothetical release. The consequences of this release were simulated using the steady-state version of the HEGADAS-5 model (HEGADASS). The steady-state model was selected because the release duration was longer than the travel time to the facility fenceline, and the averaging time of concern was very short (10 seconds). The release conditions specified a jet release that was directed downward toward the ground. Therefore, this release was simulated by initializing the model as a ground level area source (a pool in the context of the HEGADAS model). Table 6-18 presents the input parameters selected for simulating this analysis, and input parameters that require interpretation are discussed below. Much of this input was taken from Table 5-1. The rest of the input is explained in the HGSYSTEM documentation.

In this simulation the ICNT parameter was set to 1 to enable the model to provide concentration isopleths for the upper explosive limit (UEL) and lower flammability limit (LFL). The upper concentration limit (CU) was set equal to the UEL (100 % or 1.44 kg/m^3) and the lower concentration limit (CL) was set equal to LFL (3% or $5.4X10^{-2}$ kg/m^3). The calculation output step (DXFIX) was set to 0.5 meters. This enabled precise calculations in the near field region so that the distance to the LOC could be identified. The size of the area source was arbitrarily selected (see POOL DATA in Table 6-18), and a second modeling run was made to ensure that the distance to the LOC was not overly sensitive to this assumption. It has been our experience for this model and this type of release that the results are relatively insensitive to the specification of area source size.

Two-phase Gas Release (Unchoked) Example

This case described a two-phase release of ethylene oxide under unchoked conditions. The consequences of this release were simulated using the HEGADASS model, which was selected for the same reasons as in the first release example. Table 6-19 presents the input parameters selected for simulating this analysis. Much of this input was taken from Table 5-3. The rest of the input is explained in the HGSYSTEM documentation. For this case, the model was initialized in an analogous manner to the first release example using the data provided.

Two-phase Pressurized Liquid Example

This release represents a two-phase pressurized liquid release from a chlorine cylinder. The release conditions for this case represent a two-phase horizontal jet release which is directed downwind. To compute more accurate concentrations for this case, the transient version of HEGADAS should be used. This approach is preferable because the release duration is less than the averaging time (the release duration is 11 minutes and the averaging time of concern is 15 minutes). However, when the HEGADAST model was executed for

TABLE 6-18. INPUT PARAMETERS USED IN THE HEGADASS MODEL TO SIMULATE RELEASE CLASS 1 (Reference Table 5-1)

```
TITLE   SCENARIO 1 CHOKED ETHYLENE OXIDE RELEASE

CONTROL                        *  --------> DATA BLOCK: CONTROL PARAMETERS
                               *
  ICNT   =      1              *          output code (isocontours,cloud contents)
  ISURF  =      3              *          code for surface heat/water transfer
                               *
AMBIENT                        *  --------> DATA BLOCK: AMBIENT CONDITIONS
                               *
   AIRTEMP =  14.4             * C          air temperature at height z = ZAIRTEMP
   ZAIRTEMP=   4.6             * M          height at which AIRTEMP is given
   RHPERC  =  62.              * %          relative humidity
   U0      =  5.37             * M/S        wind speed at height z = Z0
   Z0      =   4.6             * M          height at which U0 is given
   TGROUND =  14.4             * C          earth's surface temperature
                               *
DISP                           *  --------> DATA BLOCK: DISPERSION DATA
                               *
   ZR      =  0.01             * M          surface roughness parameter
   PQSTAB  =  C                *            Pasquill stability class
   AVTIMC  =  10.              * S          averaging time for concentration
   CROSSW  =  2                *            <σy>formula (don't normally change)
                               *
GASDATA                        *  ---------> DATA BLOCK: GAS DATA
                               *
   GASFLOW =  .0634            * KG/S     gas emission rate (excl. water pick-up)
   TEMPGAS =  10.70            * C        temperature of emitted gas
   CPGAS   =  24.49            * J/MOLE/C specific heat of emitted gas
   MWGAS   =  44.              * KG/KMOLE molecular weight of emitted gas
   WATGAS  =  0.               * -        water pick-up by gas (don't norm.change)
   HEATGR  =  29.              * .....    gas group for natural-conv. heat flux
                               *
CLOUD                          *  --------> DATA BLOCK: CLOUD OUTPUT CONTROL
                               *
   DXFIX   =  .5               * M          fixed-size output step length
   NFIX    =  300              *            fixed steps up to distance x =
NFIX*DXFIX
   XEND    =  3000.            * M          x at which calculations are stopped
   CAMIN   =  0.00001          *  KG/M3     CA (conc.) at which calcs. are stopped
   CU      =  1.44              * KG/M3      upper concentration limit
   CL      =  0.05397          * KG/M3      lower concentration limit
                               *
POOL                           *  --------> DATA BLOCK: POOL DATA
                               *
   PLL     =   .2              * M          pool length
   PLHW    =   .1              * M          pool half-width
```

TABLE 6-19. INPUT PARAMETERS USED IN THE HEGADASS MODEL TO SIMULATE RELEASE CLASS 2 (Reference Table 5-2)

```
TITLE   SCENARIO 2 UNCHOKED ETHYLENE OXIDE

CONTROL                          *  --------> DATA BLOCK: CONTROL PARAMETERS
                                 *
    ICNT   =      1              *          output code (isocontours,cloud contents)
    ISURF  =      3              *          code for surface heat/water transfer
                                 *
AMBIENT                          *  --------> DATA BLOCK: AMBIENT CONDITIONS
                                 *
   AIRTEMP =  23.3               * C          air temperature at height z = ZAIRTEMP
   ZAIRTEMP=   6.1               * M          height at which AIRTEMP is given
   RHPERC  =  37.                * %          relative humidity
   U0      =  2.68               * M/S        wind speed at height z = Z0
   Z0      =   6.1               * M          height at which U0 is given
   TGROUND =  23.3               * C          earth's surface temperature
                                 *
DISP                             *  --------> DATA BLOCK: DISPERSION DATA
                                 *
   ZR      =  0.01               * M          surface roughness parameter
   PQSTAB  =  C                  *            Pasquill stability class
   AVTIMC  =  10.                * S          averaging time for concentration
   CROSSW  =  2                  *            <σy>formula (don't normally change)
                                 *
GASDATA                          *  ---------> DATA BLOCK: GAS DATA
                                 *
   GASFLOW =  .0503              * KG/S       gas emission rate (excl. water
pick-up)
   TEMPGAS =  10.70              * C        temperature of emitted gas
   CPGAS   =  24.49              * J/MOLE/C specific heat of emitted gas
   MWGAS   =  44.                * KG/KMOLE molecular weight of emitted gas
   WATGAS  =  0.                 * -        water pick-up by gas (don't norm.change)
   HEATGR  =  29.                * .....    gas group for natural-conv. heat flux
                                 *
CLOUD                            *  --------> DATA BLOCK: CLOUD OUTPUT CONTROL
                                 *
   DXFIX   =  .5                 * M          fixed-size output step length
   NFIX    =  300                *            fixed steps upto distance x =
NFIX*DXFIX
   XEND    =  3000.              * M          x at which calculations are stopped
   CAMIN   =  0.00001            * KG/M3      CA (conc.) at which calcs. are stopped
   CU      =  .2159              * KG/M3      upper concentration limit
   CL      =  0.05397            * KG/M3      lower concentration limit
                                 *
POOL                             *  --------> DATA BLOCK: POOL DATA
                                 *
   PLL     =   .2                * M          pool length
   PLHW    =   .1                * M          pool half-width
```

this scenario with the predefined meteorological conditions (stability class "C"), the source blanket was too thin for the model to accurately compute downwind concentrations. This resulted from the simulation of a small release rate (0.32 kg/sec) and the convective atmospheric conditions. It was found that the HEGADAST model would run for this scenario under stable, worst-case, meteorological conditions. From a pragmatic perspective, the HEGADASS model runs provide a reasonable estimate of impacts for this case because the uncertainty in σ_y (11-minutes versus 15-minute) is not very large and because the averaging times are similar and relatively long. The input used in the simulation is listed in Table 6-20. Much of this input was taken from Table 5-5. The rest of the input is explained in the HGSYSTEM documentation.

Two-phase Refrigerated Liquid Example

This case described a two-phase refrigerated release of sulfur dioxide. The consequences of this release were simulated using the PLUME and PGPLUME models. This modeling approach was selected because this case simulated a release that was directed vertically upward. The PLUME model was used to estimate initial plume dispersion and trajectory. The results from this model indicate that at the point where the plume has a velocity equivalent to that of ambient air, that the density of the plume is not sufficient to cause the plume to touch down. As a result, a transition is made into the PGPLUME model, using the PLUME model results as input. Table 6-21 presents the parameters used for the PLUME model. Much of this input was taken from Table 5-7. The rest of the input is explained in the HGSYSTEM documentation. The parameters for the PGPLUME model that were passed from the PLUME model are provided in the link file that is presented in Table 6-22. Additional data required by PGPLUME are indicated by an asterisk in column 1 of the link file. These data can be manually entered into this file or by concatenating a PGPLUME link file to it, where the appropriate values have been input. In this case the data were manually entered into the PGPLUME link file, and the file was renamed to have an extension ending with PGI (Table 6-23).

TABLE 6-20. CONCATENATED INPUT FILE FOR RELEASE CLASS 3 (Reference Table 5-3)

```
* ============== HEGADAS-S standard input file STPOOLNO.HSI
==================
*            (case: run started at pool, normal thermodynamics)

TITLE   EPA SCENARIO 3 HEGADASS RUN CHLORINE RELEASE

CONTROL                    * --------> DATA BLOCK: CONTROL PARAMETERS
                           *
    ICNT   =      0        *          output code (isocontours,cloud contents)
    ISURF  =      3        *          code for surface heat/water transfer
                           *
AMBIENT                    * --------> DATA BLOCK: AMBIENT CONDITIONS

   AIRTEMP = 21.2          * C          air temperature at height z = ZAIRTEMP
   ZAIRTEMP= 10.           * M          height at which AIRTEMP is given
   RHPERC  = 50.           * %          relative humidity
   U0      = 3             * M/S        wind speed at height z = Z0
   Z0      = 10.           * M          height at which U0 is given
   TGROUND = 21.2          * C          earth's surface temperature
                           *
DISP                       * --------> DATA BLOCK: DISPERSION DATA
                           *
   ZR      = .01           * M          surface roughness parameter
   PQSTAB  = F             *            Pasquill stability class
   AVTIMC  = 900.          * S          averaging time for concentration
   CROSSW  = 2             *            <σy>formula (don't normally change)
                           *
GASDATA                    * ---------> DATA BLOCK: GAS DATA

   GASFLOW = .3170         * KG/S     gas emission rate (excl. water pick-up)
   TEMPGAS = -34.          * C        temperature of emitted gas
   CPGAS   = 6.8           * J/MOLE/C specific heat of emitted gas
   MWGAS   = 70.9          * KG/KMOLE molecular weight of emitted gas
   WATGAS  = 0.            * -        water pick-up by gas (don't norm.change)
                           *
CLOUD                      * --------> DATA BLOCK: CLOUD OUTPUT CONTROL
                           *
   DXFIX   = 1.            * M        fixed-size output step length
   NFIX    = 1000.         *          fixed steps upto distance x = NFIX*DXFIX
   XEND    = 3000.         * M        x at which calculations are stopped
   CAMIN   = 0.000001      * KG/M3    CA (conc.) at which calcs. are stopped
   CU      = 0.0001        * KG/M3    upper concentration limit
   CL      = 0.00001       * KG/M3    lower concentration limit
                           *
POOL                       * --------> DATA BLOCK: POOL DATA
                           *
   PLL     = 1.            * M          pool length
   PLHW    = .5            * M          pool half-width
```

TABLE 6-21. PLUME MODEL INPUT FOR RELEASE CLASS 4 (Reference Table 5-4)

```
TITLE   SCENARIO 4 SO2 RELEASE

GASDATA                     * PHYSICAL PROPERTIES OF GAS
                            *
   TEMPGAS  = -10.0         * CELSIUS        TEMPERATURE OF POLLUTANT
   MFGAS    =  100.00       * PERCENT        MOLE FRACTION OF POLLUTANT
   MFH2O    =  0.0          * PERCENT        MOLE FRACTION OF WATER
   MWGAS    =  64.1         * g/mol          MOLECULAR WEIGHT POLLUTANT
   CPGAS    =  21.0         * J/mol/C        ISOBARIC SPECIFIC HEAT
                            *
PIPE                        * PIPE EXIT-PLANE (CHOKE-FRONT) CONDITIONS
                            *
   DMDT     =  4.154        * KG/S           DISCHARGE RATE
   DEXIT    =  .0127        * M              EFFECTIVE ORIFICE DIAMETER
   ZEXIT    =  .3049        * M              HEIGHT ABOVE (LEVEL) GROUND
   PHISTK   =  90.00        * DEGREES        RELEASE DISCHARGE ANGLE
   DURATION =  1585         * S              RELEASE DURATION (<0 FOR STEADY)

AMBIENT CONDITIONS          * ATMOSPHERIC AMBIENT CONDITIONS
                            *
   Z0       =   6.0         * M              REFERENCE HEIGHT
   U0       =  3.13         * M/S            WIND VELOCITY AT HEIGHT Z0
   AIRTEMP  =  18.0         * CELSIUS        AIR TEMPERATURE
   AIRPRESS =  1.00         * ATMOSPHERES    AMBIENT PRESSURE
   RHPERC   =  00.0         * PERCENT        RELATIVE HUMIDITY
                            *
DISP.                       * DISPERSION DATA
                            *
   ZR       =  0.01         * M              SURFACE ROUGHNESS PARAMETER
   PQSTAB   =  E            *                PASQUILL STABILITY CLASS
                            *
TERMINAT                    * JET/PLUME DEVELOPMENT TERMINATION CRITERIA
                            *
   SLST     =  500.         * M              LAST REQD. DOWNWIND DISP.
   DLST     =  -1E6         * M              LAST REQD. PLUME DIAMETER
   ZLST     =  -.35         * M              LAST REQD. PLUME CENTROID RISE HT.
   DXLST    =  -500         * M              LAST REQD. HORIZONTAL DISPLACEMENT
   ULST     =  -0.1         * M/S            LAST REQD. (MEAN) PLUME VELOCITY
   BETLST   =  1E-7         * PERCENT        LAST REQD. POLLUTANT CONCENTRATION
                            *
MATCH                       * MATCHING CRITERIA FOR HEGADAS/PGPLUME
                            *
   RULST    =   .2          *                LAST REQD. ABS. VALUE OF
UJET/UAMB-1
   RELST    =   .3          *                LAST REQD. JET/(JET+HEG) ENTRAINM.
   RGLST    =   .3          *                MAX. BUOYANCY EFFECT FOR ADVECTION
   RNLST    =   .1          *                MAX. BUOY. EFF. FOR PASS.
DISPERSION
```

TABLE 6-22. PGPLUME LINK FILE CREATED BY THE PLUME MODEL FOR RELEASE CLASS 4

```
TITLE SCENARIO 4 SO2 RELEASE

 GASDATA * released gas composition datablock.

   CPGAS=       21.0          * pollutant specific heat (J/mol/C).
   MWGAS=       64.1          * pollutant molecular weight (g/mol).
   GASFRAC=     1.00          * release mole-fraction pollutant (-).
   WATGAS=    0.000E-01       * release mole-fraction water-vapour (-).

 GEOMETRY * plume geometry at matching datablock.

   DXPLUME=     161.          * matching plane displacement (m).
   ZPLUME=      29.0          * centroid height above ground (m).
   DPLUME=      41.6          * near-plume (effective) diameter (m).
   PHIPLUME= -0.300           * plume axis orientation (degrees).

 STATE * plume dynamic/thermodynamic state.

   UREL=      -0.477          * plume relative velocity (m/s).
   CMASS=      7.929E-04      * nearfield mass-concentration (kg/m3).
   RREL=       1.390E-03      * plume (mean) excess density (kg/m3).
   DURATION=  1.585E+03       * (steady) release duration (s).

 AMBIENT * ambient atmosphere datablock.

   AIRTEMP=    19.2           * ambient (air) temperature (C).
   AIRPRESS= 0.997            * ambient (absolute) pressure (atm).
   RHPERC=    0.000E-01       * ambient (relative) humidity (%).
   UATM=       6.02           * wind-speed at centroid height (m/s).
   RATM=       1.20           * ambient atmosphere density (kg/m3).

 DISP * Pasquill/Gifford dispersion data.

   ZR=         1.000E-02      * ground surface roughness (m).
   PQSTAB=        E           * Pasquill/Gifford stability class (-).
  *AVTIMC=      600.          * concentration averaging time (s).

 TERMINAT * output control datablock.

   XFIRST=      161.          * first required downwind distance (m).
  *STEP=        100.          * arithmetic series step-length (m).
  *NSTEP=        10           * maximum number of (arithmetic) steps (-).
  *FACTOR=      1.20          * scale factor for geometric series (-).
  *XLAST=     1.016E+04       * last required downwind distance (m).
  *VFLAST=      2.99          * last required mole concentration (ppm).
```

Note: Parameters which are marked with a * need to by updated to run PGPLUME

TABLE 6-23. PGPLUME INPUT FOR RELEASE CLASS 4

```
*    (case of pressurised release with near-source data from HFPLUME/PLUME)
*
* NOTE: HFPLUME/PGPLUME or PLUME/PGPLUME .PGL link file is appended
*       at the end of this file]
                                *
  DISP * Pasquill/Gifford dispersion data.
                                *
   AVTIMC   -  900.             * SECS        averaging time for concentrations
                                *
    ZR-         1.000E-02         * ground surface roughness (m).
    PQSTAB-        E              * Pasquill/Gifford stability class (-).
  TERMINAT * output control datablock.
                                *             [XFIRST from HFPLUME/PLUME]
                                *
   STEP     -  100.0             * M          arithmetic-progression step length
   NSTEP    -  10                *            maximum number of such steps
   FACTOR   -  2.0               *            distance scale (geometric factor)
   XLAST    -  10000.0           * M          last required cross-section distance
   VFLAST   -  3.0               * PPM        last required centre-line concentration

* [GASDATA, GEOMETRY, STATE and AMBIENT data blocks from HFPLUME/PLUME]
    XFIRST-     161.            * first required downwind distance (m).
 TITLE SCENARIO 4 SO2 RELEASE

  GASDATA * released gas composition datablock.

    CPGAS-       21.0           * pollutant specific heat (J/mol/C).
    MWGAS-       64.1           * pollutant molecular weight (g/mol).
    GASFRAC-     1.00           * release mole-fraction pollutant (-).
    WATGAS-    0.000E-01        * release mole-fraction water-vapour (-).

  GEOMETRY * plume geometry at matching datablock.

    DXPLUME-     161.           * matching plane displacement (m).
    ZPLUME-      29.0           * centroid height above ground (m).
    DPLUME-      41.6           * near-plume (effective) diameter (m).
    PHIPLUME- -0.300            * plume axis orientation (degrees).

  STATE * plume dynamic/thermodynamic state.

    UREL-      -0.477           * plume relative velocity (m/s).
    CMASS-      7.929E-04       * nearfield mass-concentration (kg/m3).
    RREL-       1.390E-03       * plume (mean) excess density (kg/m3).

  AMBIENT * ambient atmosphere datablock.

    AIRTEMP-   19.2             * ambient (air) temperature (C).
    AIRPRESS- 0.997             * ambient (absolute) pressure (atm).
    RHPERC-   0.000E-01         * ambient (relative) humidity (%).
    UATM-      6.02             * wind-speed at centroid height (m/s).
    RATM-      1.20             * ambient atmosphere density (kg/m3).
```

The following summarizes the important model input for the PLUME model. The temperature of the gas emitted (TEMPGAS) was taken from the Phase I report. The release duration (DURATION) was set to 26.4 minutes. This parameter was then passed to PGPLUME, which incorporates the effect of release duration into the dispersion calculations once the release travel time exceeds the release duration. The release angle was set to vertical (PHISTK 90). Because this version of PLUME cannot simulate the condensation of water vapor within the jet, the relative humidity was set to 0 percent.

In the PGPLUME model, the averaging time (AVTIMC) was set to 900 seconds, which corresponds to the averaging time of the STEL. The model output parameters were selected to provide concentration listings at 100 meter intervals (STEP) for the first 1000 meters (NSTE=10) and then a geometric distance step of 1.2 beyond that distance.

Single-phase Gas Release (Choked) Example

This scenario describes an accidental release of anhydrous HF as a result of a relief valve opening during the filling of a storage vessel. There are several uncertainties regarding the definition of this scenario. The first problem is that the storage conditions specified in the resource document are unrealistic (a temperature of 165 °F and a pressure of 30 psig results in a non-equilibrium condition). Even the conditions in the exit pipe (197 °F) are out of equilibrium. In addition, from the data presented, it is unclear what the release pressure of the relief valve is (does it release at 30 psi or is this the pressure at which it resets). For the conditions defined, the thermodynamics subroutine in HFPLUME determined that the storage conditions are above saturation conditions and the model would not execute because this is a non-equilibrium situation. As a result of the uncertainty in the storage conditions provided, this release was modeled in a simplified fashion by making some assumptions regarding storage conditions.

Based on the temperature and pressure given in the definition of this scenario, or even if more reasonable storage conditions are assumed, this

release will not result in a plume that is denser than ambient air. This was demonstrated by running HFPLUME (version 2.1) for more representative storage conditions with the result that a transition was made from HFPLUME to PGPLUME.

The definition of this scenario is further complicated by the fact that the release duration is only 45 seconds. Using the HFPLUME and PGPLUME models, it is not possible to obtain an accurate 15-minute average concentration for a release of this short duration.

As a result of these issues, this case was modeled as a ground level area source with HEGADAST and assuming that the release rate and release temperatures given are correct. Thus, in modeling the impacts of such a release, we have not accounted for the fact that a release height of 3.7 meters was given. As a result of the modeling approach taken (ground level area source), we may have overstated near field impacts.

Table 6-24 presents the HEGADAST input parameters used in this analysis. Much of this input was taken from Table 5-9. The rest of the input is explained in the HGSYSTEM documentation. The following presents an overview of parameters that require additional explanation. The ICNT parameter was set to 1, which will provide contours of the cloud width and height to the upper and lower concentration limits. These contours reflect an averaging time equivalent to the setting of the AVTIMC parameter (for this scenario, it is 45 seconds). For this scenario, the lower concentration limit (CL) was set to 4.088×10^{-6} kg/m^3 (6 ppm). The model output provides the cloud width and height, to the lower concentration limit for each time step and downwind distance. Thus, one can examine the cloud width as a function of time.

The emission rate in HEGADAST is controlled by the TIMEDATA block. There are three aspects to this data block: TSTPOOL; TSTEPR; and SOURCE. The TSTPOOL input reflects the start time of the emission data. For this case it is set to 0.0, which implies that the emissions are released at the start of the simulation. This value would be set to a positive time if near field

TABLE 6-24. HEGADAST INPUT PARAMETERS FOR RELEASE CLASS 5
(Reference Table 5-5)

```
TITLE    SCENARIO 5 HF RELEASE

CONTROL                        *  --------> DATA BLOCK: CONTROL PARAMETERS
                               *
    ICNT   =      1            *          output code (isocontours,cloud contents)
    ISURF  =      3            *          code for surface heat/water transfer
                               *
AMBIENT                        *  --------> DATA BLOCK: AMBIENT CONDITIONS
                               *
   AIRTEMP = 22.               * C          air temperature at height z = ZAIRTEMP
   ZAIRTEMP= 6.1               * M          height at which AIRTEMP is given
   RHPERC  = 45.               * %          relative humidity
   UO      = 6.26              * M/S        wind speed at height z = ZO
   ZO      = 6.1               * M          height at which UO is given
   TGROUND = 22.               * C          earth's surface temperature
                               *
DISP                           *  --------> DATA BLOCK: DISPERSION DATA
                               *
   ZR      = .01               * M          surface roughness parameter
   PQSTAB  = D                 *            Pasquill stability class
   AVTIMC  =  45.              * S          averaging time for concentration
   CROSSW  = 2 , ,             *            <σy>formula (don't normally change)
                               *
GASDATA                        *  ---------> DATA BLOCK: HF DATA
                               *
   THERMOD = 2                 *          HF thermodynamics model
   CPGAS   = 29.0              * J/MOLE/C specific heat of HF
   MWGAS   = 20.01             * KG/KMOLE molecular weight of HF
   TEMPGAS = 27.00             * C        temperature of HF pool (see NOTE 1)
   HFLIQFR = 1.0               * -        liquid mass fraction of pool (see NOTE1)
                               *
CLOUD                          *  --------> DATA BLOCK: CLOUD OUTPUT CONTROL
                               *
   XSTEP   = 50.               * M          output step length
   CAMIN   = 5E-5              * KG/M3      CA (conc.) at which calcs. are stopped
   CU      = 5E-5              * KG/M3      upper concentration limit
   CL      = 4.088E-6          * KG/M3      lower concentration limit
                               *
CALC                           *  --------> DATA BLOCK: OUTPUT TIMES
                               *
   TSTAR   = 10                * S
   TSTAR   = 12                * S
   TSTAR   = 15                * S
   TSTAR   = 20                * S
   TSTAR   = 40                * S
   TSTAR   = 60                * S
   TSTAR   = 80                * S
```

TABLE 6-24 (CONTINUED)

```
   TSTAR   =  100          * S
   TSTAR   =  120          * S
   TSTAR   =  140          * S
   TSTAR   =  160          * S
   TSTAR   =  180          * S
   TSTAR   =  200          * S
   TSTAR   =  220          * S
   TSTAR   =  240          * S
   TSTAR   =  260          * S
   TSTAR   =  280          * S
   TSTAR   =  300          * S
                           *
TIMEDATA                   *  --------> DATA BLOCK: POOL DATA
                           *
   TSTPOOL =  0.           * S         start time (zero data for time<TSTPOOL)
   TSTEPR  =   5.          * S         time step

**            pool radius    ,  evaporation rate       *  time
*                (m)               (kg/s)                  (s)
*
   SOURCE=       .1          ,        .8513            *  05  SECONDS
   SOURCE=       .1          ,        .8513            *  10  SECONDS
   SOURCE=       .1          ,        .8513            *  15  SECONDS
   SOURCE=       .1          ,        .8513            *  20  SECONDS
   SOURCE=       .1          ,        .8513            *  25  SECONDS
   SOURCE=       .1          ,        .8513            *  30  SECONDS
   SOURCE=       .1          ,        .8513            *  35  SECONDS
   SOURCE=       .1          ,        .8513            *  40  SECONDS
   SOURCE=       .1          ,        .8513            *  45  SECONDS
```

dispersion were described using another model and HEGADAST was started at some distance downwind of the release. The TSTEPR parameter is used to set the time step for the emission data. For this simulation this parameter was set equal to 5 seconds. This parameter provides a check to ensure that emission data are consistent with the dispersion calculations. The SOURCE data provides a description of the size of the area source (pool in the context of the model) and the emission rate. The size of the area source was set to a radius of 0.1 meter. (Model predictions are relatively insensitive to the area source radius value beyond 100 meters.) The number of source steps to be included depends on the actual release duration and the value of TSTEP. Thus, for a 45-second release, 9 SOURCE input was used. The TSTAR parameter contained in the CALC data block specifies the times at which dispersion calculations are performed. The best way to establish the TSTAR value is to estimate the plume transport time to the distance of concern and then bracket this time by several other times. By setting TSTAR in this manner, it ensures that peak concentrations are being calculated. Also, keep in mind that computer time will increase as the number of TSTARs specified in a simulation increases. In the CLOUD data block, the parameter XSTEP is used to specify the downwind distances at which calculations are performed. For this scenario, an XSTEP of 50 was selected. For a specified TSTAR, the concentration of the cloud is computed over a distance of XSTEP. For example, if TSTAR is specified as 60 seconds and XSTEP is 50 meters, then the model will compute the concentrations at a time of 60 seconds from the time of release at 50-meter intervals in a downwind direction.

Because the release duration is 45 seconds, a σ_y averaging time of 45 seconds was used (AVTIMC). This reflects the amount of plume meandering that would occur while the plume is actually present.

The following summarizes the issues associated with these modeling runs. First, the modeling results at ground level near the point of release are conservative because this release is modeled as a ground level area source. Modeling this release using HFPLUME resulted in predicted concentrations at the fenceline of approximately 700 ppm versus 984 ppm predicted by HEGADAST.

Second, there is some confusion regarding the terminology used in the reference document for estimated cloud times. For example, the duration of the maximum concentration at the site boundary will be, by definition, a 15-minute average. From HEGADAST, the peak (45-second) concentration will persist about 20 seconds. Similarly, the peak concentration will drop to 6 ppm after about 15-20 seconds.

Third, horizontal and vertical concentration isopleths to a concentration of 6 ppm can be obtained from the HEGADAST report file (YCL and ZCL). These concentrations, however, reflect a 45-second average and are presented as a function of time. Thus, the model will provide an estimate of the area encompassed within the 6 ppm isopleth at various time sequences. From these data it is possible to determine the area or volume of the 6 ppm isopleth as a function of time. This area should be contrasted to the area that is obtained from a steady state model with a finite release duration correction, such as SLAB or HEGADASS. These models will produce an isopleth that is independent of time.

Single-phase Gas Release (Unchoked) Example

The initial phase of this release was modeled using the PLUME model. A copy of the input to this model is presented in Table 6-25. Much of this input was taken from Table 5-11. The rest of the input is explained in the HGSYSTEM documentation. The following describes the important input to this model as it pertains to this example. The molecular weight used for this simulation was a mean molecular weight based on the mean molar composition (33.1 g/g-mole). The parameter MFGAS was invoked to account for the fact that the plume is only 72.9% HCL. The MFGAS parameter computes mean cloud properties and then, based on the fraction of the pollutant of interest, the total concentration is multiplied by this fraction to estimate the concentration for the component of concern. The duration of the release (720 seconds) was input using the DURATION parameter. This value was passed to the far field dispersion model (HEGADAST or PGPLUME depending on the plume density characteristics).

TABLE 6-25. PLUME MODEL INPUT FOR RELEASE CLASS 6 (Reference Table 5-6)

```
TITLE    SCENARIO 6

GASDATA                      * PHYSICAL PROPERTIES OF GAS
                             *
   TEMPGAS  =  49.0          * CELSIUS        TEMPERATURE OF POLLUTANT
   MFGAS    =  72.95         * PERCENT        MOLE FRACTION OF POLLUTANT
   MFH2O    =  0.1           * PERCENT        MOLE FRACTION OF WATER
   MWGAS    =  33.1          * g/mol          MOLECULAR WEIGHT POLLUTANT
   CPGAS    =  21.0          * J/mol/C        ISOBARIC SPECIFIC HEAT
                             *
PIPE                         * PIPE EXIT-PLANE (CHOKE-FRONT) CONDITIONS
                             *
   DMDT     =  2.52          * KG/S           DISCHARGE RATE
   DEXIT    =  0.8636        * M              EFFECTIVE ORIFICE DIAMETER
   ZEXIT    =  8.54          * M              HEIGHT ABOVE (LEVEL) GROUND
   PHISTK   =  90.00         * DEGREES        RELEASE DISCHARGE ANGLE
   DURATION =  720           * S              RELEASE DURATION (<0 FOR STEADY)

AMBIENT CONDITIONS           * ATMOSPHERIC AMBIENT CONDITIONS
                             *
   Z0       =  10.0          * M              REFERENCE HEIGHT
   U0       =  1.0           * M/S            WIND VELOCITY AT HEIGHT Z0
   AIRTEMP  =  17.9          * CELSIUS        AIR TEMPERATURE
   AIRPRESS =  1.00          * ATMOSPHERES    AMBIENT PRESSURE
   RHPERC   =  36.0          * PERCENT        RELATIVE HUMIDITY
                             *
DISP                         * DISPERSION DATA
                             *
   ZR       =  0.01          * M              SURFACE ROUGHNESS PARAMETER
   PQSTAB   =  B             *                PASQUILL STABILITY CLASS
                             *
TERMINAT                     * JET/PLUME DEVELOPMENT TERMINATION CRITERIA
                             *
   SLST     =  500.          * M              LAST REQD. DOWNWIND DISP.
   DLST     =  -1E6          * M              LAST REQD. PLUME DIAMETER
   ZLST     =  -.35          * M              LAST REQD. PLUME CENTROID RISE HT.
   DXLST    =  -500          * M              LAST REQD. HORIZONTAL DISPLACEMENT
   ULST     =  -0.1          * M/S            LAST REQD. (MEAN) PLUME VELOCITY
   BETLST   =  1E-7          * PERCENT        LAST REQD. POLLUTANT CONCENTRATION
                             *
MATCH                        * MATCHING CRITERIA FOR HEGADAS/PGPLUME
                             *
   RULST    =  .2            *                LAST REQD. ABS. VALUE OF
UJET/UAMB-1
   RELST    =  .3            *                LAST REQD. JET/(JET+HEG) ENTRAINM.
   RGLST    =  .3            *                MAX. BUOYANCY EFFECT FOR ADVECTION
   RNLST    =  .1            *                MAX. BUOY. EFF. FOR PASS.
DISPERSION
```

The PLUME model results indicate that the density of the mixture was not sufficient to cause the plume to touchdown and result in a link to the HEGADAS model, but instead a link was provided to the PGPLUME model. It is interesting to note that if this release was modeled as a pure component, as opposed to the defined mixture, then the PLUME model would predict that the plume would impact the ground as a dense plume and a link would have been made to the HEGADAS model.

Table 6-26 provides a summary of the input used for the PGPLUME model as provided by the PLUME model. Parameters indicated by the "*" are parameters that need to be refined by the user. The final input for the PGPLUME model is provided in Table 6-27. Because the release duration is shorter than the averaging time of concern, a transient model should be used to accurately reflect average concentrations. However, this is not possible in the context of PGPLUME. In order to overcome the issue of using a different averaging time in the crosswind and along-wind planes, PGPLUME was run twice, once with the averaging time set equal to the release duration and once with the averaging time equal to the 30-minutes (IDLH for HCL).

Single-phase Liquid Release (High Volatility) Example

This scenario was modeled using the PLUME model, which provided a transition into HEGADASS. The transition from PLUME to HEGADASS was made at a downwind distance of 88.3 meters and thus HEGADASS was started at this distance using a breakpoint. The modeling was done for a 30-minute average and compared to the IDLH. Tables 6-28, 6-29 and 6-30 present the model input for the PLUME model, the PLUME link file for HEGADASS, and the HEGADASS model input file, respectively. Much of the input in Table 6-28 was taken from Table 5-13. The rest of the input is explained in the HGSYSTEM documentation.

In conducting a modeling analysis of a release that persists for the extent of time calculated in this case, it is important to keep in mind the assumptions and limitations of models like those contained in HGSYSTEM. Thus, if the travel time to the level of concern exceeds several hours, a

TABLE 6-26. PGPLUME LINK FILE CREATED BY THE PLUME MODEL FOR RELEASE CLASS 6

```
TITLE SCENARIO 6

 GASDATA * released gas composition datablock.

   CPGAS=       24.2          * pollutant specific heat (J/mol/C).
   MWGAS=       33.1          * pollutant molecular weight (g/mol).
   GASFRAC=     0.729         * release mole-fraction pollutant (-).
   WATGAS=      1.000E-03     * release mole-fraction water-vapour (-).

 GEOMETRY * plume geometry at matching datablock.

   DXPLUME=     18.6          * matching plane displacement (m).
   ZPLUME=      13.7          * centroid height above ground (m).
   DPLUME=      10.4          * near-plume (effective) diameter (m).
   PHIPLUME=    2.89          * plume axis orientation (degrees).

 STATE * plume dynamic/thermodynamic state.

   UREL=      -3.361E-02      * plume relative velocity (m/s).
   CMASS=      2.267E-02      * nearfield mass-concentration (kg/m3).
   RREL=       2.526E-04      * plume (mean) excess density (kg/m3).
   DURATION=    720.          * (steady) release duration (s).

 AMBIENT * ambient atmosphere datablock.

   AIRTEMP=    17.9           * ambient (air) temperature (C).
   AIRPRESS= 0.999            * ambient (absolute) pressure (atm).
   RHPERC=    36.1            * ambient (relative) humidity (%).
   UATM=       1.03           * wind-speed at centroid height (m/s).
   RATM=       1.21           * ambient atmosphere density (kg/m3).

 DISP * Pasquill/Gifford dispersion data.

   ZR=        1.000E-02       * ground surface roughness (m).
   PQSTAB=       C            * Pasquill/Gifford stability class (-).
  *AVTIMC=     600.            * concentration averaging time (s).

 TERMINAT * output control datablock.

   XFIRST=      18.6          * first required downwind distance (m).
  *STEP=        100.          * arithmetic series step-length (m).
  *NSTEP=        10           * maximum number of (arithmetic) steps (-).
  *FACTOR=      1.20          * scale factor for geometric series (-).
  *XLAST=     1.002E+04       * last required downwind distance (m).
  *VFLAST=      165.          * last required mole concentration (ppm).
```

Note: Parameters which are marked with a * need to by updated to run PGPLUME

TABLE 6-27. PGPLUME LINK FILE CREATED BY THE PLUME MODEL FOR RELEASE CLASS 6

```
TITLE SCENARIO 6

 GASDATA * released gas composition datablock.

   CPGAS=      24.2          * pollutant specific heat (J/mol/C).
   MWGAS=      33.1          * pollutant molecular weight (g/mol).
   GASFRAC=    0.729         * release mole-fraction pollutant (-).
   WATGAS=     1.000E-03     * release mole-fraction water-vapour (-).

 GEOMETRY * plume geometry at matching datablock.

   DXPLUME=    18.6          * matching plane displacement (m).
   ZPLUME=     13.7          * centroid height above ground (m).
   DPLUME=     10.4          * near-plume (effective) diameter (m).
   PHIPLUME=   2.89          * plume axis orientation (degrees).

 STATE * plume dynamic/thermodynamic state.

   UREL=      -3.361E-02     * plume relative velocity (m/s).
   CMASS=      2.267E-02     * nearfield mass-concentration (kg/m3).
   RREL=       2.526E-04     * plume (mean) excess density (kg/m3).
   DURATION=   720.          * (steady) release duration (s).

 AMBIENT * ambient atmosphere datablock.

   AIRTEMP=    17.9          * ambient (air) temperature (C).
   AIRPRESS=  0.999          * ambient (absolute) pressure (atm).
   RHPERC=    36.1           * ambient (relative) humidity (%).
   UATM=       1.03          * wind-speed at centroid height (m/s).
   RATM=       1.21          * ambient atmosphere density (kg/m3).

 DISP * Pasquill/Gifford dispersion data.

   ZR=         1.000E-02     * ground surface roughness (m).
   PQSTAB=        C          * Pasquill/Gifford stability class (-).
   AVTIMC=     1800.         * concentration averaging time (s).

 TERMINAT * output control datablock.

   XFIRST=     18.6          * first required downwind distance (m).
   STEP=       100.          * arithmetic series step-length (m).
   NSTEP=       10           * maximum number of (arithmetic) steps (-).
   FACTOR=     1.20          * scale factor for geometric series (-).
   XLAST=      1.002E+04     * last required downwind distance (m).
   VFLAST=     100.          * last required mole concentration (ppm).
```

TABLE 6-28. PLUME INPUT FOR RELEASE 7 (Reference Table 5-7)

```
TITLE    SCENARIO 7 EHTYLENE OXIDE RELEASE

GASDATA                      * PHYSICAL PROPERTIES OF GAS
                             *
   TEMPGAS  =  10.70         * CELSIUS        TEMPERATURE OF POLLUTANT
   MFGAS    =  100.0         * PERCENT        MOLE FRACTION OF POLLUTANT
   MFH2O    =  0.0           * PERCENT        MOLE FRACTION OF WATER
   MWGAS    =  44.1          * g/mol          MOLECULAR WEIGHT POLLUTANT
   CPGAS    =  24.49         * J/mol/C        ISOBARIC SPECIFIC HEAT
                             *
PIPE                         * PIPE EXIT-PLANE (CHOKE-FRONT) CONDITIONS
                             *
   DMDT     =  0.1220        * KG/S           DISCHARGE RATE
   DEXIT    =  6.35E-3       * M              EFFECTIVE ORIFICE DIAMETER
   ZEXIT    =  0.50          * M              HEIGHT ABOVE (LEVEL) GROUND
   PHISTK   =  0.000         * DEGREES        RELEASE DISCHARGE ANGLE
   DURATION =  -1            * S              RELEASE DURATION (<0 FOR STEADY)

AMBIENT CONDITIONS           * ATMOSPHERIC AMBIENT CONDITIONS
                             *
   Z0       =  10.0          * M              REFERENCE HEIGHT
   U0       =  2.0           * M/S            WIND VELOCITY AT HEIGHT Z0
   AIRTEMP  =  28.0          * CELSIUS        AIR TEMPERATURE
   AIRPRESS =  1.00          * ATMOSPHERES    AMBIENT PRESSURE
   RHPERC   =  50.0          * PERCENT        RELATIVE HUMIDITY
                             *
DISP                         * DISPERSION DATA
                             *
   ZR       =  0.01          * M              SURFACE ROUGHNESS PARAMETER
   PQSTAB   =  E             *                PASQUILL STABILITY CLASS
                             *
TERMINAT                     * JET/PLUME DEVELOPMENT TERMINATION CRITERIA
                             *
   SLST     =  500.          * M              LAST REQD. DOWNWIND DISP.
   DLST     =  -1E6          * M              LAST REQD. PLUME DIAMETER
   ZLST     =  -.35          * M              LAST REQD. PLUME CENTROID RISE HT.
   DXLST    =  -500          * M              LAST REQD. HORIZONTAL DISPLACEMENT
   ULST     =  -0.1          * M/S            LAST REQD. (MEAN) PLUME VELOCITY
   BETLST   =  1E-7          * PERCENT        LAST REQD. POLLUTANT CONCENTRATION
                             *
MATCH                        * MATCHING CRITERIA FOR HEGADAS/PGPLUME
                             *
   RULST    =  .2            *                LAST REQD. ABS. VALUE OF
UJET/UAMB-1
   RELST    =  .3            *                LAST REQD. JET/(JET+HEG) ENTRAINM.
   RGLST    =  .3            *                MAX. BUOYANCY EFFECT FOR ADVECTION
   RNLST    =  .1            *                MAX. BUOY. EFF. FOR PASS.
DISPERSION
```

TABLE 6-29. HEGADASS LINK FILE GENERATED BY PLUME FOR RELEASE CLASS 7

```
TITLE SCENARIO 7 EHTYLENE OXIDE RELEASE

 ****************************************************
 *    Input file for the (steady-state) heavy gas   *
 *       advection model HEGADAS-S. The file is     *
 *    generated by the near field dispersion model  *
 *      PLUME. It incorporates all the breakpoint   *
 *     data generated by PLUME together with such   *
 *      additional variables and flags needed to    *
 *   ensure physical consistency. In addition, the  *
 *    file contains variables needed to complete a  *
 *    viable input file suitable for submission to  *
 *    HEGADAS-S; Such additional data are prefixed  *
 *     by an asterisk (*) and should be physically  *
 *   and contextually sensible, but may be changed  *
 * at the user's discretion. Such data may also be  *
 *  overwritten by the addition of keywords to the  *
 *   HEGADAS-S partial input file under HGSYSTEM.   *
 ****************************************************

CONTROL * HEGADAS Control Flags Datablock.

 *ICNT=   0                 * flag controlling contour generation (-).
  ISURF=   3                * flag indicating plume/ground heat transfer (-).

AMBIENT * Ambient Atmosphere Datablock.

  ZAIRTEMP= 0.500           * height of temperature measurement (m).
  AIRTEMP=   28.0           * ambient (air) temperature (C).
  ZO=        10.0           * height of wind-speed measurement (m).
  UO=        2.00           * ambient wind-speed (m/s).
  RHPERC=   50.0            * atmosphere relative humidity (%).
 *TGROUND=   27.6           * ground surface temperature (C).

DISP * farfield/heavy-gas dispersion Data.

  ZR=       1.000E-02       * surface roughness height (m).
  PQSTAB=     E             * Pasqill/Gifford stability class.
 *AVTIMC=    600.           * concentration averaging time (s).
 *CROSSW=      2,,          * <σy> formulation selected (-).

GASDATA * Released gas Datablock.

  THERMOD=    1             * thermodynamic model flag (-).
  GASFLOW=  0.122           * HF mass flow-rate dry gas (kg/s).
  CPGAS=     24.5           * specific heat of gas (J/mol/C).
  MWGAS=     44.1           * molecular weight of gas (g/mol).
```

TABLE 6-29 (CONTINUED)

```
    GASFRAC=   1.00          * mole fraction pollutant in released gas (-).
    HEATGR=    20.0          * ground heat transfer factor (-).
    WATGAS=   0.000E-01      * mole-fraction water in released gas (-).
    TEMPGAS=  -95.7          * gas temperature immediately upon release (C).

  TRANSIT * PLUME/HEGADAS Transition Datablock.

    DISTS=     88.3          * downwind distance from release point (m).
    CONCS=    1.027E-03      * center-line ground-level molar gas fraction
(-).
    WS=       -11.3          * heavy-gas plume half-width (signed flag) (m).

 *CLOUD * Output control datablock.

   *DXFIX=     100.          * arithmetic progression step length (m).
   *NFIX=      10            * maximum number of (arithmetic) steps (-).
   *XGEOM=     1.20          * scale factor for geometric series (-).
   *XEND=    1.009E+04       * last required downwind distance (m).
   *CU=      1.292E-04       * inner contour concentration (kg/m3).
   *CL=      1.292E-05       * outer contour concentration (kg/m3).
   *CAMIN=   1.292E-05       * last required gas concentration (kg/m3).
```

TABLE 6-30. HEGADASS INPUT FILE FOR RELEASE CLASS 7

```
TITLE SCENARIO 7 EHTYLENE OXIDE RELEASE

 CONTROL * HEGADAS Control Flags Datablock.

   ICNT=    1                 * flag controlling contour generation (-).
   ISURF=   3                 * flag indicating plume/ground heat transfer (-).

 AMBIENT * Ambient Atmosphere Datablock.

   ZAIRTEMP= 0.500            * height of temperature measurement (m).
   AIRTEMP=   28.0            * ambient (air) temperature (C).
   ZO=        10.0            * height of wind-speed measurement (m).
   UO=        2.00            * ambient wind-speed (m/s).
   RHPERC=   50.0             * atmosphere relative humidity (%).
   TGROUND=   28.6            * ground surface temperature (C).

 DISP * farfield/heavy-gas dispersion Data.

   ZR=       1.000E-02        * surface roughness height (m).
   PQSTAB=     E              * Pasqill/Gifford stability class.
   AVTIMC=   1800.            * concentration averaging time (s).
   CROSSW=      2,,           * <σy> formulation selected (-).

 GASDATA * Released gas Datablock.

   THERMOD=    1              * thermodynamic model flag (-).
   GASFLOW=  0.122            * HF mass flow-rate dry gas (kg/s).
   CPGAS=     24.5            * specific heat of gas (J/mol/C).
   MWGAS=     44.1            * molecular weight of gas (g/mol).
   GASFRAC=   1.00            * mole fraction pollutant in released gas (-).
   HEATGR=    20.0            * ground heat transfer factor (-).
   WATGAS=   0.000E-01        * mole-fraction water in released gas (-).
   TEMPGAS=  -95.7            * gas temperature immediately upon release (C).

 TRANSIT * PLUME/HEGADAS Transition Datablock.

   DISTS=     88.3            * downwind distance from release point (m).
   CONCS=    1.027E-03        * center-line ground-level molar gas fraction
(-).
   WS=       -11.3            * heavy-gas plume half-width (signed flag) (m).

 CLOUD * Output control datablock.

   DXFIX=      10.            * arithmetic progression step length (m).
   NFIX=      10              * maximum number of (arithmetic) steps (-).
   XGEOM=     1.10            * scale factor for geometric series (-).
   XEND=     1.009E+04        * last required downwind distance (m).
   CU=       .1               * inner contour concentration (kg/m3).
   CL=       .0014            * outer contour concentration (kg/m3).
   CAMIN=    1.292E-05        * last required gas concentration (kg/m3).
```

persistence analysis should be conducted to ensure that such long travel times are plausible.

Single-phase Liquid Release (Low Volatility) Example

This case reflects a spill from a storage tank that contains 30 percent HCL with the balance being water. This release is assumed to be contained as a liquid pool within the tank diking.

This case was modeled using the HEGADASS model and the emission rate calculated in the scenario description. It should be noted that the emission calculations for this case reflect a very simplified screening approach. For such a release the emission rate will not be constant over time. Effects such as cooling of the pool as a result of evaporation will suppress the emission rate. Because this case is designed to compare impacts against an ERPG (60-minute average) LOC, the variations in emissions could be quite important. While the EVAP model contained in HGSYSTEM could not be completely adapted to this scenario, EVAP could provide a more realistic estimate of emissions from the pool then the rate provided from the screening calculation.

While this release is not a dense gas release, the HEGADASS model can accurately simulate both the dense gas and trace gas regions and, therefore, it is applicable to this release. Because the emissions were not denser than air, this release was modeled by only examining the HCL portion of the cloud. Thus an emission rate of 0.00427 kg/s was used. This release also could have been modeled by invoking the GASFRACT parameter, which would automatically account for the HCL fraction. This approach was not taken because it would have made obtaining cloud widths more difficult.

Table 6-31 presents the HEGADASS model input used in modeling this case. Much of this input was taken from Table 5-15. The rest of the input is explained in the HGSYSTEM documentation. In modeling this case, the CU parameter was set to 20 ppm and the CL parameter was set to 3 ppm. Thus from

TABLE 6-31. HEGADASS INPUT FILE FOR RELEASE CLASS 8 (Reference Table 5-8)

```
* ================ HEGADAS-S standard input file STPOOLNO.HSI
==================
*            (case: run started at pool, normal thermodynamics)

TITLE   SCENARIO 8 HCL EVAPORATING POOL

CONTROL                    *  --------> DATA BLOCK: CONTROL PARAMETERS
                           *
    ICNT   =      1        *          output code (isocontours,cloud contents)
    ISURF  =      3        *          code for surface heat/water transfer
                           *
AMBIENT                    *  --------> DATA BLOCK: AMBIENT CONDITIONS
                           *
   AIRTEMP = 18.5          * C          air temperature at height z = ZAIRTEMP
   ZAIRTEMP= 10.7          * M          height at which AIRTEMP is given
   RHPERC  = 58.           * %          relative humidity
   U0      = 2.24          * M/S        wind speed at height z = Z0
   Z0      = 10.7          * M          height at which U0 is given
   TGROUND = 18.5          * C          earth's surface temperature
                           *
DISP                       *  --------> DATA BLOCK: DISPERSION DATA
                           *
   ZR      = 0.01          * M          surface roughness parameter
   PQSTAB  = C             *            Pasquill stability class
   AVTIMC  = 3600.         * S          averaging time for concentration
   CROSSW  = 2             *            <σy>formula (don't normally change)
                           *
GASDATA                    *  ---------> DATA BLOCK: GAS DATA
                           *
   GASFLOW = .00427        * KG/S     gas emission rate (excl. water pick-up)
   TEMPGAS =  18.5         * C        temperature of emitted gas
   CPGAS   = 32.5          * J/MOLE/C specific heat of emitted gas
   MWGAS   = 30.2          * KG/KMOLE molecular weight of emitted gas
   WATGAS  = 0.            * -        water pick-up by gas (don't norm.change)
   HEATGR  = 29.           * .....    gas group for natural-conv. heat flux
                           *
CLOUD                      *  --------> DATA BLOCK: CLOUD OUTPUT CONTROL
                           *
   DXFIX   = 1.            * M          fixed-size output step length
   NFIX    = 200           *            fixed steps upto distance x =
NFIX*DXFIX
   XEND    = 3000.         * M          x at which calculations are stopped
   CAMIN   = 0.1E-5        * KG/M3      CA (conc.) at which calcs. are stopped
   CU      = 2.4718E-5     * KG/M3      upper concentration limit
   CL      = 3.708E-6      * KG/M3      lower concentration limit
                           *
POOL                       *  --------> DATA BLOCK: POOL DATA
                           *
   PLL     =  7.3          * M          pool length
   PLHW    =  3.66         * M          pool half-width
```

a model run, model predictions on cloud width could be obtained for these two ERPG concentration levels. The width of the 100 ppm isopleth could have been developed in an analogous manner.

6.5 SLAB

The specific input required by the SLAB model and a brief description is listed in Table 6-32. It includes information on the type of release; physical property information on the material released; release rate, height and duration; fraction of the release that is liquid; concentration averaging time; maximum downwind distance of interest; height above ground of concentration calculations; meteorological information; and site roughness characteristics. In the comments column for many of the input parameters of Table 6-32 the subsection in Section 4 is given which discusses how that parameter is calculated.

Table 6-33 shows the value of each input parameter used for the eight release class examples. In a few cases a value different from that given in Section 5 was used. Values that are different from those given in Section 5 are highlighted in Table 6-33. Those occurrences are described below. In the column header for each release class, the table in Section 5 from which the input was taken is given. The tables in Section 5, in turn, each reference the section in which the calculation was done.

The release class examples are:

Release Class (RC)	Title
1	Two-Phase Gas Release (Choked)
2	Two-Phase Gas Release (Unchoked)
3	Two-Phase Pressurized Liquid
4	Two-Phase Refrigerated Liquid
5	Single-Phase Gas Release (Choked)
6	Single-Phase Gas Release (Unchoked)
7	Single-Phase Liquid Release (High Volatility)
8	Single-Phase Liquid Release (Low Volatility)

TABLE 6-32. SLAB MODEL INPUT PARAMETERS

Input Parameter Name	Description of Input Parameter	Comments
idspl	type of release	1 = liquid pool 2 = horizontal 3 = vertical 4 = instantaneous
ncalc	number of calculation steps	
wms	molecular weight of source gas (kg/g-mole)	4.2
cps	heat capacity at constant pressure (j/kg-degK)	4.2
tbp	boiling point temperature (deg K)	4.2
cmed	initial liquid mass fraction	4.9
dhe	heat of vaporization (j/kg)	4.2
cpsl	liquid heat capacity (j/kg-deg K)	4.2
rhosl	liquid density of source material (kg/m^3)	4.2
spb	saturation pressure constant b	if unknown, spb = -1
spc	saturation pressure constant c	if unknown, spc = 0
ts	temperature of source gas (degK)	4.8
qs	mass source rate (kg/s)	4.7
as	source area (m^2)	4.12
tsd	continuous source duration (s)	4.4
qtis	instantaneous source mass (kg)	4.4
hs	source height (m)	4.14
tav	concentration averaging time (sec)	4.16
xffm	far field length (m)	

TABLE 6-32 (CONTINUED)

Input Parameter Name	Description of Input Parameter	Comments
zp(1),zp(2),zp(3),zp(4)	concentration measurement heights (m)	4.18
z_0	surface roughness height (m)	4.17.3
za	ambient wind measurement height (m)	4.17.1
ua	ambient wind speed (m/s)	4.17.1
ta	ambient temperature (deg K)	4.17.5
rh	relative humidity (%)	4.17.5
stab	stability class	4.17.2

TABLE 6-33. SLAB MODEL INPUT USED FOR THE EIGHT RELEASE CLASSES (RC). NUMBERS IN () INDICATE THE TABLE TO REFERENCE FOR SOURCE OF INPUT DATA.

Input Parameter name	Input Values RC 1 (5-1)	Input Values RC 2 (5-2)	Input Values RC 3 (5-3)	Input Values RC 4 (5-4)	Input Values RC 5 (5-5)	Input Values RC 6 (5-6)	Input Values RC 7 (5-7)	Input Values RC 8 (5-8)
idspl	2	2	2	3	2	3	2	1
ncalc	1	1	1	1	1	1	1	1
wms	.044054	.044054	.070906	.064063	.0350	.03307	.044054	.03019
cps	1078	1078	481.5	623.1	1456	1054	1078	980.98
tbp	283.85	283.85	239.15	263.13	292.67	188.15	283.85	370.2
cmed	0.0133	0.0133	0.8221	0.786	0	0	1	1
dhe	568954	568994	287775	388747	376440	442708	568994	2354863
cpsl	1972	1972	927.3	1386	2560	1655.85	1972	3475
rhosl	882.7	882.7	1562	1460	955	1194.2	882.7	993.3
spb	2507.61	2507.61	1978.34	2302.35	3404.51	-1	2507.61	-1
spc	-29.01	-29.01	-27.01	-35.97	15.06	0	-29.01	0
ts	283.85	283.85	239.09	263.13	313.6	322.04	283.85	291.48
qs	.0634	.0503	.3170	4.154	.8513	2.5151	.1220	.005365
as	.0002337	.0001882	.003020	.01344	0.003167	.585754	.014784	53.53
tsd	480	480	672	1584	[illegible]	720	7200	7200
qtis	0	0	0	0	0	0	0	0
hs	[illegible]	[illegible]	2	.3049	3.66	8.54	.5	0
tav	5	5	900	900	900	1800	1800	3600
xffm	1000	1000	2000	10000	1000	10000	10000	10000
zp(1)	0	0	0	0	0	0	0	0
z_0	.01	.01	.01	.01	.01	.01	.01	.01
za	4.57	6.10	10	6	6.1	10	10	10.7
ua	5.37	2.68	4.47	3.13	6.26	.98	2	2.24
ta	287.52	296.48	294.38	291.15	295.15	290.9	301	291.48
rh	62	37	50	42	45	36	50	58
stab	3	3	3	5	4	2	5	3

Two-phase Gas Release (Choked and Unchoked) Examples

The height of release is assumed to be ground level, even though the release occurred at 3.66 meters above the ground. As shown in Figure 5-1, it is a downward directed release. Since SLAB is not configured to handle downward directed releases, a ground level release was assumed.

Single-phase Gas Release (Choked) Example

The text describing this scenario suggested that either an instantaneous release or a 45-second-long continuous release could be used for this scenario. Even though an instantaneous release was recommended, the scenario was modeled as a continuous release with a 45 second duration.

SLAB is capable of simulating a release of any duration. In this case the scenario was also run as instantaneous, with little difference in the results. It is suggested that if the release duration is known, the actual duration of the release should be used rather than simulating the release as instantaneous. This is not to suggest that the instantaneous release option should never be used. If the release duration is very much less than the travel time to a receptor, the instantaneous option can be used.

Single-phase Gas Release (Unchoked) Example

The release is a mixture of HCL, water, and air, but the only chemical of concern is the HCL. This release was modeled as a mixture with the predicted output concentrations adjusted to account for only the HCL portion of the release. This was done by multiplying the predicted concentrations by the value of f_i, 0.7295. The apparent molecular weight, which was calculated in Section 5.6.11, and the mixture gas phase specific heat, calculated in Section 5.6.2, were used to describe the chemical.

Single-phase Liquid Release (High Volatility) Example

Because this release is a highly volatile liquid release, there is a concern that this release may actually cause a pool formation. Section 4.7.7 suggests that the release be assumed to volatilize immediately upon release, so that is what was done.

Single-phase Liquid Release (Low Volatility) Example

The release in this scenario is a liquid mixture of 30% HCL and 70% water. It forms a liquid pool, from which HCl and wter evaporate into the atmosphere, as described in Section 5.8.7. It was suggested that the release be modeled as if it were only HCL. However, for the SLAB modeling, this scenario was modeled as a mixture, with the predicted concentrations adjusted to account for the HCL-only portion of the release by multiplying the concentration results by the value of f_i, 0.01258.

SECTION 7

MODEL OUTPUT

This section gives examples of each model's output and describes how to use the output to determine the following impacts of concern:

- Maximum off-site concentration;
- Maximum distance downwind of specified concentration;
- Maximum width of specified concentration;
- Maximum time-averaged (e.g. 30 minutes) off-site concentration;
- Maximum time-averaged concentration at a specific point;
- Time at which the maximum concentration is reached at a specific point;
- Duration above specified concentration at a point;
- Time the specified concentration is reached at a point; and
- Total area impacted by specified concentration.

Not all of the above impacts of concern are available from each model. Furthermore, for certain models further manipulation of the output may be required to generate some of the impacts presented here. If so, the method is described in this section. Examples of available graphical output are presented.

Rather than discuss all output of each model, in this document only the procedures required to generate output for the specified impacts of concern are discussed. For more discussion of the output of a specific model, consult the user's guide for that model.

7.1 ADAM

By default, ADAM presents its output as a graphic representation of the cloud contour for the input concentration or dose of interest. The graphic shows a concentration (ppm) or dose (ppm-s) isopleth superimposed on an x-y coordinate system representing the north, south, east and west directions. A typical output is shown in Figure 7-1. The box to the right of the figure lists the chemical name, wind speed, source mass (instantaneous release) or source rate (continuous release), dispersion duration, maximum cloud width, and maximum centerline downwind distance to the specified concentration or dose. A hard copy of the output can be obtained by dumping the screen to the available printer.

Obtaining output on specific parameters is discussed in the following paragraphs.

Maximum off-site concentration.
Maximum time-averaged off-site concentration.
Maximum time-averaged concentration at a specific point.

The above parameters are not directly available from ADAM. However, these parameters can be estimated as long as the maximum hazard distance (labeled MAX HAZARD DIST in Figure 7-1) is greater than the distance to the site boundary or a specific point of interest. The estimates are made by invoking the re-plot routine, which is available after leaving the graphics display, and specifying that the cloud contour be re-plotted for a concentration or dose higher than the original value. If the resulting plot indicates a corresponding distance greater than the site boundary distance, the concentration or dose level must be increased and the plot re-displayed. Likewise, if the resulting distance is less than the site boundary distance, the concentration or dose should be decreased and the results re-plotted.

Since the re-plotted contours are based on the dispersion calculations for the original concentration or dose of interest, the exact distance of

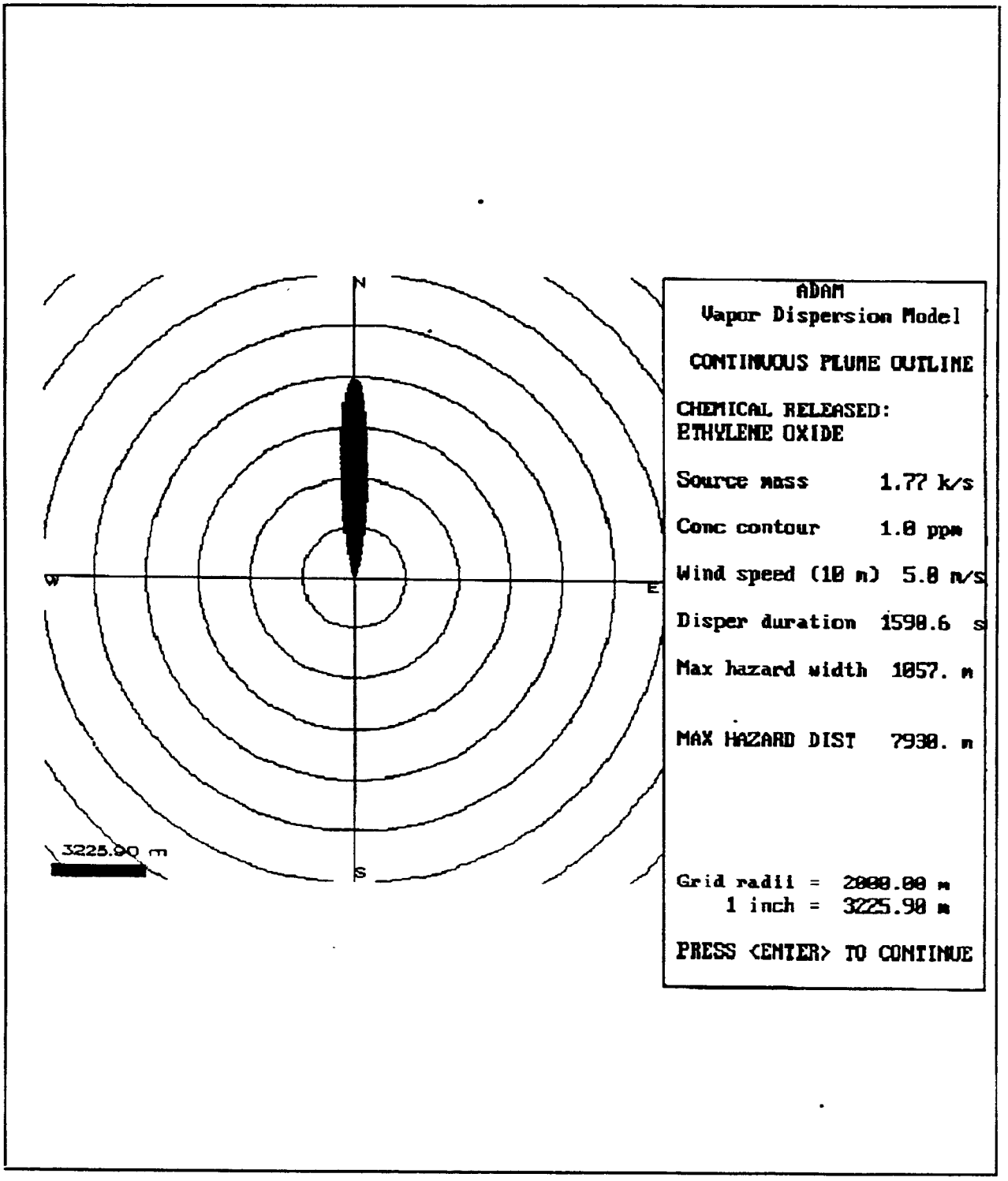

Figure 7-1. Typical ADAM Model Output

interest can not be obtained. However, this distance can be estimated by interpolating between two distances, one on each side of the distance of interest.

To determine the maximum off-site concentration, the distance to the site boundary must be used as a specific point. Then treat the maximum offsite concentration as though it were the maximum concentration at that point. This approach is only rigorously true if the emission remains at ground level.

Maximum distance downwind of specified concentration.

This parameter is displayed in the standard ADAM output (see Figure 7-1). It is labeled "MAX HAZARD DIST."

Maximum width of specified concentration.

This parameter also is displayed the standard ADAM output. It is labeled "Max hazard width."

Time at which the maximum concentration is reached at a specific point.
Duration above specified concentration at a point.
Time the specified concentration is reached at a point.

The only information available from ADAM for concentration timing is the location of the leading edge of a specific concentration. That information is made available by storing the results (called "output DATA" in ADAM) in a file. An example is given in Table 7-1. For the concentration of the contour, its distance from source as a function of time is tabulated. There is no information output describing the timing of the maximum concentration or duration at specific points. The peak concentration is given as a function of time, not location.

TABLE 7-1 EXAMPLE DATA OUTPUT FILE FROM THE ADAM MODEL

DISPERSION CALCULATION RESULTS
99 = # of Points
Contour for Concentration = 5.000000 ppm

Time Since Release (s)	Distance From Source (m)	Velocity of Plume or Puff (m/s)	Peak Concentration (ppm)	Peak Dose (ppm-s)	Contour Width (m)
16.47	27.51	1.6780	15817.	.0000	27.51
16.76	28.00	1.6774	15734.	.0000	29.04
17.25	28.82	1.6761	15598.	.0000	29.39
17.98	30.05	1.6743	15400.	.0000	29.92
19.01	31.77	1.6720	15102.	.0000	30.65
20.40	34.09	1.6690	14414.	.0000	31.63
22.24	37.14	1.6652	12957.	.0000	32.88
24.62	41.10	1.6607	10963.	.0000	34.48
27.67	46.15	1.6557	8901.8	.0000	36.47
31.54	52.53	1.6499	7045.6	.0000	38.92
36.42	60.56	1.6438	5486.7	.0000	41.92

Total area impacted by specified concentration

Although not calculated by ADAM, the ground area covered by the cloud contour can be estimated by assuming that the shape of the contour is elliptical. The hazard area within the isopleth can then be determined from the area equation of an ellipse having a major axis equal to the centerline maximum downwind distance (X_{max}) and a minor axis equal to the maximum cloud width (Y_{max}). Thus, the ground area covered by the cloud would be:

$$\text{AREA} = \left(\frac{\pi}{4}\right) \times (X_{max}) \times (Y_{max}).$$

7.2 ALOHA

ALOHA was initially designed to be a first-responders tool rather than a planning tool. Because of this, the available output are somewhat limited. The only impact output available from ALOHA is:

- Dispersion footprint;
- Concentration versus time; and
- Dose versus time.

A text summary of input required by ALOHA and examples of output are provided in Section 6.2. In addition, the output parameter, Source Strength versus Time, is also available.

The Source Strength does not indicate downwind impacts. Furthermore, it is recommended that footprints not be used in transient releases, unless it has been confirmed through point-by-point interrogation (i.e., the use of the "Concentration" option) that the footprint is not being over-estimated. The maximum output time is 60 minutes.

Three examples of ALOHA output are presented in Figures 7-2 through 7-4. The published version of ALOHA does not include tabular output. The concentration values are assumed to be for five-minute averages; other

Footprint Window

2804080279

Chemical Name: ETHYLENE OXIDE
Note: Potential or confirmed human carcinogen.
Model Run: Heavy Gas
Wind: 2 meters/sec from N

FOOTPRINT INFORMATION:
Model Run: Heavy Gas
User specified LOC: equals IDLH (800 ppm)
Max Threat Zone for LOC: 50 meters
Note: The Heavy Gas footprint is an initial screening.
For short releases it may be an overestimation.
Be sure to check concentration information at specific locations.

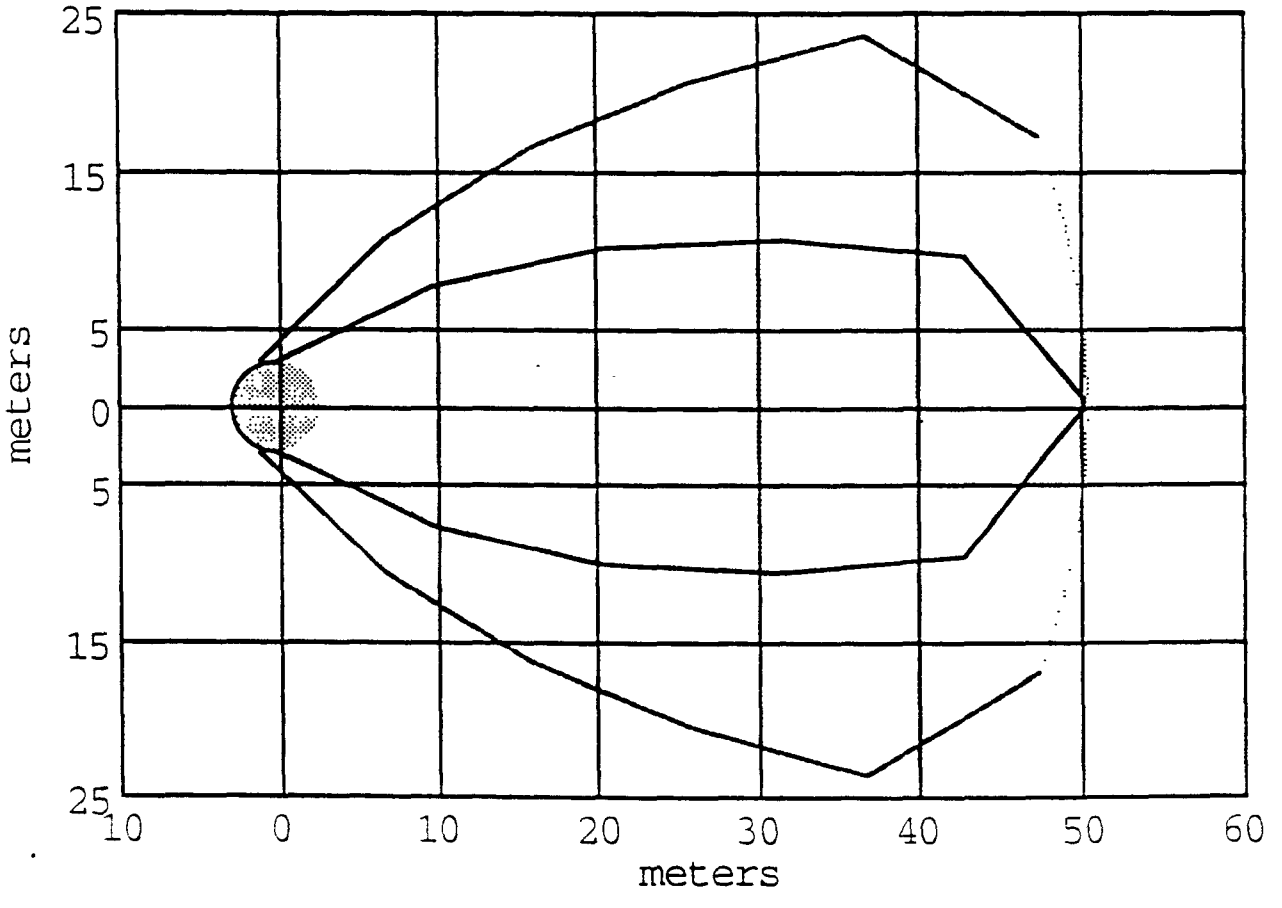

Figure 7-2. Footprint Window

Concentration Window

2804080354

```
Chemical Name: ETHYLENE OXIDE
   Note: Potential or confirmed human carcinogen.
Model Run: Heavy Gas
Building Air Exchanges Per Hour: 0.01 (User specified)


TIME DEPENDENT INFORMATION:
   Concentration/Dose Estimates at the point:
   Downwind:        100 meters
   Off Centerline: 0 meters
   Max Concentration:
      Outdoor: 279 ppm
      Indoor:  2.69 ppm
   Max Dose:
      Outdoor: 16,200 (ppm,min)
      Indoor:  78.6 (ppm,min)
   Note: Indoor graphs are shown with a dotted line.
```

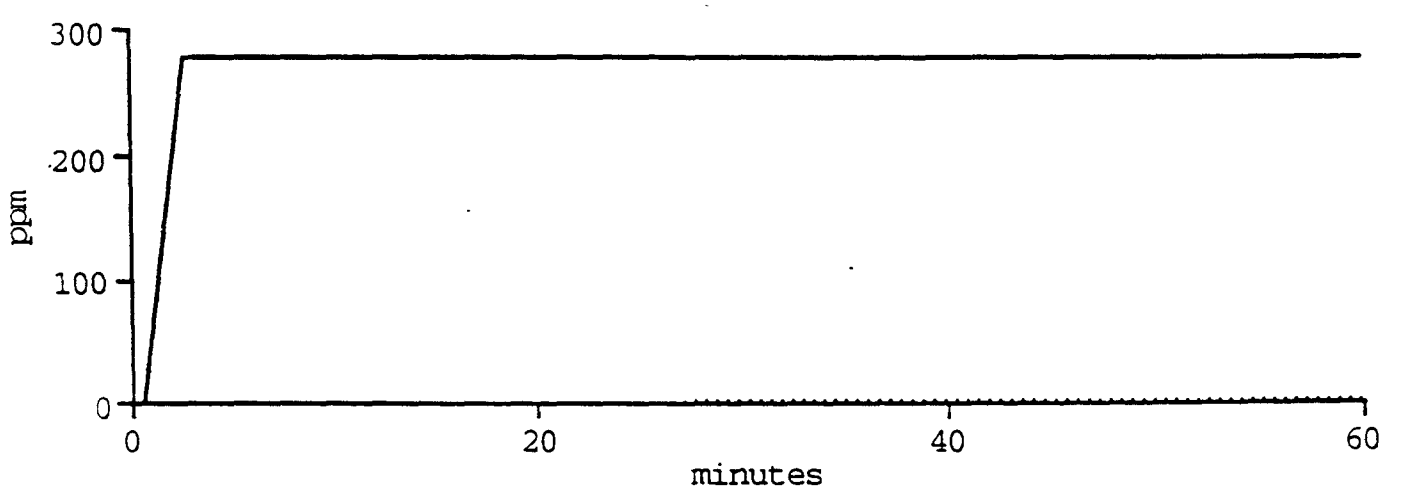

Figure 7-3. Concentration versus Time Plot

Dose Window

2804080315

```
Chemical Name: ETHYLENE OXIDE
   Note: Potential or confirmed human carcinogen.
Model Run: Heavy Gas
Building Air Exchanges Per Hour: 0.01 (User specified)


TIME DEPENDENT INFORMATION:
   Concentration/Dose Estimates at the point:
   Downwind:        100 meters
   Off Centerline: 0 meters
   Max Concentration:
      Outdoor: 279 ppm
      Indoor:  2.69 ppm
   Max Dose:
      Outdoor: 16,200 (ppm,min)
      Indoor:  78.6 (ppm,min)
   Note: Indoor graphs are shown with a dotted line.
```

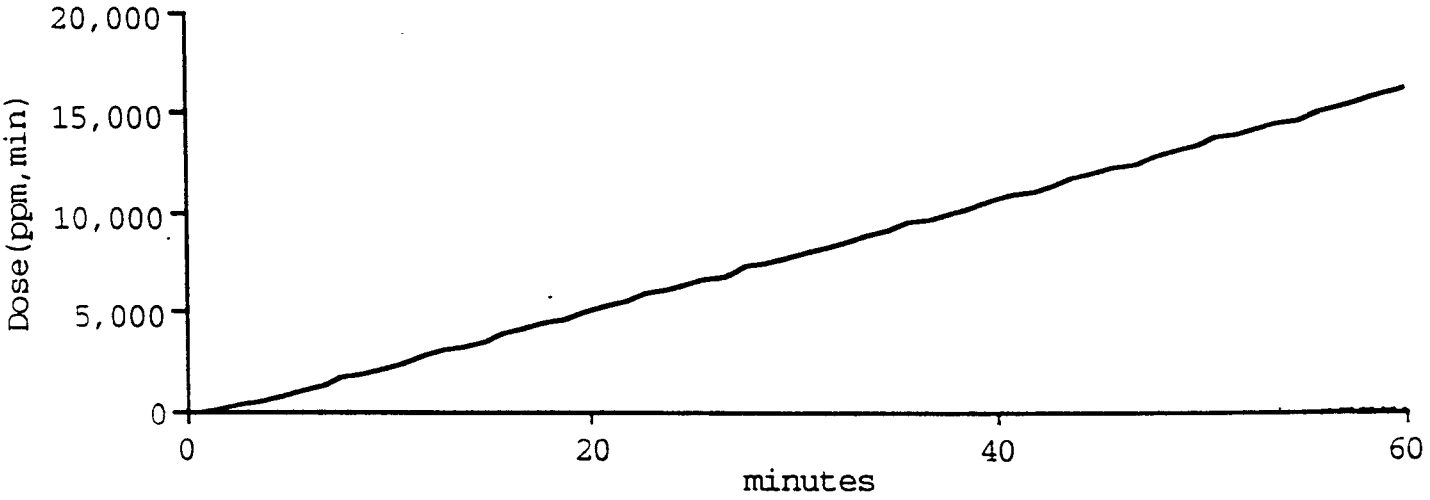

Figure 7-4. Dose versus Time Plot

averaging times are not available. The concentration of interest, however, is selectable.

Specific parameters are discussed below.

Maximum off-site concentration.
Maximum time-averaged off-site concentration.
Maximum time-averaged concentration at a specific point.
Time at which the maximum concentration is reached at a specific point.
Duration above specified concentration at a point.
Time the specified concentration is reached at a point.

To determine the maximum off-site concentration, the distance to the site boundary must be used as a specific point. Then treat the maximum off-site concentration as though it were as the maximum concentration at that point. This approach is only rigorously true if the emission remains at ground level.

Figure 7-3 shows a plot reflecting Concentration-versus-Time. The location of the point, which is selectable, is given as a pair of downwind and off-centerline distances. The maximum concentration and dosage are given numerically on the output. This plot can be used to determine maximum concentration at a point, as well as duration over some concentration (graphically). Concentration predictions for both indoor and outdoor scenarios are available.

The Dose-versus-Time parameter (Figure 7-4) contains the same numerical data as given in the Concentration-versus-Time output. The dose plot is that derived from the equation given in Section 4.16. Since the dosage is given in ppm-min, a new concentration with an averaging time larger than five minutes can be estimated by dividing the dose by the new time. Dosage predictions for both indoor and outdoor scenarios are available.

Maximum distance downwind of specified concentration

This parameter is available from the output displayed in Figure 7-2. It is labeled "Max Threat Zone for LOC."

Maximum width of specified concentration

This parameter can be approximated from the output displayed in Figure 7-2. The size of the axis on the left of Figure 7-2 represents the cross-wind width, which can be used to plot the plume.

Total area impacted by specified concentration

The Footprint output, shown in Figure 7-2, graphically presents the extent of a specified concentration. For short releases, the footprint may be over-estimated. The maximum area of impact can only be determined by a trial-and-error method.

7.3 DEGADIS

The DEGADIS model output is separated into two parts. The first gives the results from the jet sub-model. This output represents plume characteristics of the elevated jet portion of a release. An example of the output is in Table 7-2. The elevation of the jet is calculated as a function of downwind distance. Once the jet touches ground, DEGADIS switches from the jet sub-model to the ground level plume dispersion sub-model. An example of the output from that sub-model of DEGADIS is shown in Table 7-3. The example outputs given in Tables 7-2 and 7-3 are for the steady-state case. If the release is transient, the output is very similar, except that a table is created for varying times after the release. An example and discussion of a transient table is given below.

TABLE 7-2. EXAMPLE OUTPUT FROM THE JET SUB-MODEL OF DEGADIS--JETPLU/DEGADIS v2.1

```
22-DEC-1992 12: 3:48.59

 Radian case 3:  Chlorine release from a pipe attached to a one-ton cylinder
                 Two-phase release from pressurized (saturated) liquid
                 release rate: 0.3139 kg/s; initial density: 19.71 kg/m3


 Ambient Meteorological Conditions...

 Ambient windspeed at reference height:    4.4700      m/s
                     Reference height:    10.000       m
                    Surface roughness:   1.00000E-02   m

             Pasquill stability class:              C

                 Monin-Obukhov length:   -30.431      m

                   Friction velocity:     .24814      m/s
                 Ambient temperature:    294.30       K
                    Ambient pressure:    1.0000       atm
                    Ambient humidity:   7.98079E-03
                   Relative humidity:    50.000       %

             Specified averaging time:    678.00      s
                              DELTAy:     .21520
                               BETAy:     .90000
                              DELTAz:   9.62300E-02
                               BETAz:     .94770
                              GAMMAz:  -2.00000E-03

Contaminant Properties...

        Contaminant molecular weight:    70.910
                 Initial temperature:    238.70      K
             Upper level of interest:   1.00000E-05
             Lower level of interest:   1.00000E-06
               Average heat capacity:    476.44      J/kg K

NDEN flag:   2
 Mole fraction  Concentration     Density
                  (kg/m3)         (kg/m3)
    .00000        .00000         1.1936
   1.0000        19.710         19.710

ISOFL flag:   1

Release Properties...

                       Release rate:    .31390      kg/s
                 Discharge elevation:   2.0000      m
                  Discharge diameter:  7.03600E-03  m
```

TABLE 7-2 (CONTINUED)

Model Parameters...

ALFA1: 2.80000E-02
ALFA2: .37000
DISTMX: 50.000 m

Downwind Distance (m)	Elevation (m)	Centerline Mole Fraction Concentration (kg/m3) ③		Density (kg/m3)	Temp. (K)	Sigma y (m)	Sigma z (m)	At z = .000 m: Mole Fraction ④	Width to mol%: (m)	(m)	Maximum Mole Fraction ⑤	Elevation for Max Mol Frac. (m)
3.965E-13	2.05	1.00	19.7	19.7	294.	3.880E-03	3.884E-03	.000			1.00	2.05
26.7	8.63	4.489E-04	1.319E-03	1.19	294.	4.26	2.36	.000			4.489E-04	8.63
57.0	8.83	1.232E-04	3.619E-04	1.19	294.	8.27	4.45	3.445E-05	17.8	13.0	1.232E-04	8.82
84.7	8.86	6.224E-05	1.828E-04	1.19	294.	11.8	6.33	4.578E-05	25.3	20.5	6.235E-05	8.45
111.	8.86	4.113E-05	1.208E-04	1.19	294.	14.9	8.06	4.125E-05	32.1	25.1	4.235E-05	5.94
146.	8.85	2.831E-05	8.315E-05	1.19	294.	19.1	10.4	3.190E-05	41.0	29.1	3.190E-05	.000
179.	8.83	2.161E-05	6.346E-05	1.19	294.	23.0	12.5	2.461E-05	49.4	30.9	2.461E-05	.000
223.	8.81	1.609E-05	4.726E-05	1.19	294.	28.0	15.3	1.800E-05	60.1	30.3	1.800E-05	.000
273.	8.78	1.203E-05	3.533E-05	1.19	294.	33.5	18.4	1.314E-05	72.0	24.8	1.314E-05	.000
323.	8.76	9.305E-06	2.733E-05	1.19	294.	39.0	21.5	9.971E-06	83.6		9.971E-06	.000
373.	8.73	7.402E-06	2.174E-05	1.19	294.	44.4	24.6	7.822E-06	90.0		7.822E-06	.000
423.	8.71	6.026E-06	1.770E-05	1.19	294.	49.7	27.6	6.303E-06	95.4		6.303E-06	.000
473.	8.69	5.001E-06	1.469E-05	1.19	294.	55.0	30.6	5.190E-06	99.7		5.190E-06	.000
523.	8.67	4.219E-06	1.239E-05	1.19	294.	60.2	33.6	4.352E-06	103.		4.352E-06	.000
573.	8.65	3.608E-06	1.059E-05	1.19	294.	65.3	36.5	3.704E-06	106.		3.704E-06	.000
623.	8.63	3.122E-06	9.167E-06	1.19	294.	70.4	39.4	3.194E-06	107.		3.194E-06	.000
673.	8.62	2.729E-06	8.014E-06	1.19	294.	75.5	42.3	2.784E-06	108.		2.784E-06	.000
723.	8.60	2.407E-06	7.069E-06	1.19	294.	80.5	45.2	2.450E-06	108.		2.450E-06	.000
773.	8.59	2.140E-06	6.285E-06	1.19	294.	85.5	48.1	2.173E-06	107.		2.173E-06	.000
823.	8.57	1.916E-06	5.626E-06	1.19	294.	90.5	51.0	1.943E-06	104.		1.943E-06	.000
873.	8.56	1.726E-06	5.068E-06	1.19	294.	95.4	53.8	1.747E-06	101.		1.747E-06	.000
923.	8.55	1.563E-06	4.591E-06	1.19	294.	100.	56.6	1.581E-06	96.0		1.581E-06	.000
973.	8.54	1.423E-06	4.179E-06	1.19	294.	105.	59.5	1.438E-06	89.7		1.438E-06	.000
1.023E+03	8.52	1.302E-06	3.822E-06	1.19	294.	110.	62.3	1.314E-06	81.3		1.314E-06	.000
1.073E+03	8.51	1 195E-06	3.510E-06	1.19	294.	115.	65.1	1.205E-06	70.2		1.205E-06	.000
1 123E+03	8.50	1.102E-06	3.235E-06	1.19	294.	120.	67.8	1.110E-06	54.7		1.110E-06	.000
1.173E+03	8.49	1.019E-06	2.992E-06	1.19	294.	124.	70.6	1.026E-06	28.4		1.026E-06	.000
1.198E+03	8.49	9.812E-07	2.881E-06	1.19	294.	127.	72.0	9.879E-07			9.879E-07	.000

①

TABLE 7-3. EXAMPLE OUTPUT FROM THE GROUND LEVEL DISPERSION SUB-MODEL OF DEGADIS.0

```
U O A _ D E G A D I S   M O D E L   O U T P U T   - -   V E R S I O N   2.1
              *************** 22-DEC-1992 15:51:18.95 ***************

 Data input on                    22-DEC-1992 12:31:51.90
 Source program run on            22-DEC-1992 15:51:18.95

0          TITLE BLOCK

 Radian case 3:  Chlorine release from a pipe attached to a one-ton cylinder
                 Two-phase release from pressurized (saturated) liquid
                 release rate: 0.3139 kg/s; initial density: 19.71 kg/m3


      Wind velocity at reference height                      4.47  m/s
      Reference height                                      10.00  m
0     Surface roughness length                           1.000E-02  m
0     Pasquill Stability class                                C
0     Monin-Obukhov length                                -30.4     m
      Gaussian distribution constants
                     Specified averaging time              678.00  s
                                     Deltay                .21520
                                      Betay                .90000
0     Wind velocity power law constant  Alpha              .16070
      Friction velocity                                     .24814  m/s
0     Ambient Temperature                                  294.30  K
      Ambient Pressure                                       1.000  atm
      Ambient Absolute Humidity                          7.981E-03  kg/kg BDA
      Ambient Relative Humidity                             50.00  %

      Input:            Mole fraction    CONCENTRATION OF C      GAS DENSITY
                                                kg/m**3              kg/m**3
                            .00000            .00000               1.19357
                           1.00000          19.71000              19.71000

0     Specified Gas Properties:

         Molecular weight:                                        70.910
         Release temperature:                                     238.70     K
         Density at release temperature and ambient pressure:     19.710     kg/m**3
         Average heat capacity:                                   476.44     J/kg K
         Upper mole fraction contour:                            1.00000E-05
         Lower mole fraction contour:                            1.00000E-06
         Height for isopleths:                                    .00000     m
```

TABLE 7-3 (CONTINUED)

Source input data points

Initial (pure contaminant) mass in cloud: .00000 kg

Time	Contaminant Mass Rate	Source Radius	Contaminant Mass Fraction	Temperature	Enthalpy
s	kg/s	m	kg contam/kg mix	K	J/kg
.00000	.31390	4.22000E-02	1.0000	294.30	.00000
60230.	.31390	4.22000E-02	1.0000	294.30	.00000
60231.	.00000	.00000	1.0000	294.30	.00000
60232.	.00000	.00000	1.0000	294.30	.00000

0 Calculation procedure for ALPHA: 1
0 Entrainment prescription for PHI: 3
0 Layer thickness ratio used for average depth: 2.1500
0 Air entrainment coefficient used: .590
0 Gravity slumping velocity coefficient used: 1.150
0 Isothermal calculation
0 Heat transfer not included
0 Water transfer not included

TABLE 7-3 (CONTINUED)

***** CALCULATED SOURCE PARAMETERS *****

Time sec	Gas Radius m	Height m	Qstar kg/m**2/s	SZ(x=L/2.) m	Mole frac C	Density kg/m**3	Rich No.
.000000	4.220000E-02	1.100000E-05	2.61745	8.984817E-03	1.00000	19.7100	.756144
2.500000E-03	4.402756E-02	6.497224E-03	2.51689	9.330851E-03	.993858	18.9725	.756144
5.000000E-03	4.731675E-02	1.196966E-02	2.36164	9.935933E-03	.983742	17.8611	.756144
7.952711E-03	5.201731E-02	1.706137E-02	2.17499	1.078444E-02	.970118	16.5377	.756144
1.090542E-02	5.717519E 02	2.091386E-02	2.00658	1.169485E-02	.956206	15.3563	.756144
1.955035E-02	7.315855E 02	2.759510E-02	1.63891	1.439543E-02	.918929	12.8234	.756144
2.819529E-02	8.917064E 02	3.062364E-02	1.40398	1.693771E-02	.888579	11.2479	.756144
4.490576E-02	.118768	3.242206E-02	1.13704	2.129080E-02	.845507	9.51023	.756144
6.161624E-02	.146454	3.217368E-02	.984510	2.502090E-02	.815847	8.55591	.756144
8.933680E-02	.188873	3.030543E-02	.836821	3.017611E-02	.783778	7.68684	.756144
.117057	.227825	2.786473E-02	.749758	3.436799E-02	.764409	7.22770	.756144
.172885	.298301	2.270286E-02	.653236	4.070046E-02	.746995	6.85035	.756144
.228713	.360389	1.780135E-02	.605643	4.485447E-02	.747166	6.85392	.756144
.263658	.395621	1.494556E-02	.589267	4.649787E-02	.753701	6.99196	.756144

TABLE 7-3 (CONTINUED)

***** CALCULATED SOURCE PARAMETERS *****

Time sec	Gas Radius m	Height m	Qstar kg/m**2/s	SZ(x=L/2.) m	Mole frac C	Density kg/m**3	Rich No.
.298603	.419034	1.285349E-02	.585445	4.699319E-02	.764099	7.22069	.756144
.399346	.412110	1.148123E-02	.622694	4.427244E-02	.794083	7.95015	.756144
.498898	.403627	1.034069E-02	.657612	4.189124E-02	.818850	8.64531	.756144
.598449	.394419	9.363875E-03	.691420	3.975436E-02	.840267	9.32936	.756144
.759585	.379492	8.077288E-03	.743574	3.678365E-02	.869212	10.4061	.756144
.843749	.372180	7.537811E-03	.768699	3.547179E-02	.881694	10.9359	.756144
.927914	.365451	7.082606E-03	.791831	3.433208E-02	.892414	11.4284	.756144
1.00790	.359705	6.722174E-03	.811613	3.340676E-02	.901025	11.8518	.756144
1.16938	.350221	6.180213E-03	.844251	3.197469E-02	.914154	12.5513	.756144
1.25088	.346502	5.984797E-03	.857008	3.144576E-02	.918930	12.8235	.756144
1.42260	.340688	5.701425E-03	.876605	3.066765E-02	.925826	13.2349	.756144
1.59432	.337103	5.534678E-03	.888789	3.020215E-02	.929921	13.4902	.756144
1.90508	.333952	5.393740E-03	.899504	2.980437E-02	.933392	13.7133	.756144

TABLE 7-3 (CONTINUED)

***** CALCULATED SOURCE PARAMETERS *****

Time sec	Gas Radius m	Height m	Qstar kg/m**2/s	SZ(x=L/2.) m	Mole frac C	Density kg/m**3	Rich No.
2.33720	.332610	5.336527E-03	.903977	2.964218E-02	.934783	13.8046	.756144
2.94799	.332228	5.323522E-03	.905023	2.960630E-02	.935053	13.8225	.756144
3.21537	.331976	5.082750E-03	.911321	2.933861E-02	.938231	14.0354	.756144
3.39247	.330961	5.043425E-03	.914620	2.922283E-02	.939201	14.1016	.756144
8.79073	.329893	5.002260E-03	.918112	2.910116E-02	.940222	14.1717	.756144

0Source strength [kg/s] . .31390 Equivalent Primary source radius [m] : 4.22000E-02
Equivalent Primary source length [m] : 8.44000E-02 Equivalent Primary source half-width [m] : 3.31438E-02

Secondary source concentration [kg/m**3] : 13 815 Secondary source SZ [m] : 2.91012E-02

Contaminant flux rate: .91811

Secondary source mass fractions... contaminant: .974809 air: 2.49913E-02
Enthalpy: .00000 Density. 14.172

Secondary source length [m] : .65979 Secondary source half-width [m] : .25910

0 Distance (m)	Mole Fraction (6)	Concentration (kg/m**3)	Density (kg/m**3)	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z=.00 m to: 1.000E-04mole% (m)	1.000E-03mole% (m)
.330	.940	13.8	14.2	294.	.259	2.910E-02	.000	.259	.259
.380	.931	13.2	13.5	294.	.235	2.529E-02	9.419E-02	.604	.575
.430	.926	12.8	13.3	294.	.252	2.246E-02	.139	.795	.753
.563	.903	11.4	11.9	294.	.307	1.895E-02	.232	1.21	1.14
.696	.870	9.86	10.5	294.	.360	1.788E-02	.312	1.57	1.47
.845	.829	8.25	8.95	294.	.414	1.790E-02	.394	1.93	1.81
.994	.776	6.71	7.50	294	.462	1.898E-02	.471	2.27	2.12
1.36	.628	3.96	4.91	294.	.556	2.408E-02	.648	2.99	2.78
1.73	.494	2.51	3.55	294.	.625	3.080E-02	.811	3.62	3.36
2.83	.247	920	2.06	294.	.745	5.535E-02	1.25	5.18	4.76
3.94	.142	475	1.64	294	.799	8.252E-02	1.64	6.47	5.89
6.72	5.571E-02	172	1.35	294	.818	.154	2.49	9.08	8.16
9.50	3.024E-02	9 116E-02	1.28	294.	.763	.226	3.25	11.2	9.98
17.1	1.106E-02	3 280E-02	1.22	294.	.476	.418	5.04	15.9	13.8
24.6	6.015E-03	1 775E-02	1.21	294.	.112	.605	6.62	19.6	16.9
26.7	5.625E-03	1 660E-02	1.21	294	.000	.656	6.55	19.2	16.5
86.7	4 295E-04	1 262E-03	1.19	294.	.000	2.59	17.5	43.1	34.0
147.	1.482E-04	4 351E-04	1.19	294	.000	4.36	27.7	61.9	45.5
207.	7.506E-05	2 204E-04	1.19	294	.000	6.04	37.5	77.9	53.2
267.	4.550E-05	1 336E-04	1.19	294.	.000	7.65	47.0	91.8	57.8
327.	3.061E-05	8 989E-05	1.19	294.	.000	9.21	56.3	104.	59.5

(2)

TABLE 7-3 (CONTINUED)

0 Distance (m)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z=.00 m to: 1.000E-04mole% (m)	1.000E-03mole% (m)
387.	2.205E-05	6.476E-05	1.19	294.	.000	10.7	65.4	115.	58.2
447.	1.667E-05	4.895E-05	1.19	294.	.000	12.2	74.4	125.	53.2
507.	1.306E-05	3.836E-05	1.19	294.	.000	13.7	83.2	133.	43.0
567.	1.052E-05	3.090E-05	1.19	294.	.000	15.1	92.0	141.	20.7
627.	8.665E-06	2.544E-05	1.19	294.	.000	16.6	101.	148.	
687.	7.265E-06	2.133E-05	1.19	294.	.000	18.0	109.	154.	
747.	6.183E-06	1.816E-05	1.19	294.	.000	19.3	118.	159.	
807.	5.329E-06	1.565E-05	1.19	294.	.000	20.7	126.	163.	
867.	4.642E-06	1.363E-05	1.19	294.	.000	22.1	135.	167.	
927.	4.082E-06	1.199E-05	1.19	294.	.000	23.4	143.	170.	
987.	3.619E-06	1.063E-05	1.19	294.	.000	24.7	151.	171.	
1.047E+03	3.232E-06	9.490E-06	1.19	294.	.000	26.1	159.	173.	
1.107E+03	2.904E-06	8.528E-06	1.19	294.	.000	27.4	168.	173.	
1.167E+03	2.624E-06	7.707E-06	1.19	294.	.000	28.7	176.	173.	
1.227E+03	2.384E-06	7.001E-06	1.19	294.	.000	30.0	184.	171.	
1.287E+03	2.176E-06	6.389E-06	1.19	294.	.000	31.2	192.	169.	
1.347E+03	1.994E-06	5.855E-06	1.19	294.	.000	32.5	200.	166.	
1.407E+03	1.834E-06	5.386E-06	1.19	294.	.000	33.8	208.	162.	
1.467E+03	1.693E-06	4.972E-06	1.19	294.	.000	35.0	216.	157.	
1.527E+03	1.568E-06	4.605E-06	1.19	294.	.000	36.3	224.	150.	
1.587E+03	1.457E-06	4.278E-06	1.19	294.	.000	37.5	232.	142.	
1.647E+03	1.357E-06	3.985E-06	1.19	294.	.000	38.8	239.	132.	
1.707E+03	1.267E-06	3.721E-06	1.19	294.	.000	40.0	247.	120.	
1.767E+03	1.186E-06	3.483E-06	1.19	294.	.000	41.2	255.	105.	
1.827E+03	1.113E-06	3.268E-06	1.19	294.	.000	42.4	263.	85.9	
1.887E+03	1.046E-06	3.072E-06	1.19	294.	.000	43.7	271.	57.4	
1.947E+03	9.854E-07	2.894E-06	1.19	294.	.000	44.9	278.		

0

For the UFL of 1.00000E-03 mole percent, and the LFL of 1.00000E-04 mole percent:

The mass of contaminant between the UFL and LFL is: 54.399 kg.
The mass of contaminant above the LFL is: 85.514 kg.

Information on the impact of two concentrations at a single receptor height may be requested. Both the elevated jet and ground level sub-models in DEGADIS report the widths of the requested concentrations at the receptor height as a function of downwind distance. The elevated jet sub-model stops when the plume touches ground or the lowest requested concentration ceases to exist. If the lowest concentration still exists when the plume reaches the ground, the ground-level dispersion model begins. The ground-level model stops when the lowest concentration ceases to exist.

The important tables in the output for determining the impacts are the Centerline table (labeled 1 in Table 7-2) from the jet sub-model and the table (labeled 2 in Table 7-3) following the Calculated Source Parameter information in the ground-level dispersion sub-model. In both tables the width for each of the two requested concentrations as a function of distance is given. Also included is the maximum concentration as a function of downwind distance at the requested altitude. The concentrations are average concentrations for the averaging time specified. The specified averaging time should be the minimum of the release duration and the requested averaging time. Some manipulation of the reported concentrations and distances may be required if the averaging time is less than the requested averaging time or if the release is simulated as transient. See below for more discussion on interpreting the output.

Specific parameters are discussed below.

Maximum off-site concentration.
Maximum time-averaged off-site concentrations.
Maximum time-averaged concentration at a specific point.

For the jet sub-model three centerline concentrations are given. One is the concentration at the vertical center of the plume. The second is given for the altitude requested. The third is the maximum concentration. The vertical center mole fraction concentration is given in the column labeled 3 in Table 7-2. The constant altitude concentration is given in the column

labeled 4 in Table 7-2. The maximum concentration and its altitude are given in the columns labeled 5 in Table 7-2.

In the ground level sub-model the mole fraction is in the column labeled 6 in Figure 7-3. Since the release is at ground level, this value is also the maximum concentration.

The maximum concentration at any downwind location can be found by finding the downwind distance of interest in the first column of either the jet or ground level sub-model and then reading the maximum concentration from the appropriate column.

Maximum distance downwind of specified concentration.
Maximum width of specified concentration.
Total area impacted by specified concentration.

For the jet sub-model, the columns under "Width to mol%" contain the width information. For the ground level sub-model the table's last two columns contain the width information. The maximum distance downwind of the concentration is the last distance with a width for that concentration. The maximum width of the concentration can be determined by selecting the maximum width listed. The data provided are sufficient to calculate the plume dispersion area; however, DEGADIS does not do it. The area of impact at the specified height is calculated using the width/distance data.

Time at which the maximum concentration is reached at a specific point.
Duration above specified concentration at a point.
Time the specified concentration is reached at a point.

The time that a specific concentration arrives at a specific location is not explicitly available in the DEGADIS output. However, it can be estimated by dividing the distance to the location from the release site by the ambient wind speed. This method, however, becomes less reliable as the location gets

closer to the source and the higher the exit velocity of the release. The duration of impact can be estimated as being the same as the release duration.

SPECIAL CONSIDERATIONS

The above discussion of DEGADIS output is based on the assumption that the release is simulated as a continuous release. When the release duration is less than the desired averaging time, the averaging time input to DEGADIS should be the release duration. When the averaging time used is less than the one desired, the reported average concentrations must be corrected to represent the averaging time requested. When a release is simulated as transient, extra effort is necessary to determine concentrations. This section describes some of the techniques required.

When averaging time used is less than requested

When the averaging time used is less than the requested averaging time, the output must be converted to represent the requested averaging time. To extrapolate from the reported average concentration to the requested averaging time, multiply the reported average concentration by the ratio of the actual averaging time to the requested averaging time. This means that to find a concentration averaged over the requested time, a higher concentration may need to be found in the output. For example, if the release duration is 680 s and the requested averaging time is 900 s, DEGADIS should be told to average over 680 s. To convert the concentrations reported in the output to concentrations for the requested averaging time, each reported concentration must be multiplied by (680 s/900 s) or 0.756. This means that if a 900 s average concentration of 1 ppm is of interest, the output will have to be searched for a concentration of (1 ppm/0.756) or 1.32 ppm.

Transient Simulations

After each simulation, DEGADIS estimates the travel time to the distance of interest. If the travel time was longer than the release duration, a

transient simulation was performed. Because DEGADIS does not presently output time-averaged concentrations directly, additional effort is necessary for transient release simulations.

For an example, assume that a steady-state ground-level release is being simulated in which the duration of the release is 45 seconds and an averaging time of 15 minutes (900 seconds) is requested. A portion of the output from that simulation is shown in Table 7-4. In this simulation, the travel time to the location downwind (plant boundary) is greater than the release duration, so a transient simulation must be made. A portion of the transient simulation output is shown in Table 7-5. Although not used in this example, it is presented to indicate the difference between the steady-state output and the transient output.

The following procedure demonstrates how to determine the maximum downwind extent to the 6 ppm (15 min) concentration:

- From the steady-state output, the distance to 6 ppm(900 s/45 s)=120 ppm is approximately 700 m. So, use DEG4 to get the concentration time histories at 700 m and 0.8(700 m)=560 m (the factor of 0.8 was chosen from experience). DEG4 will create output similar to that shown in Table 7-6. The mole fraction at the centerline of the plume at the requested downwind distance is always presented. The mole fraction at an off-center point at the same downwind distance is optional. A dosage (D) at the point downwind can be estimated by summing predicted concentrations (in the Mole Fraction column) multiplied by he time interval between the predicted concentrations (in the Time column):

$$D = \sum F_i \, \Delta t$$

TABLE 7-4. PARTIAL LISTING OF A STEADY-STATE SIMULATION

0 Distance (m)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z= .00 m to: 6.000E-04mole% (m)	1.200E-03mole% (m)
1.23	.569	.605	1.27	295.	.965	.263	2.680E-07	.965	.965
1.28	.565	.600	1.27	295.	.890	.263	9.368E-02	1.21	1.20
1.33	.561	.594	1.26	295.	.863	.263	.133	1.32	1.30
2.73	.453	.455	1.25	295.	.705	.281	.537	2.52	2.46
7.06	.250	.229	1.22	295.	.653	.371	1.17	4.49	4.37
11.4	.155	.136	1.21	295.	.629	.476	1.66	5.94	5.76
20.9	7.367E-02	6.265E-02	1.20	295.	.538	.712	2.57	8.44	8.15
30.5	4.412E-02	3.708E-02	1.20	295.	.409	.943	3.37	10.5	10.1
54.5	2.090E-02	1.741E-02	1.19	295.	.000	1.50	4.68	13.4	12.8
114.	4.333E-03	3.585E-03	1.19	295.	.000	3.36	8.63	22.1	20.9
174.	1.861E-03	1.538E-03	1.19	295.	.000	5.03	12.4	29.6	27.8
234.	1.039E-03	8.586E-04	1.19	295.	.000	6.60	16.0	36.3	33.8
294.	6.658E-04	5.500E-04	1.19	295.	.000	8.10	19.5	42.4	39.1
354.	4.643E-04	3.835E-04	1.19	295.	.000	9.55	23.0	48.0	44.0
414.	3.430E-04	2.833E-04	1.19	295.	.000	11.0	26.4	53.1	48.3
474.	2.642E-04	2.182E-04	1.19	295.	.000	12.3	29.8	57.9	52.3
534.	2.100E-04	1.734E-04	1.19	295.	.000	13.7	33.1	62.4	56.0
594.	1.711E-04	1.413E-04	1.19	295.	.000	15.0	36.4	66.5	59.3
654.	1.422E-04	1.174E-04	1.19	295.	.000	16.3	39.6	70.5	62.3
714.	1.202E-04	9.923E-05	1.19	295.	.000	17.5	42.8	74.1	65.0
774.	1.029E-04	8.501E-05	1.19	295.	.000	18.8	46.0	77.6	67.4
834.	8.920E-05	7.367E-05	1.19	295.	.000	20.0	49.2	80.8	69.6
894.	7.809E-05	6.449E-05	1.19	295.	.000	21.3	52.3	83.8	71.6
954.	6.895E-05	5.695E-05	1.19	295.	.000	22.5	55.4	86.6	73.3

TABLE 7-5. PARTIAL LISTING OF A TRANSIENT SIMULATION

0 Time after beginning of spill 96.00000 sec

0 Distance (m)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z= .00 m to: 6.000E-04mole% (m)	1.200E-03mole% (m)
258.	2.218E-04	1.832E-04	1.1904	295.	.000	7.69	17.0	32.3	29.1
269.	3.286E-04	2.714E-04	1.1904	295.	.000	7.82	17.8	35.7	32.4
279.	4.311E-04	3.561E-04	1.1905	295.	.000	7.77	18.9	39.0	35.7
290.	5.064E-04	4.183E-04	1.1905	295.	.000	7.99	19.5	41.1	37.8
301.	5.510E-04	4.551E-04	1.1905	295.	.000	8.26	20.2	42.9	39.4
312.	5.565E-04	4.597E-04	1.1905	295.	.000	8.52	20.8	44.3	40.7
323.	5.421E-04	4.478E-04	1.1905	295.	.000	8.79	21.4	45.5	41.8
334.	5.164E-04	4.266E-04	1.1905	295.	.000	9.06	22.1	46.6	42.8
345.	4.876E-04	4.028E-04	1.1905	295.	.000	9.32	22.7	47.6	43.7
356.	4.592E-04	3.793E-04	1.1905	295.	.000	9.59	23.3	48.6	44.6
368.	4.315E-04	3.564E-04	1.1905	295.	.000	9.85	24.0	49.6	45.4
379.	4.070E-04	3.362E-04	1.1905	295.	.000	10.1	24.6	50.6	46.3
390.	3.842E-04	3.174E-04	1.1905	295.	.000	10.4	25.3	51.6	47.1
402.	3.633E-04	3.001E-04	1.1904	295.	.000	10.7	25.9	52.5	47.9
413.	3.442E-04	2.843E-04	1.1904	295.	.000	10.9	26.6	53.5	48.7
425.	3.261E-04	2.693E-04	1.1904	295.	.000	11.2	27.2	54.4	49.5
436.	3.090E-04	2.552E-04	1.1904	295.	.000	11.5	27.9	55.4	50.3
448.	2.929E-04	2.419E-04	1.1904	295.	.000	11.7	28.5	56.3	51.0
460.	2.775E-04	2.292E-04	1.1904	295.	.000	12.0	29.2	57.2	51.7
471.	2.626E-04	2.169E-04	1.1904	295.	.000	12.3	29.8	58.0	52.4
483.	2.475E-04	2.044E-04	1.1904	295.	.000	12.5	30.5	58.8	53.1
495.	2.318E-04	1.914E-04	1.1904	295.	.000	12.8	31.2	59.6	53.6
507.	2.162E-04	1.786E-04	1.1904	295.	.000	13.0	31.8	60.2	54.1
519.	1.998E-04	1.650E-04	1.1904	295.	.000	13.3	32.5	60.8	54.5
531.	1.826E-04	1.508E-04	1.1904	295.	.000	13.6	33.1	61.3	54.7
543.	1.646E-04	1.359E-04	1.1904	295.	.000	13.8	33.8	61.6	54.7
555.	1.459E-04	1.205E-04	1.1904	295.	.000	14.1	34.5	61.7	54.6
567.	1.250E-04	1.032E-04	1.1904	295.	.000	14.4	35.1	61.1	53.7
579.	1.056E-04	8.723E-05	1.1904	295.	.000	14.7	35.7	60.5	52.7
592.	8.684E-05	7.172E-05	1.1904	295.	.000	15.2	36.0	58.9	50.7

For the ULC of 1.20000E-03 mole percent, and the LLC of 6.00000E-04 mole percent:

The mass of contaminant between the ULC and LLC is: .25661 kg.
The mass of contaminant above the LLC is: 40.109 kg.

where F_i = Mole Fraction; and

Δt = time interval (1 second in this case).

The dosage can be multiplied by $1x10^6$ to put the answer into ppm•s.

- The integrated concentration time histories are 6782. ppm•s and 4173. ppm•s at 560 m and 700 m, respectively. So, the 15-minute averaged concentrations are (6782. ppm•s/900 s=)7.54 ppm and (4173. ppm•s/900 s=)4.64 ppm at 560 m and 700 m, respectively. Based on log-log interpolation, the distance to the STEL is approximately 620 m; this could be confirmed by integrating the concentration time history at 620 m.

Using the same approach, the following procedure can be used to determine the maximum cloud width to the 6 ppm (15 min) concentration:

- From the steady-state output (Table 7-4), the concentration at 620 m is approximately 159 ppm, and the maximum width to (159 ppm/1.1=)140 ppm is about 50 m at a downwind distance of 350 m (the factor of 1.1 is chosen from experience). So, use DEG4 to get the concentration time history at x=350 m, y=25 m, and z=0 m. (A total width of 50 m would be a half-width of 25 m.) The concentration history is given in Table 7-6.

- For this point (x=350 m, y=25 m, and z=0 m), the integrated concentration time history is 5329 ppm•s which gives a 15-minute averaged concentration of 5329 ppm•s/900 s=5.9 ppm. Therefore, a reasonable estimate of the maximum cloud width is 50 m.

7.4 HGSYSTEM

Multiple models are contained within HGSYSTEM. Therefore, there can be multiple output. In addition, post-processors are available which read the model output files and create files that can be imported into other programs such as Lotus® 1-2-3 or GRAPHER®. These other programs can then be used to create graphs or figures. However, in this discussion only the standard tabular output from the HGSYSTEM models will be considered.

TABLE 7-6. PARTIAL LISTING OF THE OUTPUT FROM DEG4

0 X-Direction correction was applied.
Coefficient: 4.00000E-02
Power: 1.1400
Minimum Distance: 100.00 m
0 Centerline values for the position -->
x: 350.00 m

0 Time (s)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z= .00 m to: 6.000E-04mole% (m)	1.200E-03mole% (m)
63.0	2.685E-04	2.218E-04	1.1904	295.	.000	9.58	22.8	44.4	40.1
64.0	3.067E-04	2.533E-04	1.1904	295.	.000	9.45	23.0	45.5	41.3
65.0	3.430E-04	2.833E-04	1.1904	295.	.000	9.44	23.0	46.2	42.1
66.0	3.732E-04	3.083E-04	1.1905	295.	.000	9.43	23.0	46.8	42.7
67.0	3.968E-04	3.277E-04	1.1905	295.	.000	9.43	23.1	47.2	43.1
68.0	4.146E-04	3.424E-04	1.1905	295.	.000	9.43	23.1	47.4	43.4
69.0	4.306E-04	3.557E-04	1.1905	295.	.000	9.44	23.0	47.6	43.6
70.0	4.427E-04	3.656E-04	1.1905	295.	.000	9.44	23.0	47.7	43.7
71.0	4.519E-04	3.733E-04	1.1905	295.	.000	9.44	23.0	47.8	43.8
72.0	4.594E-04	3.795E-04	1.1905	295.	.000	9.44	23.0	47.9	43.9
73.0	4.647E-04	3.838E-04	1.1905	295.	.000	9.44	23.0	48.0	44.0
74.0	4.688E-04	3.873E-04	1.1905	295.	.000	9.44	23.0	48.0	44.0
75.0	4.714E-04	3.894E-04	1.1905	295	.000	9.44	23.0	48.0	44.1
76.0	4.730E-04	3.907E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
77.0	4.742E-04	3.917E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
78.0	4.753E-04	3.926E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
79.0	4.759E-04	3.931E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
80.0	4.764E-04	3.935E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
81.0	4.766E-04	3.937E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
82.0	4.765E-04	3.936E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
83.0	4.767E-04	3.937E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
84.0	4.765E-04	3.936E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
85.0	4.764E-04	3.936E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
86.0	4.765E-04	3.936E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
87.0	4.761E-04	3.933E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
88.0	4.763E-04	3.934E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
89.0	4.762E-04	3.934E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
90.0	4.759E-04	3.931E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
91.0	4.762E-04	3.933E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
92.0	4.760E-04	3.932E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
93.0	4.761E-04	3.932E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
94.0	4.760E-04	3.932E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
95.0	4.755E-04	3.927E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1

TABLE 7-6 (CONTINUED)

0 Time (s)	Mole Fraction	Concentration (kg/m**3)	Density (kg/m**3)	Temperature (K)	Half Width (m)	Sz (m)	Sy (m)	Width at z= .00 m to: 6.000E-04mole% (m)	1.200E-03mole% (m)
96.0	4.753E-04	3.926E-04	1.1905	295.	.000	9.44	23.0	48.1	44.1
97.0	4.738E-04	3.913E-04	1.1905	295.	.000	9.44	23.0	48.0	44.1
98.0	4.713E-04	3.893E-04	1.1905	295.	.000	9.44	23.0	48.0	44.0
99.0	4.658E-04	3.848E-04	1.1905	295.	.000	9.44	23.0	48.0	44.0
100.	4.583E-04	3.786E-04	1.1905	295.	.000	9.44	23.0	47.9	43.9
101.	4.433E-04	3.662E-04	1.1905	295.	.000	9.44	23.0	47.7	43.7

0 Time (s)	Mole fraction at: y= 25.000 m z= .00000 m	Mole fraction at: y= .00000 m z= .00000 m	Mole fraction at: y= .00000 m z= .00000 m	Mole fraction at: y= .00000 m z= .00000 m
62.00000	.0000000			
63.00000	8.0425147E-05			
64.00000	9.3628549E-05			
65.00000	1.0491194E-04			
66.00000	1.1464036E-04			
67.00000	1.2258834E-04			
68.00000	1.2793180E-04			
69.00000	1.3265277E-04			
70.00000	1.3612420E-04			
71.00000	1.3881778E-04			
72.00000	1.4098159E-04			
73.00000	1.4258062E-04			
74.00000	1.4385843E-04			
75.00000	1.4461576E-04			
76.00000	1.4511603E-04			
77.00000	1.4547613E-04			
78.00000	1.4580346E-04			
79.00000	1.4599093E-04			
80.00000	1.4611341E-04			
81.00000	1.4617105E-04			
82.00000	1.4615733E-04			
83.00000	1.4617498E-04			
84.00000	1.4613995E-04			
85.00000	1.4609244E-04			
86.00000	1.4610133E-04			
87.00000	1.4599399E-04			
88.00000	1.4601977E-04			
89.00000	1.4599971E-04			
90.00000	1.4589066E-04			
91.00000	1.4595505E-04			

TABLE 7-6 (CONTINUED)

0	Time (s)	Mole fraction at: y= 25.000 m z= .00000 m	Mole fraction at: y= .00000 m z= .00000 m	Mole fraction at: y= .00000 m z= .00000 m	Mole fraction at: y= .00000 m z= .00000 m
	92.00000	1.4591968E-04			
	93.00000	1.4590477E-04			
	94.00000	1.4589936E-04			
	95.00000	1.4570884E-04			
	96.00000	1.4563420E-04			
	97.00000	1.4518097E-04			
	98.00000	1.4440163E-04			
	99.00000	1.4272115E-04			
	100.0000	1.4041359E-04			
	101.0000	1.3579899E-04			

The HGSYSTEM models are stand-alone computer programs that can be run separately or linked together to simulate all of the aspects of an atmospheric accidental release. When models are linked, the first model calculates parameters required as input by the following model. For example, the jet/plume model, HFPLUME, will calculate the touch-down of a dense plume but then, following touch-down, further calculations need to be performed by the ground-based dispersion model HEGADAS. The HFPLUME model determines when its calculations should be stopped by checking specific criteria (e.g., jet velocity). Relevant parameters are then written to an ASCII file using the same free-format arrangement as files generated by the user. The user is encouraged to examine the results of the upstream models, at least for a few cases, before allowing the models to run automatically in sequence.

HEGADASS

An example of the HEGADASS output is given in Table 7-7. The output consists of a listing of the input data, some calculated parameters (e.g. length and width of gas blanket), and a table of plume parameters as a function of downwind distance. In Table 7-7 only the first page of the output table is shown. However, the table can be multiple pages. The table length is dependent on the input parameters describing output step size and extent.

The columns of information most likely to be of interest are:

DISTANCE	-	Downwind distance in meters;
CONC	-	Concentration in per cent volume;
YCU	-	Horizontal extent of the upper concentration, CU, in meters; and
YCL	-	Horizontal extent of the lower concentration, CL, in meters;

TABLE 7-7. EXAMPLE HEGADASS OUTPUT

```
HSMAIN                                   HEGADAS-S PROGRAM ( VERSION NOV90    )                          PAGE     0
DATE 29/12/92                                  STANDARD REPORT FILE                                       TIME 11:03
-------------------------------------------------------------------------------------------------------------------
                                <<<<   SCENARIO 1 CHOKED ETHYLENE OXIDE RELEASE            >>>>
-------------------------------------------------------------------------------------------------------------------


===================================================================================================================
                                HEGADAS-S INPUT DATA
===================================================================================================================

-------------------------------------------------------------------> CONTROL data block: control parameters
OUTPUT CODE                      ICNT =      1       (output of cumulative cloud data)
SURFACE-TRANSFER CODE           ISURF =      3       (only heat transfer, no water vapour)
-------------------------------------------------------------------> AMBIENT data block: ambient data
AIR TEMP.AT HEIGHT ZAIRTEMP AIRTEMP =   30.000     CELSIUS
REF. HEIGHT FOR AIR TEMP.  ZAIRTEMP =   4.6000     M
RELATIVE HUMIDITY             RHPERC =  62.000     %
WIND VELOCITY AT HEIGHT Z0       U0 =   5.3700     M/S
REFERENCE HEIGHT FOR WIND VEL.   Z0 =   4.6000     M
EARTH-S SURFACE TEMPERATURE TGROUND =   30.000     CELSIUS
-------------------------------------------------------------------> DISP data block: dispersion data
SURFACE ROUGHNESS PARAMETER      ZR =  1.00000E-02 M
PASQUILL STABILITY CLASS     PQSTAB =      C
AVERAG. TIME FOR CONC.MEAS.  AVTIMC =   18.750     SECONDS  (value for instantaneous releases)
MONIN - OBUKHOV LENGTH        OBUKL =  -30.400     M
TYPE OF FORMULA FOR SIGMA_Y   MODSY =      2       (Briggs formula)
        with parameters:      DELTA =  5.50000E-02
                               BETA =  1.00000E-04 M**(-1)
CONST. IN GRAV. SPREADING LAW    CE =   1.1500
CONST. IN GRAV. SPREADING LAW    CD =   5.0000
-------------------------------------------------------------------> GASDATA data block: gas data
EVAPORATION RATE            GASFLOW =  6.34000E-02 KG/S
EVAPORATION FLUX               FLUX =   1.5850     KG/M2/S
TEMPERATURE OF EMITTED GAS  TEMPGAS =   10.850     CELSIUS
SPECIFIC HEAT OF EMITTED GAS  CPGAS =   24.490     J/MOLE/CELSIUS
MOLECULAR WEIGHT OF EM. GAS   MWGAS =   44.000     KG/KMOLE
PICKED-UP WATER BY EM. GAS   WATGAS =  0.00000E-01 (MOLAR FRACTION)
HEAT GROUP IN HEAT FLUX QH   HEATGR =   29.000
THERMODYNAMIC MODEL         THERMOD =      1       (normal,non-reactive gas)
-------------------------------------------------------------------> POOL data block: pool dimensions
SOURCE LENGTH                    PLL =  0.20000     M
SOURCE HALF-WIDTH               PLHW =  0.10000     M
-------------------------------------------------------------------> CLOUD data block: control of cloud output
NR. OF SOURCE OUTPUT STEPS  NSOURCE =      4
FIXED OUTPUT STEP             DXFIX =  0.50000     M
NUMBER OF FIXED STEPS          NFIX =    300
INCREASE FACTOR FOR VAR.STEPS XGEOM =   1.2000
X AT WHICH CALC. IS STOPPED    XEND =   3000.0     M
CA AT WHICH CALC. IS STOPPED  CAMIN =  1.00000E-05 KG/M3
UPPER CONCENTRATION LIMIT        CU =   1.4400     KG/M3
LOWER CONCENTRATION LIMIT        CL =  5.39700E-02 KG/M3
```

TABLE 7-7 (CONTINUED)

WIND PROFILE EXPONENT	ALPHA =	0.18986	
FRICTION VELOCITY	USTAR =	0.38898	M/S
AIR TEMP. AT GROUND LEVEL	TAP =	30.500	CELSIUS
LENGTH GAS BLANKET	L =	0.49091	M
WIDTH GAS BLANKET	B =	0.24546	M

TABLE 7-7 (CONTINUED)

HSMAIN
DATE 29/12/92

HEGADAS-S PROGRAM (VERSION NOV90)
STANDARD REPORT FILE

PAGE 1
TIME 11:03

<<<< SCENARIO 1 CHOKED ETHYLENE OXIDE RELEASE >>>>

DISTANCE (M)	CONC (X VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	RIB	TMP (DEG.C)	CA (KG/M3)
-0.245	100.	0.00	0.00	0.245	0.245	0.00	0.245	0.00		10.8	1.9
-0.123	100.	1.330E-02	0.000E-01	0.245	0.245	4.446E-03	0.245	3.862E-02	0.519	10.8	1.9
0.000E-01	100.	2.261E-02	0.000E-01	0.245	0.245	7.558E-03	0.245	6.565E-02	0.881	10.8	1.9
0.123	100.	3.058E-02	0.000E-01	0.245	0.245	1.022E-02	0.245	8.881E-02	1.19	10.8	1.9
0.245	100.	3.774E-02	0.000E-01	0.245	0.245	1.262E-02	0.245	0.110	1.47	10.8	1.9
	Take-up flux = 0.263	KG/M2/S = 6.346E-02 KG/S									
0.500	65.9	4.652E-02	0.110	0.201	0.000E-01	0.000E-01	0.396	0.121	1.13	19.5	1.2
1.00	34.3	6.524E-02	0.207	0.209	0.000E-01	0.000E-01	0.532	0.138	0.782	25.8	0.62
1.50	21.0	8.486E-02	0.284	0.220	0.000E-01	0.000E-01	0.616	0.148	0.598	27.9	0.37
2.00	14.5	0.113	0.351	0.174	0.000E-01	0.000E-01	0.613	0.165	0.529	28.8	0.26
2.50	11.0	0.143	0.407	0.126	0.000E-01	0.000E-01	0.588	0.177	0.482	29.3	0.20
3.00	8.88	0.171	0.457	8.435E-02	0.000E-01	0.000E-01	0.557	0.181	0.441	29.5	0.16
3.50	7.41	0.198	0.502	4.706E-02	0.000E-01	0.000E-01	0.520	0.179	0.404	29.7	0.13
4.00	6.34	0.225	0.543	1.304E-02	0.000E-01	0.000E-01	0.478	0.173	0.369	29.8	0.11
4.20	5.98	0.236	0.559	0.000E-01	0.000E-01	0.000E-01	0.459	0.169	0.356	29.9	0.11
4.50	5.31	0.252	0.582	0.000E-01	0.000E-01	0.000E-01	0.433	0.153	0.317	30.0	9.40E-02
5.00	4.40	0.279	0.621	0.000E-01	0.000E-01	0.000E-01	0.376	0.120	0.258	30.1	7.79E-02
5.50	3.71	0.307	0.660	0.000E-01	0.000E-01	0.000E-01	0.291	7.751E-02	0.203	30.2	6.56E-02
6.00	3.16	0.334	0.699	0.000E-01	0.000E-01	0.000E-01	0.131	2.014E-02	0.153	30.2	5.59E-02
6.50	2.73	0.362	0.737	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.106	30.3	4.82E-02
7.00	2.37	0.389	0.776	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	6.106E-02	30.3	4.20E-02
7.50	2.08	0.417	0.815	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.859E-02	30.3	3.68E-02
8.00	1.84	0.445	0.854	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-2.212E-02	30.3	3.26E-02
8.50	1.64	0.472	0.893	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-6.131E-02	30.4	2.90E-02
9.00	1.47	0.500	0.932	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-9.920E-02	30.4	2.59E-02
9.50	1.32	0.528	0.970	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.136	30.4	2.34E-02
10.0	1.20	0.556	1.01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.172	30.4	2.11E-02
10.5	1.09	0.583	1.05	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.207	30.4	1.92E-02
11.0	0.991	0.611	1.09	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.241	30.4	1.75E-02
11.5	0.908	0.639	1.13	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.275	30.4	1.60E-02
12.0	0.834	0.667	1.16	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.308	30.4	1.47E-02
12.5	0.769	0.694	1.20	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.341	30.4	1.36E-02
13.0	0.711	0.722	1.24	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.374	30.4	1.26E-02
13.5	0.659	0.750	1.28	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.406	30.4	1.17E-02
14.0	0.613	0.778	1.32	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.437	30.4	1.08E-02
14.5	0.571	0.806	1.36	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.469	30.4	1.01E-02
15.0	0.533	0.833	1.40	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.500	30.5	9.42E-03
15.5	0.499	0.861	1.44	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.531	30.5	8.81E-03
16.0	0.468	0.889	1.48	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.562	30.5	8.26E-03
16.5	0.439	0.917	1.51	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.593	30.5	7.76E-03
17.0	0.413	0.945	1.55	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.624	30.5	7.30E-03
17.5	0.389	0.973	1.59	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.655	30.5	6.88E-03
18.0	0.367	1.00	1.63	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.685	30.5	6.49E-03

TABLE 7-7 (CONTINUED)

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	RIB	TMP (DEG.C)	CA (KG/M3)
18.5	0.347	1.03	1.67	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.716	30.5	6.14E-03
19.0	0.329	1.06	1.71	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.746	30.5	5.81E-03
19.5	0.311	1.09	1.75	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.777	30.5	5.50E-03
20.0	0.296	1.11	1.79	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	-0.807	30.5	5.22E-03

Specific parameters of interest are discussed below.

Maximum off-site concentration.

Maximum time-averaged off-site concentrations.

Maximum time-averaged concentration at a specific point.

Maximum distance downwind of specified concentration.

Maximum width of specified concentration.

Total area impacted by specified concentration.

Maximum time-averaged concentrations at specific distances downwind and maximum extent downwind of a specific time-averaged concentration can be determined from the DISTANCE and CONC columns. Widths and the downwind distances at which the widths exist can be determined from the DISTANCE and either YCU or YCL columns. Although not explicitly output, the area impacted by a concentration can be determined using the width as a function of downwind distance information. The volume and mass contained within the concentrations CU and CL can be read from a secondary output of HEGADASS. A portion of that output is shown in Table 7-8.

Time at which the maximum concentration is reached at a specific point.

Duration above specified concentration at a point.

Time the specified concentration is reached at a point.

Since HEGADASS is a steady-state model, no information on the timing of an impact can be deduced from the output. However, the amount of time from the release until a specific downwind location is impacted can be estimated by assuming that the plume moves at the same speed as the ambient wind speed. This assumption breaks down, however, if the specific distance is close to the source or if the release is a jet.

TABLE 7-8. EXAMPLE OUTPUT OF HEGADASS SHOWING VOLUME OF CONCENTRATIONS

HSMAIN
DATE 29/12/92

HEGADAS-S PROGRAM (VERSION NOV90)
ISOCONCENTRATION/CLOUD-DATA FILE

PAGE 1
TIME 11:03

<<<< SCENARIO 1 CHOKED ETHYLENE OXIDE RELEASE >>>>

DISTANCE (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CUM. CONTENT (KG) C>CU	CUM. CONTENT (KG) C>CL	CUM. VOLUME (M3) C>CU	CUM. VOLUME (M3) C>CL
-0.123	0.245	4.446E-03	0.245	3.862E-02	4.485E-04	1.399E-03	2.679E-04	2.327E-03
0.000E-01	0.245	7.558E-03	0.245	6.565E-02	1.211E-03	3.776E-03	7.233E-04	6.282E-03
0.123	0.245	1.022E-02	0.245	8.881E-02	2.242E-03	6.991E-03	1.339E-03	1.163E-02
0.245	0.245	1.262E-02	0.245	0.110	3.515E-03	1.096E-02	2.099E-03	1.824E-02
0.500	0.000E-01	0.000E-01	0.396	0.121	3.515E-03	1.865E-02	2.099E-03	3.896E-02
1.00	0.000E-01	0.000E-01	0.532	0.138	3.515E-03	3.198E-02	2.099E-03	9.884E-02
1.50	0.000E-01	0.000E-01	0.616	0.148	3.515E-03	4.366E-02	2.099E-03	0.172
2.00	0.000E-01	0.000E-01	0.613	0.165	3.515E-03	5.353E-02	2.099E-03	0.252
2.50	0.000E-01	0.000E-01	0.588	0.177	3.515E-03	6.181E-02	2.099E-03	0.331
3.00	0.000E-01	0.000E-01	0.557	0.181	3.515E-03	6.867E-02	2.099E-03	0.406
3.50	0.000E-01	0.000E-01	0.520	0.179	3.515E-03	7.424E-02	2.099E-03	0.474
4.00	0.000E-01	0.000E-01	0.478	0.173	3.515E-03	7.866E-02	2.099E-03	0.532
4.20	0.000E-01	0.000E-01	0.459	0.169	3.515E-03	8.027E-02	2.099E-03	0.554
4.50	0.000E-01	0.000E-01	0.433	0.153	3.515E-03	8.218E-02	2.099E-03	0.582
5.00	0.000E-01	0.000E-01	0.376	0.120	3.515E-03	8.418E-02	2.099E-03	0.613
5.50	0.000E-01	0.000E-01	0.291	7.751E-02	3.515E-03	8.511E-02	2.099E-03	0.629
6.00	0.000E-01	0.000E-01	0.131	2.014E-02	3.515E-03	8.521E-02	2.099E-03	0.631
6.50	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
7.00	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
7.50	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
8.00	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
8.50	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
9.00	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
9.50	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
10.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
10.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
11.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
11.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
12.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
12.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
13.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
13.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
14.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
14.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
15.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
15.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
16.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
16.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
17.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
17.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
18.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
18.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
19.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
19.5	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631
20.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.515E-03	8.521E-02	2.099E-03	0.631

HEGADAST

The output from the HEGADAST model is the same as HEGADASS, except that instead of a steady-state emission assumption, the model assumes a transient release. Therefore, instead of the output consisting of a single table of plume parameters as a function of downwind distance (like HEGADASS), HEGADAST output consists of multiple tables. Each table is for a different time since the release. Also, notice that each table only displays the downwind distances which have non-zero concentrations.

Specific parameters of interest are discussed below.

Maximum off-site concentration.
Maximum time-averaged off-site concentrations.
Maximum time-averaged concentration at a specific point.
Maximum distance downwind of specified concentration.
Maximum width of specified concentration.
Total area impacted by specified concentration.

HEGADAST output consists of two types of tables: one shows the plume parameters and some concentration parameters, while the other shows the cumulative volume above specified concentrations. Examples of these two output are provided in Tables 7-9 and 7-10. To find the parameters above, the same approach is made from HEGADAST output as with HEGADASS output, except that all HEGADAST temporal "snapshots" must be used.

Time at which the maximum concentration is reached at a specific point.
Duration above specified concentration at a point.
Time the specified concentration is reached at a point.

A temporal history of a concentration can be constructed from the collection of snapshots output by HEGADAST. That is, a table showing

TABLE 7-9. EXAMPLE HEGADAST OUTPUT

```
HTMAIN                                   HEGADAS-T PROGRAM ( VERSION NOV90    )                          PAGE     0
DATE 22/12/92                                     STANDARD REPORT FILE                                    TIME 14:25
-------------------------------------------------------------------------------------------------------------------
                              <<<<   SCENARIO 5 USING EPA EMISSION ESTIMATE              >>>>
-------------------------------------------------------------------------------------------------------------------

===================================================================================================================
                              HEGADAS-T INPUT DATA
===================================================================================================================

-------------------------------------------------------------------> CONTROL data block: control parameters
OUTPUT CODE                      ICNT =      1       (output of cumulative cloud data)
SURFACE-TRANSFER CODE           ISURF =      3       (only heat transfer, no water vapour)
GAS-BLANKET FORMULATION       BLMODEL =      1       (new, non-oscillatory formulation)
CLOUD-SHAPE CORRECTION CODE   ICSCOR =      1       (correction included)
-------------------------------------------------------------------> AMBIENT data block: ambient data
AIR TEMP.AT HEIGHT ZAIRTEMP AIRTEMP =   22.000     CELSIUS
REF. HEIGHT FOR AIR TEMP.   ZAIRTEMP =  22.000     M
RELATIVE HUMIDITY            RHPERC =   45.000     %
WIND VELOCITY AT HEIGHT Z0       U0 =   6.2600     M/S
REFERENCE HEIGHT FOR WIND VEL.   Z0 =   6.1000     M
EARTH-S SURFACE TEMPERATURE TGROUND =   22.000     CELSIUS
-------------------------------------------------------------------> DISP data block: dispersion data
SURFACE ROUGHNESS PARAMETER       ZR =  1.00000E-02 M
PASQUILL STABILITY CLASS      PQSTAB =     D
AVERAG. TIME FOR CONC.MEAS.   AVTIMC =   45.000     SECONDS
MONIN - OBUKHOV LENGTH         OBUKL =  1.00000E+05 M
TYPE OF FORMULA FOR SIGMA_Y    MODSY =      2       (Briggs formula)
        with parameters:       DELTA =  4.76543E-02
                                BETA =  1.00000E-04 M**(-1)
CONST. IN GRAV. SPREADING LAW     CE =   1.1500
CONST. IN GRAV. SPREADING LAW     CD =   5.0000
TYPE OF FORMULA FOR SIGMA_X    MODSX =      3       (Chatwin/Wilson)
        with parameters:       ASIGX =   10.000
                               BSIGX =  0.10000
-------------------------------------------------------------------> GASDATA data block: gas data
TEMPERATURE OF EMITTED GAS  TEMPGAS =   27.000     CELSIUS
SPECIFIC HEAT OF EMITTED GAS  CPGAS =   29.000     J/MOLE/CELSIUS
MOLECULAR WEIGHT OF EM. GAS   MWGAS =   20.010     KG/KMOLE
PICKED-UP WATER BY EM. GAS   WATGAS =  0.00000E-01 (MOLAR FRACTION)
HEAT GROUP IN HEAT FLUX QH   HEATGR =   24.000
THERMODYNAMIC MODEL         THERMOD =      2       (hydrogen fluoride)
INITIAL LIQUID IN HF        HFLIQFR =   1.0000     (MASS FRACTION)
-------------------------------------------------------------------->TIMEDATA data block: source/breakpoint data
TIME-DEPENDENT RECORD DATA:  ITYPBR =      0       (primary pool data: radius, strength)
- skip increment for reading  INCRT =      0
- start time for data       TSTPOOL =  0.00000E-01 S
- time step between read records DT =   5.0000     S
- number of records read       NTYD =      9       (see list of pool data below for record data read)
-------------------------------------------------------------------> CLOUD data block: control of cloud output
OUTPUT STEP LENGTH            XSTEP =   50.000     M
CA AT WHICH CALC. IS STOPPED  CAMIN =  5.00000E-05 KG/M3
UPPER CONCENTRATION LIMIT        CU =  5.00000E-05 KG/M3
LOWER CONCENTRATION LIMIT        CL =  4.08800E-06 KG/M3
```

TABLE 7-9 (CONTINUED)

```
-----------------------------------------------------------------> CALC data block: control of output times
PNTS. OF TIME FOR CLOUD CALC. TSTAR =   10.000     SEC
                                        12.000     SEC
                                        15.000     SEC
                                        20.000     SEC
                                        40.000     SEC
                                        60.000     SEC
                                        80.000     SEC
                                        100.00     SEC
                                        120.00     SEC
                                        140.00     SEC
                                        160.00     SEC
                                        180.00     SEC
                                        200.00     SEC
                                        220.00     SEC
                                        240.00     SEC
                                        260.00     SEC
                                        280.00     SEC
                                        300.00     SEC

==================================================================================================

WIND PROFILE EXPONENT          ALPHA =  0.20295
FRICTION VELOCITY              USTAR =  0.40006     M/S
AIR TEMP. AT GROUND LEVEL        TAP =   22.000     CELSIUS
```

TABLE 7-9 (CONTINUED)

HTMAIN HEGADAS-T PROGRAM (VERSION NOV90) PAGE 1
DATE 22/12/92 STANDARD REPORT FILE TIME 14:25

<<<< SCENARIO 5 USING EPA EMISSION ESTIMATE >>>>

DATA FOR PRIMARY POOL AND SECONDARY VAPOUR BLANKET

TIME - TSTPOOL (S)	POOL RADIUS (M)	POOL STRENGTH (KG/S)	BLANKET RADIUS (M)	BLANKET HEIGHT (M)	BLANKET EV.RATE (KG/S)	BLANKET MASS (KG)	
0.00	0.00	0.00	-	-	-	-	
2.50	5.000E-02	0.437	0.817	7.129E-03	0.269	0.283	
5.00	0.100	0.874	1.50	5.310E-03	0.715	0.711	
7.50	0.100	0.874	2.04	2.078E-03	1.17	0.513	
8.91	0.100	0.874	2.18	0.00	1.30	0.00	blanket height reduces to zero
10.0	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
12.5	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
15.0	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
17.5	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
20.0	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
22.5	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
25.0	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
27.5	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
30.0	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
32.5	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
35.0	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
37.5	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
40.0	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
42.5	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
45.0	0.100	0.874	1.70	0.000E-01	0.874	0.000E-01	
47.5	5.000E-02	0.437	1.10	0.000E-01	0.437	0.000E-01	
50.0	0.000E-01	0.000E-01	-	-	-	-	

Maximum source radius RGMAX = 2.1752 M

Source/blanket data set; total CPU = 7 seconds

SOURCE DATA SEEN BY OBSERVERS

OBSERVER	START TIME - TSTPOOL (S)	PLACE OF DOWNWIND EDGE (M)	LENGTH (M)	HALF-WIDTH (M)	TAKE-UP FLUX (KG/M2/S)	TAKE-UP RATE (KG/S)
1	-0.4238	0.2774	0.4863	0.1923	0.1604	2.9997E-02
9	1.989	1.110	1.981	0.7840	0.1187	0.3685
17	4.402	1.783	3.235	1.287	9.7810E-02	0.8146
25	6.815	2.145	4.066	1.666	8.8839E-02	1.204
33	9.228	1.675	3.372	1.343	9.6330E-02	0.8726

TABLE 7-9 (CONTINUED)

OBSERVER	START TIME - TSTPOOL (S)	PLACE OF DOWNWIND EDGE (M)	LENGTH (M)	HALF-WIDTH (M)	TAKE-UP FLUX (KG/M2/S)	TAKE-UP RATE (KG/S)
41	11.64	1.673	3.371	1.343	9.6330E-02	0.8725
49	14.05	1.697	3.378	1.341	9.6330E-02	0.8728
57	16.47	1.695	3.392	1.336	9.6330E-02	0.8733
65	18.88	1.693	3.390	1.337	9.6330E-02	0.8733
73	21.29	1.690	3.388	1.338	9.6330E-02	0.8732
81	23.71	1.688	3.375	1.342	9.6330E-02	0.8729
89	26.12	1.686	3.375	1.342	9.6330E-02	0.8729
97	28.53	1.684	3.374	1.343	9.6330E-02	0.8728
105	30.94	1.682	3.374	1.343	9.6330E-02	0.8728
113	33.36	1.680	3.377	1.342	9.6330E-02	0.8728
121	35.77	1.677	3.375	1.342	9.6330E-02	0.8727
129	38.18	1.675	3.373	1.343	9.6330E-02	0.8726
137	40.60	1.699	3.397	1.334	9.6330E-02	0.8732
145	43.01	1.697	3.378	1.341	9.6330E-02	0.8728
153	45.42	1.210	2.724	1.076	0.1049	0.6147
161	47.83	0.5406	1.294	0.5191	0.1397	0.1878

Observer-source data set; total CPU = 15 seconds

TABLE 7-9 (CONTINUED)

```
HTMAIN                                   HEGADAS-T PROGRAM ( VERSION NOV90    )                          PAGE     2
DATE 22/12/92                                  STANDARD REPORT FILE                                       TIME 14:25
-----------------------------------------------------------------------------------------------------------------------
                                  <<<<   SCENARIO 5 USING EPA EMISSION ESTIMATE              >>>>
-----------------------------------------------------------------------------------------------------------------------
Observer-release frequency = 32; maximum value over all times of [mean error in observer concentration]/[peak conc.] = 0.470
Observer-release frequency = 16; maximum value over all times of [mean error in observer concentration]/[peak conc.] = 0.277
Observer-release frequency =  8; maximum value over all times of [mean error in observer concentration]/[peak conc.] = 6.271E-02
Observer-release frequency =  4; maximum value over all times of [mean error in observer concentration]/[peak conc.] = 3.678E-02
Convergence tolerance OBSEPS = 5.000E-02 is satisfied

Cloud shape correction performed

Observer-dispersion data set for  41 observers; total CPU =  983 seconds
```

DISPERSION DATA AT TIME = 10.00 SEC

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
0.000E-01	97.3	1.501E-02	9.116E-02	1 31	1.60	9.947E-02	1.63	0.120	0.841
50.0	8.149E-05	2.00	3.43	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	6.764E-07

DISPERSION DATA AT TIME = 12.00 SEC

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
0.000E-01	99.0	7.465E-03	0.000E-01	1.34	1.34	4.951E-02	1 34	5.988E-02	0.846
50.0	1.731E-02	2.02	3.43	0.000E-01	3.52	2.11	6.47	5.80	1.434E-04
100.	9.192E-22	3.59	6.78	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	7.613E-24

DISPERSION DATA AT TIME = 15.00 SEC

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
0.000E-01	97.3	1.427E-02	5.511E-02	1.29	1.46	9.455E-02	1.49	0.114	0.838
50.0	0.488	2.00	3.45	0.000E-01	7.24	6.85	9.06	9.96	4.080E-03
100.	2.309E-10	3.63	6.76	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.913E-12

TABLE 7-9 (CONTINUED)

DISPERSION DATA AT TIME = 20.00 SEC

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
0.000E-01	99.2	0.000E-01	0.000E-01	1.34	1.34	0.000E-01	1.34	0.000E-01	0.847
50.0	3.30	1.16	4.10	0.000E-01	10.3	5.41	12.2	7.13	2.856E-02
100.	6.448E-04	3.71	6.78	0.000E-01	0.000E-01	0.000E-01	3.52	1.25	5.352E-06

DISPERSION DATA AT TIME = 40.00 SEC

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
0.000E-01	98.6	9.841E-03	6.209E-02	1.29	1.48	6.527E-02	1.50	7.894E-02	0.846
50.0	3.23	1.17	4.13	0.000E-01	10.4	5.41	12.3	7.14	2.727E-02
100.	0.650	2.83	7.47	0.000E-01	16.2	10.2	20.0	14.5	5.375E-03
150.	0.179	4.36	10.5	0.000E-01	19.4	12.0	25.6	19.1	1.482E-03
200.	3.597E-03	6.93	13.4	0.000E-01	0.000E-01	0.000E-01	18.9	12.3	2.985E-05

DISPERSION DATA AT TIME = 60.00 SEC

DISTANCE (M)	CONC (% VOL.)	SZ (M)	SY (M)	MIDP (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CA (KG/M3)
50.0	2.15	1.27	4.07	0.000E-01	9.87	5.51	11.8	7.41	1.781E-02
100.	0.639	2.83	7.48	0.000E-01	16.1	10.2	20.0	14.5	5.290E-03
150.	0.274	4.18	10.8	0.000E-01	21.1	12.7	27.2	19.3	2.280E-03
200.	0.156	5.29	14.1	0.000E-01	25.5	14.1	33.9	22.7	1.300E-03
250.	6.708E-02	6.75	17.2	0.000E-01	26.7	14.0	38.1	25.4	5.571E-04
300.	7.965E-03	9.93	20.0	0 000E-01	10.6	3.43	33.4	23.3	6.606E-05
350.	1.856E-04	11.3	23.3	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.538E-06

TABLE 7-10. EXAMPLE OUTPUT OF HEGADAST SHOWING VOLUME OF CONCENTRATIONS

ISOCONCENTRATION AND CUMULATIVE CLOUD DATA AT TIME = 10.00 SEC

DISTANCE (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CUM.CONT. C>CU (KG)	CUM.CONT. C>CL (KG)	CUM.VOL. C>CU (M3)	CUM.VOL. C>CL (M3)
0.000E-01	1.60	9.947E-02	1.63	0.120	1.65	1.65	15.0	18.5
50.0	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.65	1.65	15.0	18.5

ISOCONCENTRATION AND CUMULATIVE CLOUD DATA AT TIME = 12.00 SEC

DISTANCE (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CUM.CONT. C>CU (KG)	CUM.CONT. C>CL (KG)	CUM.VOL. C>CU (M3)	CUM.VOL. C>CL (M3)
0.000E-01	1.34	4.951E-02	1.34	5.988E-02	0.797	0.797	6.65	8.04
50.0	3.52	2.11	6.47	5.80	0.840	0.875	527.	2.637E+03
100.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.840	0.875	527.	2.637E+03

ISOCONCENTRATION AND CUMULATIVE CLOUD DATA AT TIME = 15.00 SEC

DISTANCE (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CUM.CONT. C>CU (KG)	CUM.CONT. C>CL (KG)	CUM.VOL. C>CU (M3)	CUM.VOL. C>CL (M3)
0.000E-01	1.46	9.455E-02	1.49	0.114	1.51	1.51	13.4	16.3
50.0	7.24	6.85	9.06	9.96	3.79	3.84	3.485E+03	6.338E+03
100.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.79	3.84	3.485E+03	6.338E+03

ISOCONCENTRATION AND CUMULATIVE CLOUD DATA AT TIME = 20.00 SEC

DISTANCE (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CUM.CONT. C>CU (KG)	CUM.CONT. C>CL (KG)	CUM.VOL. C>CU (M3)	CUM.VOL. C>CL (M3)
0.000E-01	1.34	0.000E-01	1.34	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
50.0	10.3	5.41	12.2	7.13	11.3	11.4	3.917E+03	6.099E+03
100.	0.000E-01	0.000E-01	3.52	1.25	11.3	11.4	3.917E+03	6.406E+03

TABLE 7-10 (CONTINUED)

ISOCONCENTRATION AND CUMULATIVE CLOUD DATA AT TIME = 40.00 SEC

DISTANCE (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CUM.CONT. C>CU (KG)	CUM.CONT. C>CL (KG)	CUM.VOL. C>CU (M3)	CUM.VOL. C>CL (M3)
0.000E-01	1.48	6.527E-02	1.50	7.894E-02	1.05	1.05	9.28	11.3
50.0	10.4	5.41	12.3	7.14	12.0	12.0	3.936E+03	6.142E+03
100.	16.2	10.2	20.0	14.5	21.3	21.5	1.547E+04	2.655E+04
150.	19.4	12.0	25.6	19.1	26.6	27.1	3.182E+04	6.070E+04
200.	0.000E-01	0.000E-01	18.9	12.3	26.6	27.3	3.182E+04	7.699E+04

ISOCONCENTRATION AND CUMULATIVE CLOUD DATA AT TIME = 60.00 SEC

DISTANCE (M)	YCU (M)	ZCU (M)	YCL (M)	ZCL (M)	CUM.CONT. C>CU (KG),	CUM.CONT. C>CL (KG)	CUM.VOL. C>CU (M3)	CUM.VOL. C>CL (M3)
50.0	9.87	5.51	11.8	7.41	7.60	7.64	3.813E+03	6.116E+03
100.	16.1	10.2	20.0	14.5	16.8	17.0	1.532E+04	2.652E+04
150.	21.1	12.7	27.2	19.3	25.0	25.5	3.415E+04	6.334E+04
200.	25.5	14.1	33.9	22.7	32.5	33.5	5.935E+04	1.172E+05
250.	26.7	14.0	38.1	25.4	37.1	38.8	8.559E+04	1.849E+05
300.	10.6	3.43	33.4	23.3	37.2	39.8	8.813E+04	2.393E+05
350.	0.000E-01	0.000E-01	0.000E-01	0.000E-01	37.2	39.8	8.813E+04	2.393E+05

Concentration-versus-Time can be generated for a specific downwind distance. For example, in Table 7-9 the concentration at 150 meters downwind first apears at 40 seconds and is 0.179 % volume. The concentration at 150 meters downwind at 60 seconds is 0.274 % volume. Because there was no reported concentration at 150 meters downwind at 20 seconds after the release, the plume must have reached 150 meters downwind between 20 and 40 seconds after the release.

SPECIAL CONSIDERATIONS

The above discussion of the HEGADST output assumes that the release is simulated as being continuous. When the release duration is less than the desired averaging time, the averaging time used should be the release duration. When the averaging time used is less than the one desired, the reported average concentrations must be corrected to represent the averaging time requested.

When averaging time used is less than requested

When the averaging time becomes longer than the release duration, special steps have to be taken to be sure the correct time-averaged concentrations are calculated. These special steps were taken in Scenario 5 where the release duration was 45 seconds but the averaging time was 15 minutes. To compute an accurate 15-minute average concentration, the model predictions had to be integrated at fixed downwind locations to account for the variations in concentration as a function of time. This was accomplished using the HTPOST post processing utility. HTPOST is an interactive program that extracts model results from the binary data file (*.HTM) produced by the HEGADAST model. The HTPOST utility program can be run in batch mode using the DOS redirect function (HTPOST <HTPOST.INP), which sets up an input file needed to run in batch mode. A separate file is written for each downwind distance. Table 7-11 presents a copy of the file used for this analysis. One of the important aspects of this utility is the ability to integrate the predicted

concentrations in terms of sigma x. This concept becomes very important as the averaging time becomes longer than the release duration and emissions vary as a function of time.

PLUME

An example of the output from the PLUME model is shown in Table 7-12. There may be multiple pages of output in the form presented in Table 7-12. The number of pages of output depends on the distance downwind that is to be covered by the output. Note that a definition of each of the column headings is at the bottom of each table. The columns most likely to be used are x (horizontal displacement) and beta (pollutant mole-concentration).

Specific parameters of interest are discussed below.

Maximum off-site concentration.
Maximum time-averaged off-site concentrations.
Maximum time-averaged concentration at a specific point.
Maximum distance downwind of specified concentration.

Concentrations listed are given at the plume centerline (z) level. If some height other than centerline is desired, the concentration must be extrapolated to the other altitude .

Maximum width of specified concentration.
Total area impacted by specified concentration.

Widths of specified concentrations are not given directly. The area can not be calculated unless external calculations are done that also use the parameter D (plume-effective diameter).

TABLE 7-11. INPUT FILE FOR HTPOST FOR SCENARIO 5

scen5.htm	Input File
900	AVERAGING TIME in seconds. USED ONLY ONCE
2	Request a history time-series USED ONLY ONCE
1	Graph, time v. data
a62.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
62.	Distance downwind (m)
1	Graph, time v. data
a76.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
76	Distance downwind (m)
1	Graph, time v. data
a94.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
94	Distance downwind (m)
1	Graph, time v. data
a125.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
125	Distance downwind (m)
1	Graph, time v. data
a188.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
188	Distance downwind (m)
1	Graph, time v. data
a250.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
250	Distance downwind (m)
1	Graph, time v. data
a313.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
313	Distance downwind (m)
1	Graph, time v. data
a376.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
376	Distance downwind (m)
1	Graph, time v. data
a438.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
438	Distance downwind (m)
1	Graph, time v. data
a563.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
563	Distance downwind (m)
1	Graph, time v. data
a626.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration

TABLE 7-11 (CONTINUED)

626	Distance downwind (m)
1	Graph, time v. data
a688.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
688	Distance downwind (m)
1	Graph, time v. data
a751.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
751	Distance downwind (m)
1	Graph, time v. data
a876.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
876	Distance downwind (m)
1	Graph, time v. data
a939.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
939	Distance downwind (m)
1	Graph, time v. data
a1001.dat	Output file name
10 180	Min and Max TIME
1	Plot of % Volume Concentration
1001	Distance downwind (m)
0	End
0	End
0	End

TABLE 7-12. EXAMPLE PLUME OUTPUT

Output from PLUME Version NOV90 Title: SCENARIO 4 SO2 RELEASE Date: 22/12/92 Time: 08:22

Orifice conditions:

orifice temperature:-10.00C;
orifice pressure:67.19atm;
orifice diameter: 0.01m;
orifice height: 0.01m;
orifice mass-flux 5.99kg/s;
pollutant mass-flux: 5.99kg/s;
release inclination: 90.00deg;

Atmosphere conditions:

data reference height: 6.00m;
atmosphere temperature: 18.00C;
atmosphere pressure: 1.00atm;
relative humidity: 0.00%;
ambient wind-speed: 3.20m/s;
atmosphere density: 1.22kg/m3;
surface roughness: 0.0100m;
Pasquill/Gifford class: 'E'.

Flash conditions:

flash temperature:******C;
flash pressure: 1.00atm;
gas-jet velocity:379.19m/s;
flash density: 5.99kg/m3;
flash diameter: 0.06m;

x	z	D	u	phi	T	beta	r	c	dm/dt	hmd	xx
2.984E-03	1.01	0.313	138.	89.6	14.0	20.7	1.54	0.562	16.4	0.000E-01	0.365
1.681E-02	2.01	0.610	75.6	88.8	18.6	10.2	1.36	0.271	30.0	0.000E-01	0.199
4.556E-02	3.01	0.931	50.6	87.9	19.0	6.53	1.30	0.174	44.9	0.000E-01	0.133
9.221E-02	4.01	1.28	37.3	86.8	18.9	4.71	1.28	0.126	60.9	0.000E-01	9.825E-02
0.160	5.01	1.65	29.0	85.5	18.8	3.62	1.26	9.654E-02	78.3	0.000E-01	7.645E-02
0.251	6.00	2.06	23.4	84.0	18.7	2.89	1.25	7.699E-02	97.4	0.000E-01	6.147E-02
0.371	6.99	2.51	19.3	82.2	18.6	2.36	1.24	6.281E-02	119.	0.000E-01	5.046E-02
0.523	7.98	3.02	16.1	80.2	18.5	1.95	1.24	5.198E-02	143.	0.000E-01	4.195E-02
0.714	8.96	3.60	13.6	77.8	18.5	1.63	1.23	4.338E-02	170.	0.000E-01	3.514E-02
0.950	9.94	4.26	11.6	74.9	18.4	1.36	1.23	3.637E-02	203.	0.000E-01	2.956E-02
1.24	10.9	5.02	9.89	71.5	18.4	1.15	1.23	3.056E-02	240.	0.000E-01	2.490E-02
1.59	11.8	5.89	8.54	67.5	18.4	0.963	1.22	2.569E-02	285.	0.000E-01	2.098E-02
2.01	12.7	6.87	7.46	62.9	18.4	0.811	1.22	2.162E-02	338.	0.000E-01	1.769E-02
2.50	13.6	7.94	6.62	57.8	18.4	0.684	1.22	1.824E-02	400.	0.000E-01	1.495E-02
3.07	14.4	9.07	5.98	52.5	18.4	0.581	1.22	1.548E-02	471.	0.000E-01	1.270E-02
3.72	15.2	10.2	5.53	47.3	18.4	0.497	1.22	1.325E-02	550.	0.000E-01	1.089E-02
4.43	15.9	11.3	5.21	42.4	18.4	0.431	1.22	1.148E-02	634.	0.000E-01	9.440E-03
5.19	16.5	12.3	5.00	38.0	18.4	0.378	1.22	1.008E-02	722.	0.000E-01	8.291E-03
6.00	17.1	13.2	4.85	34.1	18.4	0.336	1.21	8.956E-03	812.	0.000E-01	7.374E-03
6.84	17.7	14.1	4.76	30.9	18.5	0.302	1.21	8.055E-03	902.	0.000E-01	6.636E-03
7.71	18.2	14.9	4.70	28.1	18.5	0.275	1.21	7.322E-03	992.	0.000E-01	6.035E-03
8.61	18.6	15.6	4.67	25.7	18.5	0.252	1.21	6.718E-03	1.081E+03	0.000E-01	5.539E-03
9.51	19.0	16.2	4.65	23.7	18.5	0.233	1.21	6.213E-03	1.168E+03	0.000E-01	5.124E-03
10.4	19.4	16.9	4.64	21.9	18.5	0.217	1.21	5.786E-03	1.254E+03	0.000E-01	4.773E-03
11.4	19.8	17.4	4.63	20.4	18.5	0.204	1.21	5.420E-03	1.338E+03	0.000E-01	4.473E-03
12.3	20.1	18.0	4.64	19.0	18.5	0.192	1.21	5.101E-03	1.422E+03	0.000E-01	4.210E-03
13.3	20.4	18.5	4.64	17.9	18.5	0.181	1.21	4.821E-03	1.504E+03	0.000E-01	3.979E-03
14.2	20.7	19.0	4.65	16.8	18.6	0.171	1.21	4.562E-03	1.589E+03	0.000E-01	3.767E-03
15.2	21.0	19.4	4.66	15.8	18.6	0.163	1.21	4.341E-03	1.670E+03	0.000E-01	3.585E-03
16.1	21.3	19.8	4.67	15.0	18.6	0.156	1.21	4.143E-03	1.749E+03	0.000E-01	3.422E-03
17.1	21.5	20.3	4.69	14.2	18.6	0.149	1.21	3.965E-03	1.828E+03	0.000E-01	3.275E-03
18.1	21.8	20.6	4.70	13.5	18.6	0.143	1.21	3.803E-03	1.906E+03	0.000E-01	3.141E-03
19.1	22.0	21.0	4.71	12.9	18.6	0.137	1.21	3.655E-03	1.982E+03	0.000E-01	3.020E-03
20.0	22.2	21.4	4.73	12.3	18.6	0.132	1.21	3.520E-03	2.058E+03	0.000E-01	2.908E-03
21.0	22.4	21.8	4.74	11.7	18.6	0.128	1.21	3.395E-03	2.133E+03	0.000E-01	2.806E-03
22.0	22.6	22.1	4.76	11.3	18.6	0.123	1.21	3.281E-03	2.207E+03	0.000E-01	2.712E-03
23.0	22.8	22.4	4.77	10.8	18.6	0.119	1.21	3.175E-03	2.281E+03	0.000E-01	2.624E-03
24.0	23.0	22.8	4.79	10.4	18.6	0.116	1.21	3.077E-03	2.353E+03	0.000E-01	2.543E-03
24.9	23.2	23.1	4.80	9.97	18.6	0.112	1.21	2.985E-03	2.425E+03	0.000E-01	2.468E-03
25.9	23.3	23.4	4.81	9.60	18.7	0.109	1.21	2.900E-03	2.497E+03	0.000E-01	2.398E-03

TABLE 7-12 (CONTINUED)

x	z	D	u	phi	T	beta	r	c	dm/dt	hmd	xx
26.9	23.5	23.7	4.83	9.25	18.7	0.106	1.21	2.820E-03	2.567E+03	0.000E-01	2.332E-03
27.9	23.7	24.0	4.84	8.93	18.7	0.103	1.21	2.745E-03	2.637E+03	0.000E-01	2.270E-03
28.9	23.8	24.2	4.85	8.62	18.7	0.101	1.21	2.675E-03	2.706E+03	0.000E-01	2.212E-03
29.9	24.0	24.5	4.87	8.33	18.7	9.805E-02	1.21	2.608E-03	2.775E+03	0.000E-01	2.157E-03
30.9	24.1	24.8	4.88	8.06	18.7	9.570E-02	1.21	2.546E-03	2.843E+03	0.000E-01	2.106E-03
31.9	24.2	25.0	4.89	7.80	18.7	9.348E-02	1.21	2.487E-03	2.910E+03	0.000E-01	2.057E-03
32.8	24.4	25.3	4.90	7.56	18.7	9.138E-02	1.21	2.431E-03	2.977E+03	0.000E-01	2.011E-03
33.8	24.5	25.5	4.91	7.33	18.7	8.939E-02	1.21	2.378E-03	3.043E+03	0.000E-01	1.967E-03
34.8	24.6	25.8	4.93	7.11	18.7	8.749E-02	1.21	2.327E-03	3.109E+03	0.000E-01	1.925E-03
35.8	24.8	26.0	4.94	6.90	18.7	8.569E-02	1.21	2.279E-03	3.174E+03	0.000E-01	1.886E-03
36.8	24.9	26.3	4.95	6.70	18.7	8.398E-02	1.21	2.234E-03	3.239E+03	0.000E-01	1.848E-03
37.8	25.0	26.5	4.96	6.51	18.7	8.234E-02	1.21	2.190E-03	3.304E+03	0.000E-01	1.812E-03
38.8	25.1	26.7	4.97	6.32	18.7	8.078E-02	1.21	2.148E-03	3.367E+03	0.000E-01	1.778E-03
39.8	25.2	26.9	4.98	6.15	18.7	7.928E-02	1.21	2.109E-03	3.431E+03	0.000E-01	1.745E-03
40.8	25.3	27.2	4.99	5.98	18.7	7.785E-02	1.21	2.070E-03	3.494E+03	0.000E-01	1.713E-03
41.8	25.4	27.4	5.00	5.82	18.7	7.649E-02	1.21	2.034E-03	3.556E+03	0.000E-01	1.683E-03
42.8	25.5	27.6	5.01	5.66	18.7	7.517E-02	1.21	1.999E-03	3.618E+03	0.000E-01	1.654E-03
43.8	25.6	27.8	5.02	5.52	18.7	7.391E-02	1.21	1.965E-03	3.680E+03	0.000E-01	1.627E-03
44.8	25.7	28.0	5.03	5.37	18.8	7.270E-02	1.21	1.933E-03	3.741E+03	0.000E-01	1.600E-03
45.8	25.8	28.2	5.04	5.24	18.8	7.154E-02	1.21	1.902E-03	3.802E+03	0.000E-01	1.574E-03
46.8	25.9	28.4	5.05	5.10	18.8	7.042E-02	1.21	1.872E-03	3.862E+03	0.000E-01	1.550E-03
47.8	26.0	28.6	5.06	4.97	18.8	6.934E-02	1.21	1.844E-03	3.922E+03	0.000E-01	1.526E-03
48.8	26.1	28.8	5.07	4.85	18.8	6.830E-02	1.21	1.816E-03	3.982E+03	0.000E-01	1.503E-03
49.8	26.1	29.0	5.08	4.73	18.8	6.729E-02	1.21	1.789E-03	4.042E+03	0.000E-01	1.481E-03
50.7	26.2	29.2	5.08	4.61	18.8	6.632E-02	1.21	1.763E-03	4.100E+03	0.000E-01	1.460E-03
51.7	26.3	29.3	5.09	4.50	18.8	6.539E-02	1.21	1.739E-03	4.159E+03	0.000E-01	1.439E-03
52.7	26.4	29.5	5.10	4.39	18.8	6.449E-02	1.21	1.714E-03	4.217E+03	0.000E-01	1.419E-03
53.7	26.5	29.7	5.11	4.29	18.8	6.361E-02	1.21	1.691E-03	4.275E+03	0.000E-01	1.400E-03
54.7	26.5	29.9	5.12	4.19	18.8	6.277E-02	1.21	1.669E-03	4.333E+03	0.000E-01	1.382E-03
55.7	26.6	30.1	5.12	4.09	18.8	6.195E-02	1.21	1.647E-03	4.390E+03	0.000E-01	1.363E-03
56.7	26.7	30.2	5.13	3.99	18.8	6.115E-02	1.21	1.626E-03	4.447E+03	0.000E-01	1.346E-03
57.7	26.7	30.4	5.14	3.90	18.8	6.038E-02	1.21	1.605E-03	4.504E+03	0.000E-01	1.329E-03
58.7	26.8	30.6	5.15	3.81	18.8	5.964E-02	1.21	1.585E-03	4.560E+03	0.000E-01	1.313E-03
59.7	26.9	30.7	5.15	3.72	18.8	5.891E-02	1.21	1.566E-03	4.616E+03	0.000E-01	1.297E-03
60.7	26.9	30.9	5.16	3.63	18.8	5.821E-02	1.21	1.547E-03	4.672E+03	0.000E-01	1.281E-03
61.7	27.0	31.1	5.17	3.55	18.8	5.753E-02	1.21	1.529E-03	4.727E+03	0.000E-01	1.266E-03
62.7	27.1	31.2	5.18	3.47	18.8	5.687E-02	1.21	1.512E-03	4.782E+03	0.000E-01	1.252E-03
63.7	27.1	31.4	5.18	3.39	18.8	5.622E-02	1.21	1.494E-03	4.837E+03	0.000E-01	1.238E-03
64.7	27.2	31.5	5.19	3.31	18.8	5.559E-02	1.21	1.478E-03	4.891E+03	0.000E-01	1.224E-03
65.7	27.2	31.7	5.20	3.23	18.8	5.498E-02	1.21	1.462E-03	4.945E+03	0.000E-01	1.210E-03
66.7	27.3	31.8	5.20	3.16	18.8	5.439E-02	1.21	1.446E-03	4.999E+03	0.000E-01	1.197E-03
67.7	27.4	32.0	5.21	3.09	18.8	5.381E-02	1.21	1.430E-03	5.053E+03	0.000E-01	1.185E-03
68.7	27.4	32.1	5.22	3.02	18.8	5.325E-02	1.21	1.415E-03	5.106E+03	0.000E-01	1.172E-03
69.7	27.5	32.3	5.22	2.95	18.8	5.270E-02	1.21	1.401E-03	5.159E+03	0.000E-01	1.160E-03
70.7	27.5	32.4	5.23	2.88	18.8	5.217E-02	1.21	1.387E-03	5.212E+03	0.000E-01	1.148E-03
71.7	27.6	32.6	5.23	2.82	18.8	5.165E-02	1.21	1.373E-03	5.265E+03	0.000E-01	1.137E-03
72.7	27.6	32.7	5.24	2.75	18.8	5.114E-02	1.21	1.359E-03	5.317E+03	0.000E-01	1.126E-03
73.7	27.7	32.9	5.25	2.69	18.8	5.064E-02	1.21	1.346E-03	5.369E+03	0.000E-01	1.115E-03
74.7	27.7	33.0	5.25	2.63	18.8	5.016E-02	1.21	1.333E-03	5.421E+03	0.000E-01	1.104E-03
75.7	27.7	33.1	5.26	2.57	18.8	4.969E-02	1.21	1.321E-03	5.472E+03	0.000E-01	1.094E-03
76.7	27.8	33.3	5.26	2.51	18.8	4.923E-02	1.21	1.308E-03	5.524E+03	0.000E-01	1.084E-03
77.7	27.8	33.4	5.27	2.45	18.9	4.878E-02	1.21	1.296E-03	5.575E+03	0.000E-01	1.074E-03
78.7	27.9	33.5	5.27	2.39	18.9	4.834E-02	1.21	1.285E-03	5.625E+03	0.000E-01	1.064E-03

TABLE 7-12 (CONTINUED)

x	z	D	u	phi	T	beta	r	c	dm/dt	hmd	xx
79.7	27.9	33.7	5.28	2.34	18.9	4.791E-02	1.21	1.273E-03	5.676E+03	0.000E-01	1.055E-03
80.7	28.0	33.8	5.28	2.28	18.9	4.749E-02	1.21	1.262E-03	5.726E+03	0.000E-01	1.045E-03
81.7	28.0	33.9	5.29	2.23	18.9	4.707E-02	1.21	1.251E-03	5.776E+03	0.000E-01	1.036E-03
82.7	28.0	34.1	5.29	2.17	18.9	4.667E-02	1.21	1.240E-03	5.826E+03	0.000E-01	1.027E-03
83.7	28.1	34.2	5.30	2.12	18.9	4.628E-02	1.21	1.230E-03	5.875E+03	0.000E-01	1.019E-03
84.7	28.1	34.3	5.31	2.07	18.9	4.589E-02	1.21	1.220E-03	5.925E+03	0.000E-01	1.010E-03
85.7	28.1	34.4	5.31	2.02	18.9	4.552E-02	1.21	1.210E-03	5.974E+03	0.000E-01	1.002E-03

Gas Composition:

mole-fraction water-vapour: 0.00E-01%;
mole-fraction dry-air: 0.00E-01%;
mole-fraction pollutant gas: 1.00E+02%;
exit-plane relative humidity: 0.00E-01%;
pollutant molecular weight: 64. g/mol;
pollutant specific heat: 0.33 kJ/kg/C;

Interpretation:

x: horizontal displacement (m);
z: plume-axis height (m);
D: plume effective diameter (m);
u: mean plume velocity (m/s);
phi: plume axis inclination (degrees);
T: mean plume temperature (C);

Interpretation:

beta: pollutant mole-concentration (%);
r: jet mean density (kg/m3);
c: pollutant concentration (kg/m3);
xx: mass-fraction pollutant (-);
hmd: plume relative humidity (%);
y H2O: plume relative humidity (%);

Time at which the maximum concentration is reached at a specific point.
Duration above specified concentration at a point.
Time the specified concentration is reached at a point.

The release is assumed to be steady-state; thus the timing of the impacts is not available.

PGPLUME

An example output from PGPLUME is shown in Table 7-13. This example shows only one page of output from the model; however, there may be multiple pages of output, depending on the number of output steps requested. Each output consists of a cross-section of the plume at a distance downwind.

Specific paramters of interest are discussed below.

Maximum off-site concentration.
Maximum time-averaged off-site concentrations.
Maximum time-averaged concentration at a specific point.
Maximum distance downwind of specified concentration.

Each cross-section needs to be examined to determine the maximum concentration. The maximum concentration can exist anywhere in the plane or at a specific altitude. For a specific downwind distance, the cross-sections on either side of that distance can provide bounding values. A concentration at the desired location can be interpolated using the two concentrations at two downwind distances and the desired downwind distance.

Maximum width of specified concentration.
Total area impacted by specified concentration.

Widths of the specified concentrations are not given directly. However, the area can be calculated using external calculations with the cross-

TABLE 7-13. EXAMPLE PGPLUME OUTPUT

Output from PGPLUME Version Jan92 mo Title: SCENARIO 4 SO2 RELEASE Date: 01/12/92 Time: 20:57

Cross-Section Data:

downwind displacement:	0.161	km;
peak mole-concentration gas:	1.20E-02	%;
plume averaging time:	15.	mins;
transverse plume "width":	39.	m;
maximum concentration height:	29.	m;

Cross-Section Data:

peak excess-velocity:	-29.	cm/s;
peak excess-density:	0.56	g/m3;
peak mass-concentration:	0.32	g/m3;
vertical plume "height":	13.	m;
section centroid height:	29.	m.

Virtual Source Data:

downwind displacement:	-5.24E+02	m;
height above ground:	29.	m;
source mass-flux pollutant:	6.0	kg/s;
matching achieved:	"Perfect" match	;

Table of Mole-Concentration gas (ppm) at several heights (z)(m) above (level) ground, and at several distances (y)(m) measured horizontally off-axis:

height (m) above (level) ground.	0.000E-01	7.82	15.6	23.5	31.3	39.1	46.9	54.7	62.5	70.4
0.000E-01	17.7	17.3	16.3	14.7	12.8	10.7	8.59	6.63	4.91	3.49
16.3	73.1	71.7	67.5	61.1	53.1	44.4	35.6	27.5	20.3	14.5
19.5	90.8	89.0	83.9	75.9	66.0	55.1	44.2	34.1	25.3	18.0
22.7	106.	104.	98.0	88.7	77.1	64.4	51.7	39.8	29.5	21.0
25.8	117.	114.	108.	97.4	84.6	70.7	56.7	43.7	32.4	23.1
29.0	120.	118.	111.	100.	87.3	72.9	58.5	45.1	33.4	23.8
32.2	117.	114.	108.	97.3	84.6	70.7	56.7	43.7	32.4	23.1
35.3	106.	104.	98.0	88.6	77.1	64.4	51.7	39.8	29.5	21.0
38.5	90.8	89.0	83.8	75.8	65.9	55.1	44.2	34.1	25.2	18.0
41.7	72.9	71.5	67.3	60.9	53.0	44.2	35.5	27.4	20.3	14.4

height (m) above (level) ground.

horizontal off-axis displacement (m).

Near-field Matching Data:

mean plume velocity-excess:	-49.	cm/s;
mean plume density-excess:	1.4	g/m3;
mean plume concentration gas:	0.79	g/m3;
effective plume "diameter":	42.	m;
plume downwind displacement:	1.61E+02	m;
plume centroid height:	29.	m;
plume cross-sectional area:	1.36E+03	m2;
mean plume inclination:	-0.30	degrees;

Atmosphere Conditions:

atmosphere density:	1.2	kg/m3;
atmosphere temperature:	21.	C;
atmosphere pressure:	1.00	atm;
relative humidity:	0.00E-01	%;
ambient wind-speed:	6.0	m/s;
surface roughness:	1.00E-02	m;
Pasquill/Gifford class:	E	(-);

Pasquill/Gifford Matching Data:

peak excess-velocity:	-29.	cm/s;
peak density-excess:	0.56	g/m3;
peak concentration gas:	0.32	g/m3;
peak mole concentration gas:	1.20E-02	%;
peak concentration height:	29.	m;
plume averaging time:	15.	mins;
transverse plume "width":	39.	m;
vertical plume "height":	13.	m.

sectional data. Each cross-section gives the concentration distribution at a specific distance downwind. By combining all the cross-sections, an entire plume's shape at any altitude could be mathematically created. Furthermore, a three-dimensional shape of a specific concentration could be deduced, and the area of that concentration could then be calculated. PGPLUME, however, does not presently perform such a calculation. Instead, another software package would need to be created, or an existing software package capable of mathematical manipulation (e.g. Lotus 1-2-3) would need to be used.

All cross-sections must be used to create a contour of the concentration. To do this, first the cross-sections are connected mathematically to form the entire three-dimensional outline of the concentration. This three-dimensional outline could then be cut, mathematically, by horizontal planes to determine the area of the concentration at any altitude.

Time at which the maximum concentration is reached at a specific point.
Duration above specified concentration at a point.
Time the specified concentration is reached at a point.

The release is assumed to be steady-state; thus the timing of the impacts is not available through PCPLUME.

7.5 SLAB

Except for total area, SLAB provides responses for each of the requested parameters, with only a single model run required for each of the scenarios. An example of a SLAB output is presented in Table 7-14. In order to determine the area of the cloud at a specified concentration, Golden Software's UTIL program, which is part of their SURFUR system, was used. That software determines the area inside an isopleth by gridding and interpolating the predicted concentrations from the model output. Because interpolation is used, the area of the isopleth represents the cloud as it exists in the raw model output. However, the inaccuracies caused by the interpolation are not

TABLE 7-14. EXAMPLE SLAB OUTPUT

```
            SESSION INFORMATION

INPUT DATA FILE NAME :  epalagl.dta
OUTPUT LIST FILE NAME : epalagl.LST


GRAPHICS DATA FILE NAME : epalagl.DAT
GRAPHICS PLOT FILE NAME : epalagl.XZ

problem input

 idspl =        2
 ncalc =        1
 wms   =  .044054
 cps   =  1121.00
 tbp   =   283.85
 cmed0 =      .02
 dhe   =  579450.
 cpsl  =  1954.00
 rhosl =   882.70
 spb   =  2507.61
 spc   =   -29.01
 ts    =   283.85
 qs    =      .06
 as    =      .00
 tsd   =     480.
 qtis  =      .00
 hs    =      .00
 tav   =     5.00
 xffm  =  1000.00
 zp(1) =      .00
 zp(2) =     3.66
 zp(3) =      .00
 zp(4) =      .00
 z0    =  .010000
 za    =     4.57
```

TABLE 7-14 (CONTINUED)

ua	=	5.37
ta	=	287.52
rh	=	62.00
stab	=	3.00

release gas properties

molecular weight of source gas (kg)	- wms	=	4.4054E-02
vapor heat capacity, const. p. (j/kg-k)	- cps	=	1.1210E+03
temperature of source gas (k)	- ts	=	2.8385E+02
density of source gas (kg/m3)	- rhos	=	1.8914E+00
boiling point temperature	- tbp	=	2.8385E+02
liquid mass fraction	- cmed0	=	1.7200E-02
liquid heat capacity (j/kg-k)	- cpsl	=	1.9540E+03
heat of vaporization (j/kg)	- dhe	=	5.7945E+05
liquid source density (kg/m3)	- rhosl	=	8.8270E+02
saturation pressure constant	- spa	=	9.8399E+00
saturation pressure constant (k)	- spb	=	2.5076E+03
saturation pressure constant (k)	- spc	=	-2.9010E+01

spill characteristics

spill type	- idspl	=	2
mass source rate (kg/s)	- qs	=	6.3400E-02
continuous source duration (s)	- tsd	=	4.8000E+02
continuous source mass (kg)	- qtcs	=	3.0432E+01
instantaneous source mass (kg)	- qtis	=	0.0000E+00
source area (m2)	- as	=	2.3260E-04
vertical vapor velocity (m/s)	- ws	=	0.0000E+00
source half width (m)	- bs	=	7.6256E-03
source height (m)	- hs	=	0.0000E+00
horizontal vapor velocity (m/s)	- us	=	1.4164E+02

TABLE 7-14 (CONTINUED)

field parameters

concentration averaging time (s)	- tav	=	5.0000E+00
mixing layer height (m)	- hmx	=	2.0800E+03
maximum downwind distrace (m)	- xffm	=	1.0000E+03
concentration measurement height (m)	- zp(1)	=	0.0000E+00
	- zp(2)	=	3.6600E+00
	- zp(3)	=	0.0000E+00
	- zp(4)	=	0.0000E+00

ambient meteorological properties

molecular weight of ambient air (kg)	- wmae	=	2.8847E-02
heat capacity of ambient air at const p. (j/kg-k)	- cpaa	=	1.0113E+03
density of ambient air (kg/m3)	- rhoa	=	1.2227E+00
ambient measurement height (m)	- za	=	4.5700E+00
ambient atmospheric pressure (pa=n/m2=j/m3)	- pa	=	1.0133E+05
ambient wind speed (m/s)	- ua	=	5.3700E+00
ambient temperature (k)	- ta	=	2.8752E+02
relative humidity (percent)	- rh	=	6.2000E+01
ambient friction velocity (m/s)	- uastr	=	3.9267E-01
atmospheric stability class value	- stab	=	3.0000E+00
inverse monin-obukhov length (1/m)	- ala	=	-3.2907E-02
surface roughness height (m)	- z0	=	1.0000E-02

additional parameters

sub-step multiplier	- ncalc	=	1
number of calculational sub-steps	- nssm	=	3
acceleration of gravity (m/s2)	- grav	=	9.8067E+00
gas constant (j/mol- k)	- rr	=	8.3143E+00
von karman constant	- xk	=	4.1000E-01

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TABLE 7-14 (CONTINUED)

instantaneous spatially averaged cloud parameters

x	zc	h	bb	b	bbx	bx	cv	rho	t	u	ua
1.00E+00	0.00E+00	1.08E-02	1.08E-02	9.71E-03	0.00E+00	0.00E+00	1.00E+00	1.92E+00	2.84E+02	1.42E+02	1.89E-01
1.02E+00	0.00E+00	1.09E-01	5.44E-02	3.04E-02	1.66E-02	1.66E-02	1.35E-01	1.32E+00	2.85E+02	2.10E+01	1.44E+00
1.04E+00	0.00E+00	1.27E-01	6.34E-02	3.29E-02	3.59E-02	3.59E-02	1.16E-01	1.31E+00	2.86E+02	1.81E+01	1.56E+00
1.06E+00	0.00E+00	1.46E-01	7.28E-02	3.52E-02	5.85E-02	5.85E-02	1.00E-01	1.29E+00	2.86E+02	1.59E+01	1.68E+00
1.08E+00	0.00E+00	1.66E-01	8.29E-02	3.74E-02	8.48E-02	8.48E-02	8.74E-02	1.29E+00	2.86E+02	1.40E+01	1.79E+00
1.12E+00	0.00E+00	1.88E-01	9.38E-02	3.96E-02	1.15E-01	1.15E-01	7.67E-02	1.28E+00	2.86E+02	1.25E+01	1.89E+00
1.15E+00	0.00E+00	2.11E-01	1.05E-01	4.18E-02	1.51E-01	1.51E-01	6.76E-02	1.27E+00	2.86E+02	1.12E+01	1.99E+00
1.19E+00	0.00E+00	2.36E-01	1.18E-01	4.39E-02	1.93E-01	1.93E-01	5.97E-02	1.27E+00	2.87E+02	1.02E+01	2.09E+00
1.24E+00	0.00E+00	2.63E-01	1.32E-01	4.61E-02	2.41E-01	2.41E-01	5.29E-02	1.26E+00	2.87E+02	9.24E+00	2.18E+00
1.30E+00	0.00E+00	2.93E-01	1.46E-01	4.82E-02	2.98E-01	2.98E-01	4.69E-02	1.26E+00	2.87E+02	8.45E+00	2.28E+00
1.36E+00	0.00E+00	3.24E-01	1.62E-01	5.02E-02	3.64E-01	3.64E-01	4.16E-02	1.25E+00	2.87E+02	7.76E+00	2.37E+00
1.44E+00	0.00E+00	3.58E-01	1.79E-01	5.23E-02	4.41E-01	4.41E-01	3.69E-02	1.25E+00	2.87E+02	7.17E+00	2.45E+00
1.53E+00	0.00E+00	3.94E-01	1.97E-01	5.43E-02	5.31E-01	5.31E-01	3.27E-02	1.25E+00	2.87E+02	6.66E+00	2.54E+00
1.64E+00	0.00E+00	4.33E-01	2.17E-01	5.62E-02	6.36E-01	6.35E-01	2.90E-02	1.24E+00	2.87E+02	6.22E+00	2.62E+00
1.76E+00	0.00E+00	4.75E-01	2.38E-01	5.81E-02	7.58E-01	7.57E-01	2.57E-02	1.24E+00	2.87E+02	5.84E+00	2.70E+00
1.90E+00	0.00E+00	5.20E-01	2.60E-01	5.99E-02	9.00E-01	9.00E-01	2.27E-02	1.24E+00	2.87E+02	5.51E+00	2.78E+00
2.07E+00	0.00E+00	5.69E-01	2.84E-01	6.16E-02	1.07E+00	1.07E+00	2.01E-02	1.24E+00	2.87E+02	5.23E+00	2.86E+00
2.26E+00	0.00E+00	6.21E-01	3.10E-01	6.31E-02	1.26E+00	1.26E+00	1.77E-02	1.24E+00	2.87E+02	4.99E+00	2.93E+00
2.48E+00	0.00E+00	6.77E-01	3.38E-01	6.45E-02	1.48E+00	1.48E+00	1.55E-02	1.23E+00	2.87E+02	4.78E+00	3.01E+00
2.75E+00	0.00E+00	7.38E-01	3.69E-01	6.59E-02	1.75E+00	1.75E+00	1.35E-02	1.23E+00	2.87E+02	4.61E+00	3.08E+00
3.05E+00	0.00E+00	8.05E-01	4.02E-01	6.73E-02	2.05E+00	2.05E+00	1.17E-02	1.23E+00	2.87E+02	4.46E+00	3.16E+00
3.41E+00	0.00E+00	8.79E-01	4.39E-01	6.86E-02	2.41E+00	2.41E+00	1.01E-02	1.23E+00	2.87E+02	4.34E+00	3.23E+00
3.83E+00	0.00E+00	9.61E-01	4.80E-01	6.98E-02	2.83E+00	2.83E+00	8.67E-03	1.23E+00	2.87E+02	4.24E+00	3.31E+00
4.31E+00	0.00E+00	1.05E+00	5.26E-01	7.11E-02	3.31E+00	3.31E+00	7.37E-03	1.23E+00	2.87E+02	4.16E+00	3.38E+00
4.88E+00	0.00E+00	1.15E+00	5.77E-01	7.20E-02	3.88E+00	3.88E+00	6.20E-03	1.23E+00	2.87E+02	4.11E+00	3.46E+00
5.54E+00	0.00E+00	1.27E+00	6.34E-01	7.30E-02	4.54E+00	4.54E+00	5.17E-03	1.23E+00	2.87E+02	4.07E+00	3.54E+00
6.31E+00	0.00E+00	1.40E+00	7.00E-01	7.39E-02	5.31E+00	5.31E+00	4.27E-03	1.23E+00	2.87E+02	4.06E+00	3.63E+00
7.21E+00	0.00E+00	1.55E+00	7.74E-01	7.48E-02	6.21E+00	6.21E+00	3.49E-03	1.23E+00	2.87E+02	4.06E+00	3.71E+00
8.25E+00	0.00E+00	1.72E+00	8.60E-01	7.58E-02	7.25E+00	7.25E+00	2.82E-03	1.22E+00	2.87E+02	4.07E+00	3.80E+00
9.47E+00	0.00E+00	1.91E+00	9.57E-01	7.66E-02	8.47E+00	8.47E+00	2.26E-03	1.22E+00	2.87E+02	4.10E+00	3.89E+00
1.09E+01	0.00E+00	2.14E+00	1.07E+00	7.74E-02	9.90E+00	9.90E+00	1.79E-03	1.22E+00	2.87E+02	4.14E+00	3.98E+00
1.26E+01	0.00E+00	2.39E+00	1.20E+00	7.82E-02	1.16E+01	1.16E+01	1.41E-03	1.22E+00	2.87E+02	4.19E+00	4.07E+00
1.45E+01	0.00E+00	2.68E+00	1.35E+00	7.88E-02	1.35E+01	1.35E+01	1.10E-03	1.22E+00	2.88E+02	4.25E+00	4.16E+00
1.67E+01	0.00E+00	3.02E+00	1.52E+00	7.92E-02	1.57E+01	1.57E+01	8.54E-04	1.22E+00	2.88E+02	4.33E+00	4.26E+00

TABLE 7-14 (CONTINUED)

x	zc	h	bb	b	bbx	bx	cv	rho	t	u	ua
1.94E+01	0.00E+00	3.41E+00	1.72E+00	7.94E-02	1.84E+01	1.84E+01	6.57E-04	1.22E+00	2.88E+02	4.41E+00	4.35E+00
2.24E+01	0.00E+00	3.86E+00	1.95E+00	7.96E-02	2.14E+01	2.14E+01	5.03E-04	1.22E+00	2.88E+02	4.49E+00	4.45E+00
2.60E+01	0.00E+00	4.37E+00	2.21E+00	7.97E-02	2.50E+01	2.50E+01	3.84E-04	1.22E+00	2.88E+02	4.58E+00	4.55E+00
3.02E+01	0.00E+00	4.96E+00	2.52E+00	7.97E-02	2.92E+01	2.92E+01	2.91E-04	1.22E+00	2.88E+02	4.67E+00	4.65E+00
3.50E+01	0.00E+00	5.63E+00	2.88E+00	7.97E-02	3.40E+01	3.40E+01	2.20E-04	1.22E+00	2.88E+02	4.76E+00	4.75E+00
4.07E+01	0.00E+00	6.41E+00	3.29E+00	7.96E-02	3.97E+01	3.97E+01	1.66E-04	1.22E+00	2.88E+02	4.85E+00	4.85E+00
4.73E+01	0.00E+00	7.29E+00	3.77E+00	7.94E-02	4.63E+01	4.63E+01	1.25E-04	1.22E+00	2.88E+02	4.95E+00	4.95E+00
5.50E+01	0.00E+00	8.30E+00	4.32E+00	7.92E-02	5.40E+01	5.40E+01	9.37E-05	1.22E+00	2.88E+02	5.05E+00	5.05E+00
6.40E+01	0.00E+00	9.42E+00	4.99E+00	7.93E-02	6.30E+01	6.30E+01	7.02E-05	1.22E+00	2.88E+02	5.14E+00	5.14E+00
7.44E+01	0.00E+00	1.07E+01	5.77E+00	7.96E-02	7.34E+01	7.34E+01	5.25E-05	1.22E+00	2.88E+02	5.23E+00	5.24E+00
8.66E+01	0.00E+00	1.21E+01	6.68E+00	7.97E-02	8.56E+01	8.56E+01	3.93E-05	1.22E+00	2.88E+02	5.33E+00	5.33E+00
1.01E+02	0.00E+00	1.38E+01	7.74E+00	7.99E-02	9.98E+01	9.98E+01	2.93E-05	1.22E+00	2.88E+02	5.42E+00	5.43E+00
1.17E+02	0.00E+00	1.57E+01	8.96E+00	8.00E-02	1.16E+02	1.16E+02	2.19E-05	1.22E+00	2.88E+02	5.52E+00	5.52E+00
1.37E+02	0.00E+00	1.78E+01	1.04E+01	8.01E-02	1.36E+02	1.36E+02	1.64E-05	1.22E+00	2.88E+02	5.61E+00	5.61E+00
1.59E+02	0.00E+00	2.03E+01	1.20E+01	8.02E-02	1.58E+02	1.58E+02	1.22E-05	1.22E+00	2.88E+02	5.70E+00	5.71E+00
1.86E+02	0.00E+00	2.31E+01	1.39E+01	8.03E-02	1.85E+02	1.85E+02	9.11E-06	1.22E+00	2.88E+02	5.80E+00	5.80E+00
2.16E+02	0.00E+00	2.63E+01	1.61E+01	8.04E-02	2.15E+02	2.15E+02	6.80E-06	1.22E+00	2.88E+02	5.89E+00	5.89E+00
2.52E+02	0.00E+00	2.99E+01	1.87E+01	8.04E-02	2.51E+02	2.51E+02	5.08E-06	1.22E+00	2.88E+02	5.98E+00	5.99E+00
2.94E+02	0.00E+00	3.41E+01	2.17E+01	8.05E-02	2.93E+02	2.93E+02	3.79E-06	1.22E+00	2.88E+02	6.07E+00	6.08E+00
3.42E+02	0.00E+00	3.88E+01	2.51E+01	8.05E-02	3.41E+02	3.41E+02	2.84E-06	1.22E+00	2.88E+02	6.15E+00	6.17E+00
3.99E+02	0.00E+00	4.41E+01	2.90E+01	8.05E-02	3.98E+02	3.98E+02	2.12E-06	1.22E+00	2.88E+02	6.24E+00	6.26E+00
4.65E+02	0.00E+00	5.02E+01	3.36E+01	8.06E-02	4.64E+02	4.64E+02	1.59E-06	1.22E+00	2.88E+02	6.33E+00	6.35E+00
5.42E+02	0.00E+00	5.72E+01	3.88E+01	8.06E-02	5.41E+02	5.41E+02	1.19E-06	1.22E+00	2.88E+02	6.42E+00	6.44E+00
6.31E+02	0.00E+00	6.51E+01	4.49E+01	8.06E-02	6.30E+02	6.30E+02	8.93E-07	1.22E+00	2.88E+02	6.51E+00	6.53E+00
7.36E+02	0.00E+00	7.40E+01	5.18E+01	8.06E-02	7.35E+02	7.35E+02	6.71E-07	1.22E+00	2.88E+02	6.60E+00	6.62E+00
8.58E+02	0.00E+00	8.42E+01	5.98E+01	8.06E-02	8.57E+02	8.57E+02	5.05E-07	1.22E+00	2.88E+02	6.68E+00	6.71E+00
1.00E+03	0.00E+00	9.57E+01	6.88E+01	8.07E-02	9.99E+02	9.99E+02	3.81E-07	1.22E+00	2.88E+02	6.77E+00	6.79E+00

TABLE 7-14 (CONTINUED)

x	cm	cmv	cmda	cmw	cmwv	wc	vg	ug	w	v	vx
1.00E+00	1.00E+00	9.83E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	2.52E+03	7.82E+00	0.00E+00
1.02E+00	1.93E-01	1.93E-01	8.02E-01	5.19E-03	5.19E-03	0.00E+00	7.25E-04	0.00E+00	9.06E+00	1.58E+00	4.35E-01
1.04E+00	1.66E-01	1.66E-01	8.28E-01	5.36E-03	5.36E-03	0.00E+00	1.56E-03	0.00E+00	6.86E+00	1.35E+00	4.50E-01
1.06E+00	1.45E-01	1.45E-01	8.49E-01	5.50E-03	5.50E-03	0.00E+00	2.45E-03	0.00E+00	5.36E+00	1.17E+00	4.63E-01
1.08E+00	1.28E-01	1.28E-01	8.67E-01	5.61E-03	5.61E-03	0.00E+00	3.43E-03	0.00E+00	4.30E+00	1.02E+00	4.73E-01
1.12E+00	1.13E-01	1.13E-01	8.82E-01	5.71E-03	5.71E-03	0.00E+00	4.49E-03	0.00E+00	3.50E+00	8.88E-01	4.82E-01
1.15E+00	9.97E-02	9.97E-02	8.95E-01	5.79E-03	5.79E-03	0.00E+00	5.67E-03	0.00E+00	2.90E+00	7.79E-01	4.90E-01
1.19E+00	8.84E-02	8.84E-02	9.06E-01	5.86E-03	5.86E-03	0.00E+00	6.98E-03	0.00E+00	2.42E+00	6.85E-01	4.97E-01
1.24E+00	7.86E-02	7.86E-02	9.16E-01	5.93E-03	5.93E-03	0.00E+00	8.42E-03	0.00E+00	2.05E+00	6.03E-01	5.03E-01
1.30E+00	6.99E-02	6.99E-02	9.24E-01	5.98E-03	5.98E-03	0.00E+00	1.00E-02	0.00E+00	1.75E+00	5.32E-01	5.08E-01
1.36E+00	6.21E-02	6.21E-02	9.32E-01	6.03E-03	6.03E-03	0.00E+00	1.18E-02	0.00E+00	1.51E+00	4.70E-01	5.13E-01
1.44E+00	5.53E-02	5.53E-02	9.39E-01	6.08E-03	6.08E-03	0.00E+00	1.37E-02	0.00E+00	1.31E+00	4.16E-01	5.17E-01
1.53E+00	4.91E-02	4.91E-02	9.45E-01	6.12E-03	6.12E-03	0.00E+00	1.58E-02	0.00E+00	1.14E+00	3.69E-01	5.20E-01
1.64E+00	4.37E-02	4.37E-02	9.50E-01	6.15E-03	6.15E-03	0.00E+00	1.80E-02	0.00E+00	1.01E+00	3.28E-01	5.23E-01
1.76E+00	3.87E-02	3.87E-02	9.55E-01	6.18E-03	6.18E-03	0.00E+00	2.04E-02	0.00E+00	9.01E-01	2.93E-01	5.25E-01
1.90E+00	3.43E-02	3.43E-02	9.59E-01	6.21E-03	6.21E-03	0.00E+00	2.29E-02	0.00E+00	8.11E-01	2.63E-01	5.27E-01
2.07E+00	3.03E-02	3.03E-02	9.63E-01	6.24E-03	6.24E-03	0.00E+00	2.55E-02	0.00E+00	7.36E-01	2.38E-01	5.29E-01
2.26E+00	2.67E-02	2.67E-02	9.67E-01	6.26E-03	6.26E-03	0.00E+00	2.82E-02	0.00E+00	6.76E-01	2.17E-01	5.30E-01
2.48E+00	2.35E-02	2.35E-02	9.70E-01	6.28E-03	6.28E-03	0.00E+00	3.08E-02	0.00E+00	6.26E-01	2.00E-01	5.31E-01
2.75E+00	2.05E-02	2.05E-02	9.73E-01	6.30E-03	6.30E-03	0.00E+00	3.34E-02	0.00E+00	5.85E-01	1.87E-01	5.32E-01
3.05E+00	1.78E-02	1.78E-02	9.76E-01	6.32E-03	6.32E-03	0.00E+00	3.57E-02	0.00E+00	5.52E-01	1.76E-01	5.32E-01
3.41E+00	1.54E-02	1.54E-02	9.78E-01	6.33E-03	6.33E-03	0.00E+00	3.79E-02	0.00E+00	5.26E-01	1.69E-01	5.33E-01
3.83E+00	1.32E-02	1.32E-02	9.80E-01	6.35E-03	6.35E-03	0.00E+00	3.97E-02	0.00E+00	5.04E-01	1.63E-01	5.33E-01
4.31E+00	1.12E-02	1.12E-02	9.82E-01	6.36E-03	6.36E-03	0.00E+00	4.10E-02	0.00E+00	4.88E-01	1.60E-01	5.33E-01
4.88E+00	9.44E-03	9.44E-03	9.84E-01	6.37E-03	6.37E-03	0.00E+00	4.18E-02	0.00E+00	4.75E-01	1.59E-01	5.32E-01
5.54E+00	7.88E-03	7.88E-03	9.86E-01	6.38E-03	6.38E-03	0.00E+00	4.20E-02	0.00E+00	4.65E-01	1.59E-01	5.32E-01
6.31E+00	6.51E-03	6.51E-03	9.87E-01	6.39E-03	6.39E-03	0.00E+00	4.15E-02	0.00E+00	4.57E-01	1.60E-01	5.31E-01
7.21E+00	5.32E-03	5.32E-03	9.88E-01	6.40E-03	6.40E-03	0.00E+00	4.05E-02	0.00E+00	4.52E-01	1.62E-01	5.30E-01
8.25E+00	4.30E-03	4.30E-03	9.89E-01	6.40E-03	6.40E-03	0.00E+00	3.90E-02	0.00E+00	4.48E-01	1.65E-01	5.29E-01
9.47E+00	3.45E-03	3.45E-03	9.90E-01	6.41E-03	6.41E-03	0.00E+00	3.70E-02	0.00E+00	4.45E-01	1.68E-01	5.28E-01
1.09E+01	2.74E-03	2.74E-03	9.91E-01	6.42E-03	6.42E-03	0.00E+00	3.46E-02	0.00E+00	4.43E-01	1.71E-01	5.27E-01
1.26E+01	2.15E-03	2.15E-03	9.91E-01	6.42E-03	6.42E-03	0.00E+00	3.20E-02	0.00E+00	4.41E-01	1.75E-01	5.25E-01
1.45E+01	1.68E-03	1.68E-03	9.92E-01	6.42E-03	6.42E-03	0.00E+00	2.92E-02	0.00E+00	4.40E-01	1.79E-01	5.23E-01
1.67E+01	1.30E-03	1.30E-03	9.92E-01	6.42E-03	6.42E-03	0.00E+00	2.65E-02	0.00E+00	4.39E-01	1.83E-01	5.22E-01
1.94E+01	1.00E-03	1.00E-03	9.93E-01	6.43E-03	6.43E-03	0.00E+00	2.37E-02	0.00E+00	4.38E-01	1.87E-01	5.20E-01
2.24E+01	7.68E-04	7.68E-04	9.93E-01	6.43E-03	6.43E-03	0.00E+00	2.11E-02	0.00E+00	4.37E-01	1.91E-01	5.18E-01

TABLE 7-14 (CONTINUED)

x	cm	cmv	cmda	cmw	cmwv	wc	vg	ug	w	v	vx
2.60E+01	5.86E-04	5.86E-04	9.93E-01	6.43E-03	6.43E-03	0.00E+00	1.86E-02	0.00E+00	4.36E-01	1.95E-01	5.16E-01
3.02E+01	4.45E-04	4.45E-04	9.93E-01	6.43E-03	6.43E-03	0.00E+00	1.63E-02	0.00E+00	4.35E-01	1.99E-01	5.14E-01
3.50E+01	3.36E-04	3.36E-04	9.93E-01	6.43E-03	6.43E-03	0.00E+00	1.42E-02	0.00E+00	4.33E-01	2.03E-01	5.12E-01
4.07E+01	2.53E-04	2.53E-04	9.93E-01	6.43E-03	6.43E-03	0.00E+00	1.23E-02	0.00E+00	4.31E-01	2.07E-01	5.11E-01
4.73E+01	1.91E-04	1.91E-04	9.93E-01	6.43E-03	6.43E-03	0.00E+00	1.07E-02	0.00E+00	4.29E-01	2.11E-01	5.09E-01
5.50E+01	1.43E-04	1.43E-04	9.93E-01	6.43E-03	6.43E-03	0.00E+00	9.18E-03	0.00E+00	4.26E-01	2.15E-01	5.07E-01
6.40E+01	1.07E-04	1.07E-04	9.93E-01	6.43E-03	6.43E-03	0.00E+00	7.88E-03	0.00E+00	4.24E-01	2.18E-01	5.06E-01
7.44E+01	8.02E-05	8.02E-05	9.93E-01	6.43E-03	6.43E-03	0.00E+00	6.73E-03	0.00E+00	4.21E-01	2.22E-01	5.05E-01
8.66E+01	6.00E-05	6.00E-05	9.94E-01	6.43E-03	6.43E-03	0.00E+00	5.74E-03	0.00E+00	4.18E-01	2.25E-01	5.04E-01
1.01E+02	4.48E-05	4.48E-05	9.94E-01	6.43E-03	6.43E-03	0.00E+00	4.88E-03	0.00E+00	4.14E-01	2.29E-01	5.03E-01
1.17E+02	3.35E-05	3.35E-05	9.94E-01	6.43E-03	6.43E-03	0.00E+00	4.14E-03	0.00E+00	4.10E-01	2.32E-01	5.02E-01
1.37E+02	2.50E-05	2.50E-05	9.94E-01	6.43E-03	6.43E-03	0.00E+00	3.51E-03	0.00E+00	4.07E-01	2.35E-01	5.01E-01
1.59E+02	1.86E-05	1.86E-05	9.94E-01	6.43E-03	6.43E-03	0.00E+00	2.97E-03	0.00E+00	4.03E-01	2.38E-01	5.01E-01
1.86E+02	1.39E-05	1.39E-05	9.94E-01	6.43E-03	6.43E-03	0.00E+00	2.51E-03	0.00E+00	3.98E-01	2.41E-01	5.00E-01
2.16E+02	1.04E-05	1.04E-05	9.94E-01	6.43E-03	6.43E-03	0.00E+00	2.13E-03	0.00E+00	3.94E-01	2.43E-01	5.00E-01
2.52E+02	7.75E-06	7.75E-06	9.94E-01	6.43E-03	6.43E-03	0.00E+00	1.79E-03	0.00E+00	3.90E-01	2.45E-01	5.00E-01
2.94E+02	5.79E-06	5.79E-06	9.94E-01	6.43E-03	6.43E-03	0.00E+00	1.51E-03	0.00E+00	3.85E-01	2.47E-01	5.00E-01
3.42E+02	4.33E-06	4.33E-06	9.94E-01	6.43E-03	6.43E-03	0.00E+00	1.26E-03	0.00E+00	3.80E-01	2.49E-01	5.00E-01
3.99E+02	3.24E-06	3.24E-06	9.94E-01	6.43E-03	6.43E-03	0.00E+00	1.06E-03	0.00E+00	3.75E-01	2.50E-01	5.00E-01
4.65E+02	2.43E-06	2.43E-06	9.94E-01	6.43E-03	6.43E-03	0.00E+00	8.98E-04	0.00E+00	3.71E-01	2.51E-01	5.00E-01
5.42E+02	1.82E-06	1.82E-06	9.94E-01	6.43E-03	6.43E-03	0.00E+00	7.66E-04	0.00E+00	3.66E-01	2.51E-01	5.01E-01
6.31E+02	1.36E-06	1.36E-06	9.94E-01	6.43E-03	6.43E-03	0.00E+00	6.46E-04	0.00E+00	3.60E-01	2.51E-01	5.01E-01
7.36E+02	1.02E-06	1.02E-06	9.94E-01	6.43E-03	6.43E-03	0.00E+00	5.46E-04	0.00E+00	3.55E-01	2.50E-01	5.02E-01
8.58E+02	7.71E-07	7.71E-07	9.94E-01	6.43E-03	6.43E-03	0.00E+00	4.55E-04	0.00E+00	3.50E-01	2.49E-01	5.02E-01
1.00E+03	5.81E-07	5.81E-07	9.94E-01	6.43E-03	6.43E-03	0.00E+00	3.75E-04	0.00E+00	3.44E-01	2.47E-01	5.03E-01

TABLE 7-14 (CONTINUED)

time averaged (tav = 5. s) volume concentration: concentration contour parameters

c(x,y,z,t) = cc(x) * (erf(xa)-erf(xb)) * (erf(ya)-erf(yb)) * (exp(-za*za)+exp(-zb*zb))

c(x,y,z,t) = concentration (volume fraction) at (x,y,z,t)
x = downwind distance (m)
y = crosswind horizontal distance (m)
z = height (m)
t = time (s)

erf = error functon
xa = (x-xc+bx)/(sr2*betax)
xb = (x-xc-bx)/(sr2*betax)
ya = (y+b)/(sr2*betac)
yb = (y-b)/(sr2*betac)
exp = exponential function
za = (z-zc)/(sr2*sig)
zb = (z+zc)/(sr2*sig)
sr2 = sqrt(2.0)

x	cc(x)	b(x)	betac(x)	zc(x)	sig(x)	t	xc(t)	bx(t)	betax(t)
1.00E+00	0.00E+00	9.71E-03	2.71E-03	0.00E+00	6.23E-03	0.00E+00	1.00E+00	0.00E+00	0.00E+00
1.02E+00	4.18E-02	3.04E-02	2.61E-02	0.00E+00	6.29E-02	1.34E-03	1.02E+00	1.66E-02	1.35E-04
1.04E+00	3.86E-02	3.29E-02	3.13E-02	0.00E+00	7.32E-02	3.33E-03	1.04E+00	3.59E-02	2.93E-04
1.06E+00	3.58E-02	3.52E-02	3.68E-02	0.00E+00	8.42E-02	6.00E-03	1.06E+00	5.85E-02	4.78E-04
1.08E+00	3.35E-02	3.74E-02	4.27E-02	0.00E+00	9.58E-02	9.53E-03	1.08E+00	8.48E-02	6.92E-04
1.12E+00	3.14E-02	3.96E-02	4.91E-02	0.00E+00	1.08E-01	1.42E-02	1.12E+00	1.15E-01	9.43E-04
1.15E+00	2.95E-02	4.18E-02	5.59E-02	0.00E+00	1.22E-01	2.02E-02	1.15E+00	1.51E-01	1.23E-03
1.19E+00	2.77E-02	4.39E-02	6.32E-02	0.00E+00	1.36E-01	2.80E-02	1.19E+00	1.93E-01	1.57E-03
1.24E+00	2.61E-02	4.61E-02	7.11E-02	0.00E+00	1.52E-01	3.81E-02	1.24E+00	2.41E-01	1.97E-03
1.30E+00	2.46E-02	4.82E-02	7.97E-02	0.00E+00	1.69E-01	5.09E-02	1.30E+00	2.98E-01	2.43E-03
1.36E+00	2.32E-02	5.02E-02	8.89E-02	0.00E+00	1.87E-01	6.72E-02	1.36E+00	3.64E-01	2.97E-03
1.44E+00	2.18E-02	5.23E-02	9.88E-02	0.00E+00	2.07E-01	8.79E-02	1.44E+00	4.41E-01	3.60E-03
1.53E+00	2.05E-02	5.43E-02	1.09E-01	0.00E+00	2.28E-01	1.14E-01	1.53E+00	5.31E-01	4.34E-03
1.64E+00	1.93E-02	5.62E-02	1.21E-01	0.00E+00	2.50E-01	1.46E-01	1.64E+00	6.35E-01	5.19E-03
1.76E+00	1.82E-02	5.81E-02	1.33E-01	0.00E+00	2.74E-01	1.87E-01	1.76E+00	7.57E-01	6.19E-03
1.90E+00	1.71E-02	5.99E-02	1.46E-01	0.00E+00	3.00E-01	2.37E-01	1.90E+00	9.00E-01	7.35E-03
2.07E+00	1.60E-02	6.16E-02	1.60E-01	0.00E+00	3.28E-01	2.99E-01	2.07E+00	1.07E+00	8.70E-03

TABLE 7-14 (CONTINUED)

x	ε(x)	h(x)	betac(x)	zc(x)	sig(x)
2.26E+00	1.50E-02	6.31E-02	1.75E-01	0.00E+00	3.58E-01
2.48E+00	1.40E-02	6.45E-02	1.92E-01	0.00E+00	3.91E-01
2.75E+00	1.31E-02	6.59E-02	2.10E-01	0.00E+00	4.26E-01
3.05E+00	1.21E-02	6.73E-02	2.29E-01	0.00E+00	4.65E-01
3.41E+00	1.12E-02	6.86E-02	2.51E-01	0.00E+00	5.08E-01
3.83E+00	1.03E-02	6.98E-02	2.74E-01	0.00E+00	5.55E-01
4.31E+00	9.42E-03	7.11E-02	3.01E-01	0.00E+00	6.07E-01
4.88E+00	8.59E-03	7.20E-02	3.31E-01	0.00E+00	6.66E-01
5.54E+00	7.78E-03	7.30E-02	3.64E-01	0.00E+00	7.33E-01
6.31E+00	6.99E-03	7.39E-02	4.02E-01	0.00E+00	8.08E-01
7.21E+00	6.25E-03	7.48E-02	4.46E-01	0.00E+00	8.94E-01
8.25E+00	5.54E-03	7.58E-02	4.95E-01	0.00E+00	9.92E-01
9.47E+00	4.89E-03	7.66E-02	5.52E-01	0.00E+00	1.10E+00
1.09E+01	4.30E-03	7.74E-02	6.18E-01	0.00E+00	1.23E+00
1.26E+01	3.76E-03	7.82E-02	6.94E-01	0.00E+00	1.38E+00
1.45E+01	3.28E-03	7.88E-02	7.82E-01	0.00E+00	1.55E+00
1.67E+01	2.85E-03	7.92E-02	8.82E-01	0.00E+00	1.75E+00
1.94E+01	2.47E-03	7.94E-02	9.98E-01	0.00E+00	1.97E+00
2.24E+01	2.15E-03	7.96E-02	1.13E+00	0.00E+00	2.23E+00
2.60E+01	1.86E-03	7.97E-02	1.29E+00	0.00E+00	2.52E+00
3.02E+01	1.61E-03	7.97E-02	1.47E+00	0.00E+00	2.86E+00
3.50E+01	1.39E-03	7.97E-02	1.68E+00	0.00E+00	3.25E+00
4.07E+01	1.20E-03	7.96E-02	1.92E+00	0.00E+00	3.70E+00
4.73E+01	1.04E-03	7.94E-02	2.21E+00	0.00E+00	4.21E+00
5.50E+01	8.97E-04	7.92E-02	2.53E+00	0.00E+00	4.79E+00
6.40E+01	7.75E-04	7.93E-02	2.93E+00	0.00E+00	5.44E+00
7.44E+01	6.70E-04	7.96E-02	3.39E+00	0.00E+00	6.17E+00
8.66E+01	5.78E-04	7.97E-02	3.92E+00	0.00E+00	7.01E+00
1.01E+02	5.00E-04	7.99E-02	4.54E+00	0.00E+00	7.96E+00
1.17E+02	4.31E-04	8.00E-02	5.27E+00	0.00E+00	9.05E+00
1.37E+02	3.73E-04	8.01E-02	6.10E+00	0.00E+00	1.03E+01
1.59E+02	3.22E-04	8.02E-02	7.07E+00	0.00E+00	1.17E+01
1.86E+02	2.78E-04	8.03E-02	8.19E+00	0.00E+00	1.33E+01
2.16E+02	2.40E-04	8.04E-02	9.49E+00	0.00E+00	1.52E+01
2.52E+02	2.08E-04	8.04E-02	1.10E+01	0.00E+00	1.73E+01

t	xc(t)	bx(t)	betax(t)
3.75E-01	2.26E+00	1.26E+00	1.03E-02
4.67E-01	2.48E+00	1.48E+00	1.21E-02
5.79E-01	2.75E+00	1.75E+00	1.43E-02
7.15E-01	3.05E+00	2.05E+00	1.68E-02
8.77E-01	3.41E+00	2.41E+00	1.97E-02
1.07E+00	3.83E+00	2.83E+00	2.31E-02
1.30E+00	4.31E+00	3.31E+00	2.71E-02
1.58E+00	4.88E+00	3.88E+00	3.17E-02
1.90E+00	5.54E+00	4.54E+00	3.71E-02
2.28E+00	6.31E+00	5.31E+00	4.34E-02
2.72E+00	7.21E+00	6.21E+00	5.07E-02
3.24E+00	8.25E+00	7.25E+00	5.92E-02
3.83E+00	9.47E+00	8.47E+00	6.92E-02
4.52E+00	1.09E+01	9.90E+00	8.08E-02
5.32E+00	1.26E+01	1.16E+01	9.44E-02
6.24E+00	1.45E+01	1.35E+01	1.10E-01
7.29E+00	1.67E+01	1.57E+01	1.29E-01
8.49E+00	1.94E+01	1.84E+01	1.50E-01
9.87E+00	2.24E+01	2.14E+01	1.75E-01
1.14E+01	2.60E+01	2.50E+01	2.04E-01
1.32E+01	3.02E+01	2.92E+01	2.38E-01
1.53E+01	3.50E+01	3.40E+01	2.78E-01
1.77E+01	4.07E+01	3.97E+01	3.24E-01
2.04E+01	4.73E+01	4.63E+01	3.78E-01
2.34E+01	5.50E+01	5.40E+01	4.41E-01
2.70E+01	6.40E+01	6.30E+01	5.14E-01
3.10E+01	7.44E+01	7.34E+01	5.99E-01
3.56E+01	8.66E+01	8.56E+01	6.99E-01
4.09E+01	1.01E+02	9.98E+01	8.15E-01
4.70E+01	1.17E+02	1.16E+02	9.51E-01
5.39E+01	1.37E+02	1.36E+02	1.11E+00
6.19E+01	1.59E+02	1.58E+02	1.29E+00
7.10E+01	1.86E+02	1.85E+02	1.51E+00
8.15E+01	2.16E+02	2.15E+02	1.76E+00
9.35E+01	2.52E+02	2.51E+02	2.05E+00

TABLE 7-14 (CONTINUED)

x	cc(x)	b(x)	betac(x)	zc(x)	sig(x)	t	xc(t)	bx(t)	betax(t)
2.94E+02	1.80E-04	8.05E-02	1.27E+01	0.00E+00	1.97E+01	1.07E+02	2.94E+02	2.93E+02	2.39E+00
3.42E+02	1.56E-04	8.05E-02	1.48E+01	0.00E+00	2.24E+01	1.23E+02	3.42E+02	3.41E+02	2.79E+00
3.99E+02	1.35E-04	8.05E-02	1.71E+01	0.00E+00	2.55E+01	1.42E+02	3.99E+02	3.98E+02	3.25E+00
4.65E+02	1.17E-04	8.06E-02	1.98E+01	0.00E+00	2.90E+01	1.62E+02	4.65E+02	4.64E+02	3.79E+00
5.42E+02	1.01E-04	8.06E-02	2.29E+01	0.00E+00	3.30E+01	1.87E+02	5.42E+02	5.41E+02	4.41E+00
6.31E+02	8.76E-05	8.06E-02	2.64E+01	0.00E+00	3.76E+01	2.14E+02	6.31E+02	6.30E+02	5.15E+00
7.36E+02	7.60E-05	8.06E-02	3.05E+01	0.00E+00	4.27E+01	2.46E+02	7.36E+02	7.35E+02	6.00E+00
8.58E+02	6.60E-05	8.06E-02	3.52E+01	0.00E+00	4.86E+01	2.83E+02	8.58E+02	8.57E+02	7.00E+00
1.00E+03	5.73E-05	8.07E-02	4.05E+01	0.00E+00	5.53E+01	3.25E+02	1.00E+03	9.99E+02	8.16E+00

time averaged (tav = 5. s) volume concentration: concentration in the z = .00 plane.

downwind distance x (m)	time of max conc (s)	cloud duration (s)	effective half width bbc (m)	average concentration (volume fraction) at (x,y,z) y/bbc= 0.0	y/bbc= 0.5	y/bbc= 1.0	y/bbc= 1.5	y/bbc= 2.0	y/bbc= 2.5
1.00E+00	2.40E+02	4.80E+02	1.08E-02	1.00E+00	1.00E+00	5.31E-01	1.31E-02	9.52E-06	0.00E+00
1.02E+00	2.40E+02	4.80E+02	5.44E-02	2.53E-01	1.79E-01	5.94E-02	8.25E-03	4.37E-04	8.44E-06
1.04E+00	2.40E+02	4.80E+02	6.34E-02	2.18E-01	1.53E-01	5.04E-02	7.21E-03	4.15E-04	9.23E-06
1.06E+00	2.40E+02	4.80E+02	7.28E-02	1.89E-01	1.32E-01	4.34E-02	6.33E-03	3.86E-04	9.48E-06
1.08E+00	2.40E+02	4.80E+02	8.29E-02	1.66E-01	1.15E-01	3.77E-02	5.57E-03	3.54E-04	9.37E-06
1.12E+00	2.40E+02	4.80E+02	9.38E-02	1.46E-01	1.01E-01	3.30E-02	4.92E-03	3.23E-04	9.02E-06
1.15E+00	2.40E+02	4.80E+02	1.05E-01	1.29E-01	8.89E-02	2.90E-02	4.36E-03	2.92E-04	8.52E-06
1.19E+00	2.40E+02	4.80E+02	1.18E-01	1.14E-01	7.85E-02	2.56E-02	3.86E-03	2.63E-04	7.94E-06
1.24E+00	2.40E+02	4.80E+02	1.32E-01	1.01E-01	6.95E-02	2.26E-02	3.43E-03	2.37E-04	7.32E-06
1.30E+00	2.40E+02	4.80E+02	1.46E-01	8.94E-02	6.16E-02	2.00E-02	3.05E-03	2.12E-04	6.70E-06
1.36E+00	2.40E+02	4.80E+02	1.62E-01	7.93E-02	5.46E-02	1.78E-02	2.71E-03	1.90E-04	6.10E-06
1.44E+00	2.40E+02	4.80E+02	1.79E-01	7.04E-02	4.84E-02	1.58E-02	2.40E-03	1.70E-04	5.53E-06
1.53E+00	2.40E+02	4.80E+02	1.97E-01	6.25E-02	4.30E-02	1.40E-02	2.13E-03	1.52E-04	4.98E-06
1.64E+00	2.40E+02	4.80E+02	2.17E-01	5.54E-02	3.81E-02	1.24E-02	1.89E-03	1.35E-04	4.47E-06
1.76E+00	2.40E+02	4.80E+02	2.38E-01	4.91E-02	3.37E-02	1.10E-02	1.68E-03	1.20E-04	4.00E-06
1.90E+00	2.40E+02	4.80E+02	2.60E-01	4.34E-02	2.98E-02	9.70E-03	1.48E-03	1.06E-04	3.57E-06
2.07E+00	2.40E+02	4.80E+02	2.84E-01	3.83E-02	2.63E-02	8.56E-03	1.31E-03	9.42E-05	3.17E-06
2.26E+00	2.40E+02	4.80E+02	3.10E-01	3.37E-02	2.32E-02	7.53E-03	1.15E-03	8.30E-05	2.80E-06
2.48E+00	2.40E+02	4.80E+02	3.38E-01	2.96E-02	2.03E-02	6.60E-03	1.01E-03	7.29E-05	2.47E-06
2.75E+00	2.40E+02	4.80E+02	3.69E-01	2.58E-02	1.77E-02	5.76E-03	8.83E-04	6.37E-05	2.17E-06
3.05E+00	2.40E+02	4.80E+02	4.03E-01	2.24E-02	1.54E-02	5.00E-03	7.67E-04	5.54E-05	1.88E-06
3.41E+00	2.40E+02	4.80E+02	4.39E-01	1.93E-02	1.33E-02	4.31E-03	6.61E-04	4.78E-05	1.63E-06

TABLE 7-14 (CONTINUED)

downwind distance x (m)	time of max conc (s)	cloud duration (s)	effective half width bbc (m)	average concentration (volume fraction) at (x,y,z) y/bbc= 0.0	y/bbc= 0.5	y/bbc= 1.0	y/bbc= 1.5	y/bbc= 2.0	y/bbc= 2.5
3.83E+00	2.40E+02	4.80E+02	4.80E-01	1.66E-02	1.14E-02	3.70E-03	5.67E-04	4.10E-05	1.40E-06
4.31E+00	2.41E+02	4.80E+02	5.26E-01	1.41E-02	9.67E-03	3.14E-03	4.81E-04	3.48E-05	1.19E-06
4.88E+00	2.41E+02	4.80E+02	5.77E-01	1.18E-02	8.14E-03	2.64E-03	4.05E-04	2.93E-05	1.00E-06
5.54E+00	2.41E+02	4.80E+02	6.35E-01	9.87E-03	6.78E-03	2.20E-03	3.38E-04	2.45E-05	8.35E-07
6.31E+00	2.41E+02	4.80E+02	7.00E-01	8.15E-03	5.60E-03	1.82E-03	2.79E-04	2.02E-05	6.91E-07
7.21E+00	2.41E+02	4.80E+02	7.76E-01	6.65E-03	4.57E-03	1.48E-03	2.28E-04	1.65E-05	5.64E-07
8.25E+00	2.41E+02	4.80E+02	8.61E-01	5.38E-03	3.70E-03	1.20E-03	1.84E-04	1.33E-05	4.56E-07
9.47E+00	2.41E+02	4.80E+02	9.60E-01	4.31E-03	2.96E-03	9.61E-04	1.47E-04	1.07E-05	3.64E-07
1.09E+01	2.42E+02	4.80E+02	1.07E+00	3.41E-03	2.35E-03	7.62E-04	1.17E-04	8.46E-06	2.90E-07
1.26E+01	2.42E+02	4.80E+02	1.20E+00	2.68E-03	1.84E-03	5.99E-04	9.18E-05	6.65E-06	2.27E-07
1.45E+01	2.42E+02	4.80E+02	1.36E+00	2.09E-03	1.44E-03	4.67E-04	7.16E-05	5.19E-06	1.78E-07
1.67E+01	2.43E+02	4.80E+02	1.53E+00	1.62E-03	1.11E-03	3.61E-04	5.54E-05	4.01E-06	1.38E-07
1.94E+01	2.43E+02	4.80E+02	1.73E+00	1.25E-03	8.56E-04	2.78E-04	4.26E-05	3.09E-06	1.06E-07
2.24E+01	2.43E+02	4.80E+02	1.96E+00	9.53E-04	6.55E-04	2.13E-04	3.26E-05	2.36E-06	8.11E-08
2.60E+01	2.44E+02	4.80E+02	2.23E+00	7.25E-04	4.99E-04	1.62E-04	2.48E-05	1.80E-06	6.14E-08
3.02E+01	2.45E+02	4.80E+02	2.55E+00	5.50E-04	3.78E-04	1.23E-04	1.88E-05	1.36E-06	4.66E-08
3.50E+01	2.46E+02	4.80E+02	2.91E+00	4.15E-04	2.85E-04	9.27E-05	1.42E-05	1.03E-06	3.53E-08
4.07E+01	2.46E+02	4.80E+02	3.33E+00	3.13E-04	2.15E-04	6.98E-05	1.07E-05	7.76E-07	2.66E-08
4.73E+01	2.48E+02	4.80E+02	3.82E+00	2.35E-04	1.62E-04	5.25E-05	8.04E-06	5.83E-07	2.00E-08
5.50E+01	2.49E+02	4.80E+02	4.39E+00	1.76E-04	1.21E-04	3.93E-05	6.03E-06	4.37E-07	1.50E-08
6.40E+01	2.50E+02	4.80E+02	5.07E+00	1.32E-04	9.07E-05	2.95E-05	4.52E-06	3.27E-07	1.13E-08
7.44E+01	2.52E+02	4.80E+02	5.87E+00	9.87E-05	6.79E-05	2.20E-05	3.38E-06	2.45E-07	8.48E-09
8.66E+01	2.54E+02	4.80E+02	6.80E+00	7.38E-05	5.07E-05	1.65E-05	2.52E-06	1.83E-07	6.24E-09
1.01E+02	2.56E+02	4.80E+02	7.87E+00	5.51E-05	3.79E-05	1.23E-05	1.88E-06	1.37E-07	4.56E-09
1.17E+02	2.59E+02	4.80E+02	9.12E+00	4.11E-05	2.83E-05	9.17E-06	1.41E-06	1.02E-07	3.54E-09
1.37E+02	2.62E+02	4.80E+02	1.06E+01	3.07E-05	2.11E-05	6.84E-06	1.05E-06	7.61E-08	2.62E-09
1.59E+02	2.66E+02	4.80E+02	1.22E+01	2.29E-05	1.57E-05	5.11E-06	7.83E-07	5.67E-08	1.96E-09
1.86E+02	2.70E+02	4.80E+02	1.42E+01	1.71E-05	1.17E-05	3.81E-06	5.84E-07	4.23E-08	1.43E-09
2.16E+02	2.75E+02	4.80E+02	1.64E+01	1.27E-05	8.76E-06	2.84E-06	4.36E-07	3.16E-08	1.07E-09
2.52E+02	2.81E+02	4.80E+02	1.91E+01	9.52E-06	6.54E-06	2.12E-06	3.26E-07	2.36E-08	7.78E-10
2.94E+02	2.88E+02	4.80E+02	2.21E+01	7.11E-06	4.89E-06	1.59E-06	2.43E-07	1.76E-08	5.89E-10
3.42E+02	2.96E+02	4.80E+02	2.56E+01	5.31E-06	3.65E-06	1.19E-06	1.82E-07	1.32E-08	4.37E-10
3.99E+02	3.05E+02	4.80E+02	2.96E+01	3.97E-06	2.73E-06	8.87E-07	1.36E-07	9.86E-09	3.15E-10

TABLE 7-14 (CONTINUED)

downwind distance x (m)	time of max conc (s)	cloud duration (s)	effective half width bbc (m)	average concentration (volume fraction) at (x,y,z) y/bbc= 0.0	y/bbc= 0.5	y/bbc= 1.0	y/bbc= 1.5	y/bbc= 2.0	y/bbc= 2.5
4.65E+02	3.15E+02	4.80E+02	3.43E+01	2.97E-06	2.04E-06	6.64E-07	1.02E-07	7.36E-09	2.73E-10
5.42E+02	3.28E+02	4.80E+02	3.96E+01	2.23E-06	1.53E-06	4.97E-07	7.63E-08	5.53E-09	1.89E-10
6.31E+02	3.43E+02	4.80E+02	4.58E+01	1.67E-06	1.15E-06	3.73E-07	5.72E-08	4.14E-09	1.23E-10
7.36E+02	3.60E+02	4.80E+02	5.29E+01	1.26E-06	8.64E-07	2.80E-07	4.30E-08	3.13E-09	1.07E-10
8.58E+02	3.80E+02	4.80E+02	6.10E+01	9.46E-07	6.50E-07	2.11E-07	3.24E-08	2.34E-09	9.25E-11
1.00E+03	4.03E+02	4.80E+02	7.02E+01	7.13E-07	4.90E-07	1.59E-07	2.44E-08	1.77E-09	5.35E-11

time averaged (tav = 5. s) volume concentration: concentration in the z = 3.66 plane.

downwind distance x (m)	time of max conc (s)	cloud duration (s)	effective half width bbc (m)	average concentration (volume fraction) at (x,y,z) y/bbc= 0.0	y/bbc= 0.5	y/bbc= 1.0	y/bbc= 1.5	y/bbc= 2.0	y/bbc= 2.5
1.00E+00	2.40E+02	4.80E+02	1.08E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.02E+00	2.40E+02	4.80E+02	5.44E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.04E+00	2.40E+02	4.80E+02	6.34E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.06E+00	2.40E+02	4.80E+02	7.28E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.08E+00	2.40E+02	4.80E+02	8.29E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.12E+00	2.40E+02	4.80E+02	9.38E-02	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.15E+00	2.40E+02	4.80E+02	1.05E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.19E+00	2.40E+02	4.80E+02	1.18E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.24E+00	2.40E+02	4.80E+02	1.32E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.30E+00	2.40E+02	4.80E+02	1.46E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.36E+00	2.40E+02	4.80E+02	1.62E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.44E+00	2.40E+02	4.80E+02	1.79E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.53E+00	2.40E+02	4.80E+02	1.97E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.64E+00	2.40E+02	4.80E+02	2.17E-01	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
1.76E+00	2.40E+02	4.80E+02	2.38E-01	1.14E-40	7.83E-41	2.54E-41	3.89E-42	2.79E-43	9.81E-45
1.90E+00	2.40E+02	4.80E+02	2.60E-01	2.50E-34	1.72E-34	5.59E-35	8.56E-36	6.14E-37	2.06E-38
2.07E+00	2.40E+02	4.80E+02	2.84E-01	4.07E-29	2.80E-29	9.09E-30	1.39E-30	1.00E-31	3.37E-33
2.26E+00	2.40E+02	4.80E+02	3.10E-01	7.66E-25	5.26E-25	1.71E-25	2.62E-26	1.89E-27	6.37E-29
2.48E+00	2.40E+02	4.80E+02	3.38E-01	2.74E-21	1.88E-21	6.11E-22	9.36E-23	6.75E-24	2.28E-25
2.75E+00	2.40E+02	4.80E+02	3.69E-01	2.55E-18	1.75E-18	5.68E-19	8.71E-20	6.29E-21	2.14E-22

TABLE 7-14 (CONTINUED)

Downwind distance x (m)	Time of max conc (s)	cloud duration (s)	effective half width bbc (m)	average concentration (volume fraction) at (x, y/bbc= 0.0	y/bbc= 0.5	y/bbc= 1.0	y/bbc= 1.5	y/bbc= 2.0	y/bbc= 2.5
3.05E+00	2.40E+02	4.80E+02	4.03E-01	7.89E-16	5.43E-16	1.76E-16	2.70E-17	1.95E-18	6.63E-20
3.41E+00	2.40E+02	4.80E+02	4.39E-01	9.91E-14	6.81E-14	2.21E-14	3.39E-15	2.45E-16	8.34E-18
3.83E+00	2.40E+02	4.80E+02	4.80E-01	5.85E-12	4.02E-12	1.31E-12	2.00E-13	1.45E-14	4.94E-16
4.31E+00	2.41E+02	4.80E+02	5.26E-01	1.83E-10	1.26E-10	4.09E-11	6.27E-12	4.53E-13	1.55E-14
4.88E+00	2.41E+02	4.80E+02	5.77E-01	3.34E-09	2.29E-09	7.44E-10	1.14E-10	8.26E-12	2.82E-13
5.54E+00	2.41E+02	4.80E+02	6.35E-01	3.78E-08	2.60E-08	8.44E-09	1.29E-09	9.37E-11	3.20E-12
6.31E+00	2.41E+02	4.80E+02	7.00E-01	2.88E-07	1.98E-07	6.42E-08	9.85E-09	7.13E-10	2.44E-11
7.21E+00	2.41E+02	4.80E+02	7.76E-01	1.52E-06	1.05E-06	3.40E-07	5.21E-08	3.77E-09	1.29E-10
8.25E+00	2.41E+02	4.80E+02	8.61E-01	5.98E-06	4.11E-06	1.33E-06	2.04E-07	1.48E-08	5.07E-10
9.47E+00	2.41E+02	4.80E+02	9.60E-01	1.78E-05	1.22E-05	3.97E-06	6.09E-07	4.41E-08	1.51E-09
1.09E+01	2.42E+02	4.80E+02	1.07E+00	4.19E-05	2.88E-05	9.35E-06	1.43E-06	1.04E-07	3.56E-09
1.26E+01	2.42E+02	4.80E+02	1.20E+00	8.02E-05	5.51E-05	1.79E-05	2.74E-06	1.99E-07	6.80E-09
1.45E+01	2.42E+02	4.80E+02	1.36E+00	1.29E-04	8.85E-05	2.87E-05	4.41E-06	3.19E-07	1.10E-08
1.67E+01	2.43E+02	4.80E+02	1.53E+00	1.80E-04	1.24E-04	4.01E-05	6.15E-06	4.46E-07	1.53E-08
1.94E+01	2.43E+02	4.80E+02	1.73E+00	2.22E-04	1.52E-04	4.95E-05	7.59E-06	5.50E-07	1.89E-08
2.24E+01	2.43E+02	4.80E+02	1.96E+00	2.47E-04	1.70E-04	5.52E-05	8.46E-06	6.13E-07	2.10E-08
2.60E+01	2.44E+02	4.80E+02	2.23E+00	2.53E-04	1.74E-04	5.66E-05	8.67E-06	6.28E-07	2.14E-08
3.02E+01	2.45E+02	4.80E+02	2.55E+00	2.43E-04	1.67E-04	5.42E-05	8.31E-06	6.02E-07	2.06E-08
3.50E+01	2.46E+02	4.80E+02	2.91E+00	2.21E-04	1.52E-04	4.92E-05	7.55E-06	5.47E-07	1.88E-08
4.07E+01	2.46E+02	4.80E+02	3.33E+00	1.92E-04	1.32E-04	4.28E-05	6.56E-06	4.75E-07	1.63E-08
4.73E+01	2.48E+02	4.80E+02	3.82E+00	1.61E-04	1.11E-04	3.59E-05	5.51E-06	3.99E-07	1.37E-08
5.50E+01	2.49E+02	4.80E+02	4.39E+00	1.32E-04	9.05E-05	2.94E-05	4.51E-06	3.26E-07	1.12E-08
6.40E+01	2.50E+02	4.80E+02	5.07E+00	1.05E-04	7.24E-05	2.35E-05	3.60E-06	2.61E-07	9.00E-09
7.44E+01	2.52E+02	4.80E+02	5.87E+00	8.28E-05	5.69E-05	1.85E-05	2.83E-06	2.05E-07	7.11E-09
8.66E+01	2.54E+02	4.80E+02	6.80E+00	6.44E-05	4.42E-05	1.44E-05	2.20E-06	1.60E-07	5.44E-09
1.01E+02	2.56E+02	4.80E+02	7.87E+00	4.96E-05	3.41E-05	1.11E-05	1.70E-06	1.23E-07	4.11E-09
1.17E+02	2.59E+02	4.80E+02	9.12E+00	3.79E-05	2.60E-05	8.45E-06	1.30E-06	9.39E-08	3.26E-09
1.37E+02	2.62E+02	4.80E+02	1.06E+01	2.88E-05	1.98E-05	6.43E-06	9.85E-07	7.14E-08	2.46E-09
1.59E+02	2.66E+02	4.80E+02	1.22E+01	2.18E-05	1.50E-05	4.86E-06	7.46E-07	5.40E-08	1.87E-09
1.86E+02	2.70E+02	4.80E+02	1.42E+01	1.64E-05	1.13E-05	3.67E-06	5.63E-07	4.07E-08	1.38E-09
2.16E+02	2.75E+02	4.80E+02	1.64E+01	1.24E-05	8.51E-06	2.76E-06	4.24E-07	3.07E-08	1.04E-09
2.52E+02	2.81E+02	4.80E+02	1.91E+01	9.30E-06	6.40E-06	2.08E-06	3.18E-07	2.31E-08	7.61E-10
2.94E+02	2.88E+02	4.80E+02	2.21E+01	6.99E-06	4.80E-06	1.56E-06	2.39E-07	1.73E-08	5.79E-10
3.42E+02	2.96E+02	4.80E+02	2.56E+01	5.24E-06	3.60E-06	1.17E-06	1.79E-07	1.30E-08	4.31E-10

TABLE 7-14 (CONTINUED)

downwind distance x (m)	time of max conc (s)	cloud duration (s)	effective half width bbc (m)	average concentration (volume fraction) at (x,y,z) y/bbc= 0.0	y/bbc= 0.5	y/bbc= 1.0	y/bbc= 1.5	y/bbc= 2.0	y/bbc= 2.5
3.99E+02	3.05E+02	4.80E+02	2.96E+01	3.93E-06	2.70E-06	8.78E-07	1.35E-07	9.76E-09	3.12E-10
4.65E+02	3.15E+02	4.80E+02	3.43E+01	2.95E-06	2.03E-06	6.59E-07	1.01E-07	7.31E-09	2.71E-10
5.42E+02	3.28E+02	4.80E+02	3.96E+01	2.22E-06	1.52E-06	4.94E-07	7.58E-08	5.50E-09	1.88E-10
6.31E+02	3.43E+02	4.80E+02	4.58E+01	1.66E-06	1.14E-06	3.71E-07	5.70E-08	4.12E-09	1.22E-10
7.36E+02	3.60E+02	4.80E+02	5.29E+01	1.25E-06	8.61E-07	2.79E-07	4.29E-08	3.12E-09	1.06E-10
8.58E+02	3.80E+02	4.80E+02	6.10E+01	9.43E-07	6.48E-07	2.10E-07	3.23E-08	2.34E-09	9.22E-11
1.00E+03	4.03E+02	4.80E+02	7.02E+01	7.11E-07	4.89E-07	1.59E-07	2.43E-08	1.76E-09	5.34E-11

time-averaged (tav = 5. s) volume concentration: maximum concentration (volume fraction) along centerline.

downwind distance x (m)	height z (m)	maximum concentration c(x,0,z)	time of max conc (s)	cloud duration (s)
1.00E+00	0.00E+00	1.00E+00	2.40E+02	4.80E+02
1.02E+00	0.00E+00	2.53E-01	2.40E+02	4.80E+02
1.04E+00	0.00E+00	2.18E-01	2.40E+02	4.80E+02
1.06E+00	0.00E+00	1.89E-01	2.40E+02	4.80E+02
1.08E+00	0.00E+00	1.66E-01	2.40E+02	4.80E+02
1.12E+00	0.00E+00	1.46E-01	2.40E+02	4.80E+02
1.15E+00	0.00E+00	1.29E-01	2.40E+02	4.80E+02
1.19E+00	0.00E+00	1.14E-01	2.40E+02	4.80E+02
1.24E+00	0.00E+00	1.01E-01	2.40E+02	4.80E+02
1.30E+00	0.00E+00	8.94E-02	2.40E+02	4.80E+02
1.36E+00	0.00E+00	7.93E-02	2.40E+02	4.80E+02
1.44E+00	0.00E+00	7.04E-02	2.40E+02	4.80E+02
1.53E+00	0.00E+00	6.25E-02	2.40E+02	4.80E+02
1.64E+00	0.00E+00	5.54E-02	2.40E+02	4.80E+02
1.76E+00	0.00E+00	4.91E-02	2.40E+02	4.80E+02
1.90E+00	0.00E+00	4.34E-02	2.40E+02	4.80E+02
2.07E+00	0.00E+00	3.83E-02	2.40E+02	4.80E+02
2.26E+00	0.00E+00	3.37E-02	2.40E+02	4.80E+02
2.48E+00	0.00E+00	2.96E-02	2.40E+02	4.80E+02

TABLE 7-14 (CONTINUED)

downwind distance x (m)	height z (m)	maximum concentration c(x,0,z)	time of max conc (s)	cloud duration (s)
2.75E+00	0.00E+00	2.58E-02	2.40E+02	4.80E+02
3.05E+00	0.00E+00	2.24E-02	2.40E+02	4.80E+02
3.41E+00	0.00E+00	1.93E-02	2.40E+02	4.80E+02
3.83E+00	0.00E+00	1.66E-02	2.40E+02	4.80E+02
4.31E+00	0.00E+00	1.41E-02	2.41E+02	4.80E+02
4.88E+00	0.00E+00	1.18E-02	2.41E+02	4.80E+02
5.54E+00	0.00E+00	9.87E-03	2.41E+02	4.80E+02
6.31E+00	0.00E+00	8.15E-03	2.41E+02	4.80E+02
7.21E+00	0.00E+00	6.65E-03	2.41E+02	4.80E+02
8.25E+00	0.00E+00	5.38E-03	2.41E+02	4.80E+02
9.47E+00	0.00E+00	4.31E-03	2.41E+02	4.80E+02
1.09E+01	0.00E+00	3.41E-03	2.42E+02	4.80E+02
1.26E+01	0.00E+00	2.68E-03	2.42E+02	4.80E+02
1.45E+01	0.00E+00	2.09E-03	2.42E+02	4.80E+02
1.67E+01	0.00E+00	1.62E-03	2.43E+02	4.80E+02
1.94E+01	0.00E+00	1.25E-03	2.43E+02	4.80E+02
2.24E+01	0.00E+00	9.53E-04	2.43E+02	4.80E+02
2.60E+01	0.00E+00	7.25E-04	2.44E+02	4.80E+02
3.02E+01	0.00E+00	5.50E-04	2.45E+02	4.80E+02
3.50E+01	0.00E+00	4.15E-04	2.46E+02	4.80E+02
4.07E+01	0.00E+00	3.13E-04	2.46E+02	4.80E+02
4.73E+01	0.00E+00	2.35E-04	2.48E+02	4.80E+02
5.50E+01	0.00E+00	1.76E-04	2.49E+02	4.80E+02
6.40E+01	0.00E+00	1.32E-04	2.50E+02	4.80E+02
7.44E+01	0.00E+00	9.87E-05	2.52E+02	4.80E+02
8.66E+01	0.00E+00	7.38E-05	2.54E+02	4.80E+02
1.01E+02	0.00E+00	5.51E-05	2.56E+02	4.80E+02
1.17E+02	0.00E+00	4.11E-05	2.59E+02	4.80E+02
1.37E+02	0.00E+00	3.07E-05	2.62E+02	4.80E+02
1.59E+02	0.00E+00	2.29E-05	2.66E+02	4.80E+02
1.86E+02	0.00E+00	1.71E-05	2.70E+02	4.80E+02
2.16E+02	0.00E+00	1.27E-05	2.75E+02	4.80E+02
2.52E+02	0.00E+00	9.52E-06	2.81E+02	4.80E+02
2.94E+02	0.00E+00	7.11E-06	2.88E+02	4.80E+02

TABLE 7-14 (CONTINUED)

downwind distance x (m)	height z (m)	maximum concentration c(x,0,z)	time of max conc (s)	cloud duration (s)
3.42E+02	0.00E+00	5.31E-06	2.96E+02	4.80E+02
3.99E+02	0.00E+00	3.97E-06	3.05E+02	4.80E+02
4.65E+02	0.00E+00	2.97E-06	3.15E+02	4.80E+02
5.42E+02	0.00E+00	2.23E-06	3.28E+02	4.80E+02
6.31E+02	0.00E+00	1.67E-06	3.43E+02	4.80E+02
7.36E+02	0.00E+00	1.26E-06	3.60E+02	4.80E+02
8.58E+02	0.00E+00	9.46E-07	3.80E+02	4.80E+02
1.00E+03	0.00E+00	7.13E-07	4.03E+02	4.80E+02

believed to be significant. A simpler alternative for those willing to accept a cruder approximation, is to approximate the enclosed area by assuming it to be roughly equivalent to the area of an ellipse having the same maximum length and width.

The output from a SLAB simulation includes:

- The input to the model;
- Instantaneous spatially averaged cloud parameters (two tables);
- Time-averaged concentration parameters;
- Time-averaged concentrations at specified heights (up to four tables); and
- Time-averaged concentration along centerline.

Of these, the specified concentrations at specified heights and along the centerline are most important. Note that each simulation has one averaging time output. The instantaneous, spatially averaged cloud parameters could be used in determining other averaging times, but it is more efficient to rerun the model if a different averaging time is required.

If maximum concentrations and/or maximum downwind extent are desired regardless of altitude, the centerline concentration table should be used. The centerline may be elevated. If the maximum values are only wanted for a specific altitude, normally surface level, the concentration tables at specified heights should be used. If the plume is always at ground level the column labeled "y/bbc= 0.0" for the "z = .00 plane" table should agree with the column labeled "maximum concentration" for the centerline table.

Specific parameters of interest are discussed below. In this discussion, it is assumed that all parameters to be found are for a specified height. For numerical examples, the "z = .00 plane" table in Table 7-14 is being used. For maximum distances and concentrations, the columns labeled

"downwind distance" and "y/bbc = 0.0" are used. The distances are given in meters, and the concentrations are given as volume fraction. To convert the concentrations to ppm, multiply the fractions by $1x10^6$.

Maximum off-site concentration.

Maximum time-averaged off-site concentrations.

Maximum time-averaged concentration at a specific point.

Maximum distance downwind of specified concentration.

Finding the concentration at a specific distance downwind (or the distance downwind of a specific concentration) requires interpolation. For example, to find the downwind distance of 30,000 ppm, locate two concentrations in the "y/bbc = 0.0" column which are on either side of 30,000 ppm or the fraction 3.00E-02. These two concentrations are 3.37E-02 and 2.96E-02. They correspond to distances 2.26E+00 and 2.48E+00 meters, respectively. By performing a linear interpolation between the two concentrations and distances, a downwind distance of 2.46 meters for 30,000 ppm is calculated. A concentration at a specific distance can be found by finding the closest entry in the "Downwind Distance" column for the distance desired and interpolating the concentration.

Maximum width of specified concentration

To find the maximum width of a concentration, a little more effort is required. The columns labeled "y/bbc" represent the concentrations at the scaled cross-wind distances. Since the off-centerline distances are scaled and are not actual distance values, they must be changed to actual values before interpolation can be done.

Using a concentration of 30,000 ppm again for an example, find the actual cross-wind distances of the concentration through interpolation for a number of downwind distances. Then select the maximum calculated half-width and double it for the total width. For the downwind distance of 1.76 meters, the half-width of the 3.00E-02 concentration lies between "y/bbc = 0.5" and

"y/bbc = 1.0". The value of bbc at that distance is 2.38E-01. Interpolating the value of y/bbc gives a value of 0.581. The actual distance is then 0.138 meters. Repeating these calculations for a number of other distances leads to the following list:

x(m)	half-width(m)
1.24E+00	1.22E-01
1.30E+00	1.28E-01
1.36E+00	1.35E-01
1.44E+00	1.40E-01
1.53E+00	1.43E-01
1.64E+00	1.43E-01
1.76E+00	1.38E-01

The largest half-width is 0.143 meters so the largest width is 0.29 meters.

Time at which the maximum concentration is reached at a specific point.
Duration above specified concentration at a point.
Time the specified concentration is reached at a point.

The time that a maximum concentration is reached and the duration of a concentration is listed in both types of tables as a function of the downwind distance. Therefore, these values can be interpolated the same way that concentration is interpolated. Duration of some concentration, other than the maximum, at a specific point cannot be determined directly from the concentration output.

Total area impacted by specified concentration.

As stated above, to calculate the area impacted by a specified concentration, a third-party software package is required. The concentration tables would be used as input or, if a cruder estimate is acceptable, approximating the shape of the contour by assuming it to be an ellipse. In the latter case, the area enclosed by the contour would be estimated by the following equation:

$$\text{AREA} = \left(\frac{\pi}{4}\right) \times (X_{max}) \times (Y_{max}).$$

where:

X_{max} is the centerline maximum downwind distance and Y_{max} is the maximum contour width.

SECTION 8

DETERMINING INPUT FOR MODELING "WORST CASE" IMPACTS

Accidental releases can occur at any time. For this reason the "worst-case" impact from a release is sometimes needed. Examples of impacts of concern are given in Section 7.0. To determine a worst-case impact, one should consider input that provides maximum or most-effective release rate and worst meteorological dispersion conditions. Maximum release rate from a tank occurs when the tank is assumed the most full and the hole size is the biggest possible (i.e., a full cylinder breaks in half). For most releases the most-effective release rate is equal to the maximum release rate. For reasons discussed below this may not be the case for jets. Worst meteorological conditions for non-jet ground level releases are those associated with very stable atmospheric conditions and low wind speeds, conditions normally give poor dispersion. For other releases multiple stability classes and wind speeds need to be modeled to determine the worst meteorological conditions.

This section discusses the effects which specific input can have on the type of models considered in this study. This section also discusses the mechanics of running a model multiple times and how this document can be used in an off-site consequence analysis.

8.1 MODEL INPUT

Unfortunately, it is not simple to specify all input conditions for determining the worst-case since, in source-term models, the same input plays multiple roles. For example, high wind speeds can lead to high evaporative rates from surface liquid pools, but are also associated with decreased atmospheric stability (and enhanced dispersion). On the other hand, the relationship between ambient temperature and worst-case predicted impact is

more straightforward--higher ambient temperatures tend to result in higher emission rates and more tendency for the release to behave as a denser-than-air release. A denser-than-air release can lead to higher ground level releases.

Models handle several transport zones: jet zone, gravitational slumping zone, transition from gravitational spread to atmospheric dispersion zone, and finally the atmospheric dispersion zone. Figure 8-1 illustrates these zones. Worst-case input varies by each zone and thus downwind distance. For example, high wind speed will probably have little effect in the jet zone, but a major impact in the atmospheric dispersion zone. Stability class will have little effect in the jet and gravitational slump zones. As the release dispersion becomes dominated by atmospheric mixing the stability class becomes more important.

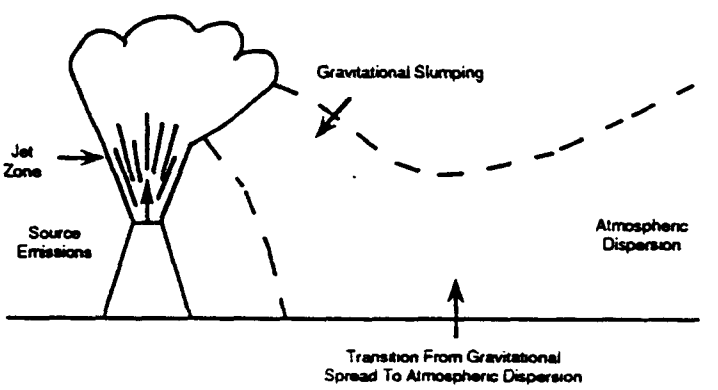

Figure 8-1. Dispersion Zone Schematic

The worst-case input is a function of the impact of concern. The input conditions which lead to the largest distance downwind of a given concentration may not be the same as those which lead to a maximum area impact. Moreover, when determining a maximum downwind distance, the worst-case input for the zone of low concentration may be different from the worst-case input for a high concentration.

There is a need for extensive sensitivity analysis studies to determine what input parameters are most important for a particular model. The user should assess each model input according to the results of such sensitivity analyses. In determining worst-case conditions, normally one or a few of the input are varied so as to bracket the maximum impact. Listed here are some of the input and internal assumptions that may have an effect on determining impacts.

8.1.1 Exit Velocity, Emission Rate, and Jets

If a non-source-term model is being used, varying the exit velocity should be done only when considering whether some other parameter should also be changed for self consistency. Increasing an exit velocity means that either the release diameter must be decreased or the total volume (emission rate) flowing through the hole must be increased. The emission rate is related to the exit velocity as shown in Section 4.12.

Jets are defined in terms of the comparison of the exit velocity with the ambient wind speed. At low ambient wind speeds a jet will have significant mixing. As the ambient wind speed approaches the exit velocity, the transport of high concentrations is enhanced due to decreased mixing from velocity differences. Thus, the assumption that worst-case conditions occur at low wind speeds does not necessarily hold true for jet releases. In fact, for high velocity releases, higher wind speeds may lead to higher impacts.

When a liquid or gas release results in a gas and/or aerosol jet, some new concerns are encountered. Assuming the emission rate and exit velocity are varied to insure mass conservation, increasing the emission rate of a jet can lead to a decrease in concentration impacts. This effect depends on the concentration level of concern. An increase in emission rate leads to an increase in exit velocity. This in turn leads to greater turbulence and greater mixing in the near-field, causing the higher concentrations to be dissipated faster. The lower concentrations that exist beyond the jet regime of the release may reach further downwind.

Jets are only slightly dependent on the stability class. Only after the jet portion of a release is complete does the plume become dependent on the stability class. This means that little, if any differences in near-field impacts of jet releases are due to varying the stability class.

8.1.2 Release Temperature

The colder the release temperature of the vapor, the more likely that the release will behave as a dense gas. Higher release temperatures for the vapor lead to a lower density which will decrease the tendency to behave as a dense gas. If there is uncertainty in the release temperature, the coldest temperature should be used. In most of the examples in this document the release temperature is calculated. In cases where the temperature is not known or calculated, use the lower temperature of boiling point or ambient temperature.

8.1.3 Release Diameter

In most source-term models, a hole size or release diameter is requested. As this parameter changes it can affect both the emission rate and the exit velocity.

8.1.4 Release Height

For dense gases, an elevated release may fall quickly to the ground. The greater the density difference between the release and the ambient temperature, the more likely that the release will fall toward the ground.

8.1.5 Ground Temperature

For liquid releases, the higher the temperature of the surface on which the liquid falls, the greater the rate of evaporation. Higher ground temperatures should be used for maximum emission rates.

For gas releases, the ground temperature is not as significant in its effect as for liquid releases. In gas releases, the ground temperature affects both the released material and air in the atmosphere similarly. Because of this, differences between the release gas and air aren't enhanced or decreased significantly.

8.1.6 Meteorology

Ambient Temperature

If a source-term model is being used, the ambient temperature can have a large effect if the species is released as a liquid and the temperature is varied above or below the boiling point of the liquid released. In that case the temperature will affect the emission rate and the initial concentration of a release.

Ambient temperature can also affect the dispersion of a release. If the ambient temperature is higher than the release temperature, the released plume will tend to be denser than the ambient air (although this is also dependent on molecular weight) and the plume may descend. Conversely, if the release temperature is higher than the ambient temperature, the plume may tend to ascend. Moving the vertical location of a plume can have large effects on impacts, especially in the near-field where gradients are the largest.

Wind Speed

If a source-term model is being used, an increase in the wind speed can increase the rate of evaporation of a liquid release. However, the increased wind speed also increases the rate of dispersion of the release in the atmosphere.

Stability Class

Stability class for complex models should be treated in much the same way as for Gaussian models. However, since many of the releases are from elevated sources, the most stable conditions will not always lead to the largest ground-level impacts. As in the Gaussian model used to simulate an elevated release, an unstable atmosphere can mix the effluent to the ground at higher concentrations than does a stable atmosphere.

Unlike Gaussian model simulations, there may be releases in complex model simulations that are almost independent of the stability class--at least in the near field. Jets and strongly buoyant (positively and negatively) releases are driven by momentum turbulence rather than atmospheric turbulence.

Once a release is no longer a jet and is not denser-than-air, it is not different from other plumes that can be simulated by a Gaussian model. If a release is not a jet and is at ground level, it will likely be influenced by the same worst-case meteorological conditions as a Gaussian model.

8.2 SIMULATION MECHANICS

The ADAM and ALOHA models are interactive. If multiple simulations are needed, they must be run one at a time with a user controlling the input as the simulation is done. DEGADIS, HGSYSTEM, and SLAB are non-interactive models. Computer files can be set up that will allow these models to run multiple simulations automatically.

For the purpose of this discussion, it is assumed that worst-case meteorological conditions are being sought. It is possible that, if a model is being used for planning purposes, non-meteorological parameters could be varied. For example, relief valve hole size and storage pressure can be varied for the purpose of finding the configuration that will minimize impacts.

The DEGADIS model simulates one set of conditions (meteorological and non-meteorological) per run. If multiple cases are to be run, separate input files must be created for each simulation. Each output must then be manually scanned for the desired impact of concern.

The SLAB model can simulate multiple sets of meteorological parameters in a single run. The results of all the meteorological simulations are given in a single output for one set of non-meteorological parameters. If non-meteorological parameters are to be varied, separate input files must be created for each simulation.

The HGSYSTEM models provide a user-efficient method of running multiple meteorological and non-meteorological conditions. This attribute is illustrated in the following example using Scenario 3. In this example only meteorological parameters are being varied. However, other parameters could be varied as well.

To identify worst-case meteorological conditions for this scenario, the HEGADASS model was executed for 14 different combinations of wind speed and atmospheric stability class. A file containing each meteorological condition was prepared. Table 8-1 presents an example of such a file. Then a standard HEGADASS input file was prepared, and the meteorological conditions were commented out by placing a * in column 1 (Table 8-2). The file containing the meteorological data was then concatenated into the HEGADASS input file using a DOS batch file. The resulting input file for stability A and 1.0 m/s wind speed is shown in Table 8-3. By incorporating the CALL command into the DOS batch file, multiple model runs can be executed in sequence. Table 8-4 presents the batch file used to perform these screening runs. The batch file can also be expanded to extract model results for direct importation into a graphical software package.

Table 8-5 summarizes the results of this analysis. This table presents, for each meteorological condition, the concentration at a specific distance (100 meters) and the distance to the LOC. These data were extracted from the

TABLE 8-1. EXAMPLE OF A METEOROLOGICAL DATA FILE TO IDENTIFY WOR[illegible]SE IMPACTS

```
AMBIENT                    * --------> DATA BLOCK: AMBIENT CONDITIONS

   UO      = 1.0           * M/S       wind speed at height z = [illegible]
                           *
DISP                       * --------> DATA BLOCK: DISPERSION DATA
                           *
   PQSTAB  = a             *           Pasquill stability class
```

TABLE 8-2. HEGADASS INPUT FILE TO IDENTIFY WORST CASE METEOROLOGICAL CONDITIONS

```
* ============ HEGADAS-S standard input file STPOOLNO.HSI==============*
        (case: run started at pool, normal thermodynamics)

TITLE   EPA SCENARIO 3 HEGADASS RUN CHLORINE RELEASE

CONTROL                    *  --------> DATA BLOCK: CONTROL PARAMETERS
                           *
    ICNT   =      0        *          output code (isocontours,cloud contents)
    ISURF  =      3        *            code for surface heat/water transfer
                           *
AMBIENT                    *  --------> DATA BLOCK: AMBIENT CONDITIONS

   AIRTEMP =  21.3         * C          air temperature at height z = ZAIRTEMP
   ZAIRTEMP=  10.          * M          height at which AIRTEMP is given
   RHPERC  =  50.          * %          relative humidity
*  U0      =  4.47         * M/S        wind speed at height z = Z0
   Z0      =  10.          * M          height at which U0 is given
   TGROUND =  21.3         * C          earth's surface temperature
                           *
DISP                       *  --------> DATA BLOCK: DISPERSION DATA
                           *
   ZR      =  .01          * M          surface roughness parameter
*  PQSTAB  =  C            *            Pasquill stability class
   AVTIMC  =  900.         * S          averaging time for concentration
   CROSSW  =  2            *          <sigma-y>formula (don't normally change)
                           *
GASDATA                    *  ---------> DATA BLOCK: GAS DATA

   GASFLOW =  .3139        * KG/S     gas emission rate (excl. water pick-up)
   TEMPGAS = -34.          * C          temperature of emitted gas
   CPGAS   =  34.          * J/MOLE/C   specific heat of emitted gas
   MWGAS   =  70.9         * KG/KMOLE   molecular weight of emitted gas
   WATGAS  =  0.           * -        water pick-up by gas (don't norm.change)
                           *
CLOUD                      *  --------> DATA BLOCK: CLOUD OUTPUT CONTROL
                           *
   DXFIX   =  1.           * M          fixed-size output step length
   NFIX    =  1000.        *          fixed steps upto distance x = NFIX*DXFIX
   XEND    =  3000.        * M          x at which calculations are stopped
   CAMIN   =  0.000001     * KG/M3      CA (conc.) at which calcs. are stopped
   CU      =  0.0001       * KG/M3      upper concentration limit
   CL      =  0.00001      * KG/M3      lower concentration limit
                           *
POOL                       *  --------> DATA BLOCK: POOL DATA
                           *
   PLL     =  1.           * M          pool length
   PLHW    =  .5           * M          pool half-width
```

TABLE 8-3. CONCATENATED INPUT FILE FOR SCENARIO 3

```
* ============= HEGADAS-S standard input file STPOOLNO.HSI ==============*
          (case: run started at pool, normal thermodynamics)

TITLE   EPA SCENARIO 3 HEGADASS RUN CHLORINE RELEASE

CONTROL                    *  --------> DATA BLOCK: CONTROL PARAMETERS
                           *
    ICNT   =      0        *          output code (isocontours,cloud contents)
    ISURF  =      3        *            code for surface heat/water transfer
                           *
AMBIENT                    *  --------> DATA BLOCK: AMBIENT CONDITIONS

   AIRTEMP =  21.3         * C          air temperature at height z = ZAIRTEMP
   ZAIRTEMP=  10.          * M          height at which AIRTEMP is given
   RHPERC  =  50.          * %          relative humidity
   U0      =  1.0          * M/S        wind speed at height z = Z0
   Z0      =  10.          * M          height at which U0 is given
   TGROUND =  21.3         * C          earth's surface temperature
                           *
DISP                       *  --------> DATA BLOCK: DISPERSION DATA
                           *
   ZR      =  .01          * M          surface roughness parameter
   PQSTAB  =  a            *            Pasquill stability class
   AVTIMC  =  900.         * S          averaging time for concentration
   CROSSW  =  2            *          <sigma-y>formula (don't normally change)
                           *
GASDATA                    *  ---------> DATA BLOCK: GAS DATA

   GASFLOW =  .3139        * KG/S     gas emission rate (excl. water pick-up)
   TEMPGAS = -34.          * C          temperature of emitted gas
   CPGAS   =  34.          * J/MOLE/C   specific heat of emitted gas
   MWGAS   =  70.9         * KG/KMOLE   molecular weight of emitted gas
   WATGAS  =  0.           * -        water pick-up by gas (don't norm.change)
                           *
CLOUD                      *  --------> DATA BLOCK: CLOUD OUTPUT CONTROL
                           *
   DXFIX   =  1.           * M          fixed-size output step length
   NFIX    =  1000.        *          fixed steps upto distance x = NFIX*DXFIX
   XEND    =  3000.        * M          x at which calculations are stopped
   CAMIN   =  0.000001     * KG/M3      CA (conc.) at which calcs. are stopped
   CU      =  0.0001       * KG/M3      upper concentration limit
   CL      =  0.00001      * KG/M3      lower concentration limit
                           *
POOL                       *  --------> DATA BLOCK: POOL DATA
                           *
   PLL     =  1.           * M          pool length
   PLHW    =  .5           * M          pool half-width
```

TABLE 8-4. DOS BATCH FILE TO IDENTIFY WORST CASE METEOROLOGY FOR CASE 3

```
rem screening run to identify worst case met
rem there are 14 different combinations of ws and stability
rem in files named met1.dat ... met15.dat.  These are then
rem concatenated to the base model input (scen3s.hsi) to form a
rem new input file (scen3s?).  This process is then repeated.
rem
call hegadass scen3s.hsi  met1.dat scen3s1
call hegadass scen3s.hsi  met2.dat scen3s2
call hegadass scen3s.hsi  met3.dat scen3s3
call hegadass scen3s.hsi  met4.dat scen3s4
call hegadass scen3s.hsi  met5.dat scen3s5
call hegadass scen3s.hsi  met6.dat scen3s6
call hegadass scen3s.hsi  met7.dat scen3s7
call hegadass scen3s.hsi  met8.dat scen3s8
call hegadass scen3s.hsi  met9.dat scen3s9
call hegadass scen3s.hsi  met10.dat scen3s10
call hegadass scen3s.hsi  met11.dat scen3s11
call hegadass scen3s.hsi  met12.dat scen3s12
call hegadass scen3s.hsi  met13.dat scen3s13
call hegadass scen3s.hsi  met14.dat scen3s14
rem to extract data from hegadass model run for input to a graphical program
call  get2col scen3s1.hsr sen3s1.dat 1 2
rem format on program get2col is model output file name, data output file name
rem and columns to be extracted (distance and concentration).
```

HEGADAS model runs by using the interactive utility program HSPOST and by reviewing HEGADAS output. The finite release duration option in the HSPOST utility was selected because this option corrects the predicted concentrations for release duration. For this example, while a steady-state model could be used to examine the effects at the fenceline, at the distance to the STEL, release duration becomes quite important under some meteorological conditions.

This approach in identifying worst-case meteorological conditions becomes quite efficient because, once the model is set up for a given problem, alternate cases can be run with very little additional input from the user. This utility for file concatenation within HGSYSTEM can be used with all of the models, and any parameter can be varied in an analogous manner. Thus, a sensitivity analysis can quickly be performed for a specific problem, and the results can be simply translated into a graphical presentation.

As indicated in the data presented in Table 8-5 for selected meteorological conditions, the distance to the LOC for this case can be quite large (8343 meters for stability class F with a 1 meter per second wind speed). Such results should be reviewed from a meteorological perspective to ensure that they are reasonable. For this case, the plume travel time to the LOC would be approximately 2.3 hours. One of the assumptions of HGSYSTEM models (and many other models of this type) is that wind speed, wind direction, and stability class do not change over time. For example, if the plume travel time to a specified LOC is 6 hours, this implies that meteorological conditions do not vary over that time period. The validity of this assumption can be tested by reviewing historical meteorological data and examining what level of persistence is observed for worst-case meteorological conditions.

If the maximum concentration at 100 meters downwind were the output parameter of primary concern, Table 8-5 indicates that the worst-case concentration is associated with meteorological conditions of stability class D with a wind speed of 1 meter per second. These conditions are different than the worst-case conditions for maximum distance to LOC--a clear example of

TABLE 8-5. IDENTIFICATION OF WORST-CASE METEOROLOGY FOR SCENARIO 3

Case Number	Pasquill Stability Class	Wind Speed (m/s)	Concentration at 100 m (ppm)	Downwind Distance to LOC (m)
1	A	1	891	591
2	A	3	58.4	370
3	B	1	2100	792
4	B	3	119.6	487
5	C	1	3660	1224
6	C	3	319	745
7	D	1	5000	3455
8	D	3	825	1983
9	D	5	391	1566
10	D	10	175	1086
11	E	1	4280	7119
12	E	3	1670	6098
13	F	1	3480	8343
14	F	3	2150	8343

the determination of worst-case conditions being influenced by the selection of which output parameter is the most important criterion.

8.3 USING THIS DOCUMENT FOR OFF-SITE CONSEQUENCE ANALYSIS

This document provides guidance on the use of dispersion models, preparing input, and interpreting the output from dispersion models used for determining off-site impacts of potential accidental releases. Thus, the guidance provided in this document is only one part of the full analysis required to determine off-site impacts.

A comprehensive methodology to determine the impact of a release scenario (worst-case, most-likely, etc.) comprises the following steps:

1. Use of Process Hazard Analysis techniques like WHAT-IF, HAZOP, FMEA, and Fault-Tree to identify the release scenario and mode of failure.

2. Use of release rate algorithms to calculate the amount released, evaporation algorithms to calculate the vapor cloud formation and atmospheric dispersion models to calculate the transport of the vapor cloud.

3. Use of Consequence Analysis algorithms to predict the number of people or sensitive natural resources impacted by the potential vapor cloud.

By their nature the steps above provide a methodology that tends to be site-specific. The Process Hazard Analysis techniques are to be used for specific plant operations (e.g. transfer from storage tank to process area) and result in the identification of one or more release scenarios. Additionally, failure rate data for the various components in the scenario can be used to estimate the probability of the event.

The second set of algorithms (release rates, evaporation and dispersion) tend to be more generic (note there may still be some significant site specific parameters like surface roughness, meteorology, etc.). However for most applications (i.e. flat terrain) the standard release rate, evaporation, and dispersion algorithms discussed in this document can be applied.

The third set of algorithms also use site-specific information. To calculate the number of people impacted one has to determine the population distribution around the plant. Some of the additional factors to be considered relate to the number of people who are indoors/outdoors, age distribution of the vulnerable population, seasonal and day/night population variations. Additionally, frequency data related to meteorology (e.g. STAR data providing the distribution of wind speed, wind direction, stability class) can be used to determine the likelihood of a particular impact.

It is important to emphasize that the above outlined scheme is a general framework which can be applied at various levels of complexity. In it's simplest form, a WHAT-IF Process Hazard Analysis followed by dispersion algorithms can be used to define a vulnerability zone (circle with radius equal to the downwind distance to the concentration level of concern). This analysis would provide an approximate number of people impacted. On the other hand, a full-fledged Fault-Tree analysis with failure mode data, followed by a site specific atmospheric dispersion and consequence analysis (using site-specific meteorology and population distribution) can be used to generate risk contours surrounding the plant. The level of detail required to do the analysis should be dictated by the impact potential of the release scenario (which is dependent upon the release size, meteorology, toxicity/flammability characteristics, and population distribution). It is possible to have a large plant-site with minimum impact potential (e.g. due to rural location or due to the nature of chemicals handled) while on the other hand it is possible to have a very small plant operation that could have significant impact (e.g. plant is located in an urban area or small facility that handles highly toxic/flammable chemicals).

SECTION 9

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APPENDIX A

Relationships Between Selected SI Units

This document provides answers to all calcuations in SI units (Le Système International d'Unités). This Appendix is to provide some relationships between the base SI units and derived SI units. The base SI units used in this document are given in Table A-1. The derived units used in this document are given in Table A-2.

Table A-1. Base SI Units

QUANTITY	NAME	SYMBOL
Length	meter	m
Mass	kilogram	kg
Time	second	s
Temperature	kelvin	°K
Amount of substance	kilogram mole	kmol

Table A-2. Derived SI Units

QUANTITY	NAME	SYMBOL
Force	newton	N (= kg m / s^2)
Pressure	pascal	Pa (= N / m^2)
Energy, work	joule	J (= N m)

Two examples of calculations which will be seen in the document and how to derive the final units are given below.

<u>Example Density of Vapor State Calculation</u>

$$\rho_a = \frac{p_a M_a}{RT_a} = \frac{(101325\text{Pa})(28.9\text{kg/kmol})}{(8314\text{J/kmol°K})(296.48\text{°K})}$$

$$= 1.188 \text{ Pa kg/J}$$

$$= 1.188 \text{ (N/m}^2\text{)(kg)/(N m)}$$

$$= 1.188 \text{ kg/m}^3$$

Example Emission Rate Calculation

$$E = A_o F \left(\frac{\lambda M p_s}{R T_s^2} \right) \left(\frac{T_s}{C_{pl}} \right)^{\frac{1}{2}}$$

$$= (3.888 \times 10^{-5} m^2)(0.7347)$$

$$\left(\frac{(2.878 \times 10^5 J/kg)(70.91 kg/kmol)(6.951 \times 10^5 Pa)}{(8314 J/kmol°K)(294.3°K)^2} \right)$$

$$\left(\frac{294.3°K}{927.13 J/kg°K} \right)^{\frac{1}{2}}$$

$$= 0.3170 \ m^2 \ Pa \ (kg/J)^{\frac{1}{2}}$$

$$= 0.3170 \ m^2 \ (N/m^2) \ (kg/N \ m)^{\frac{1}{2}}$$

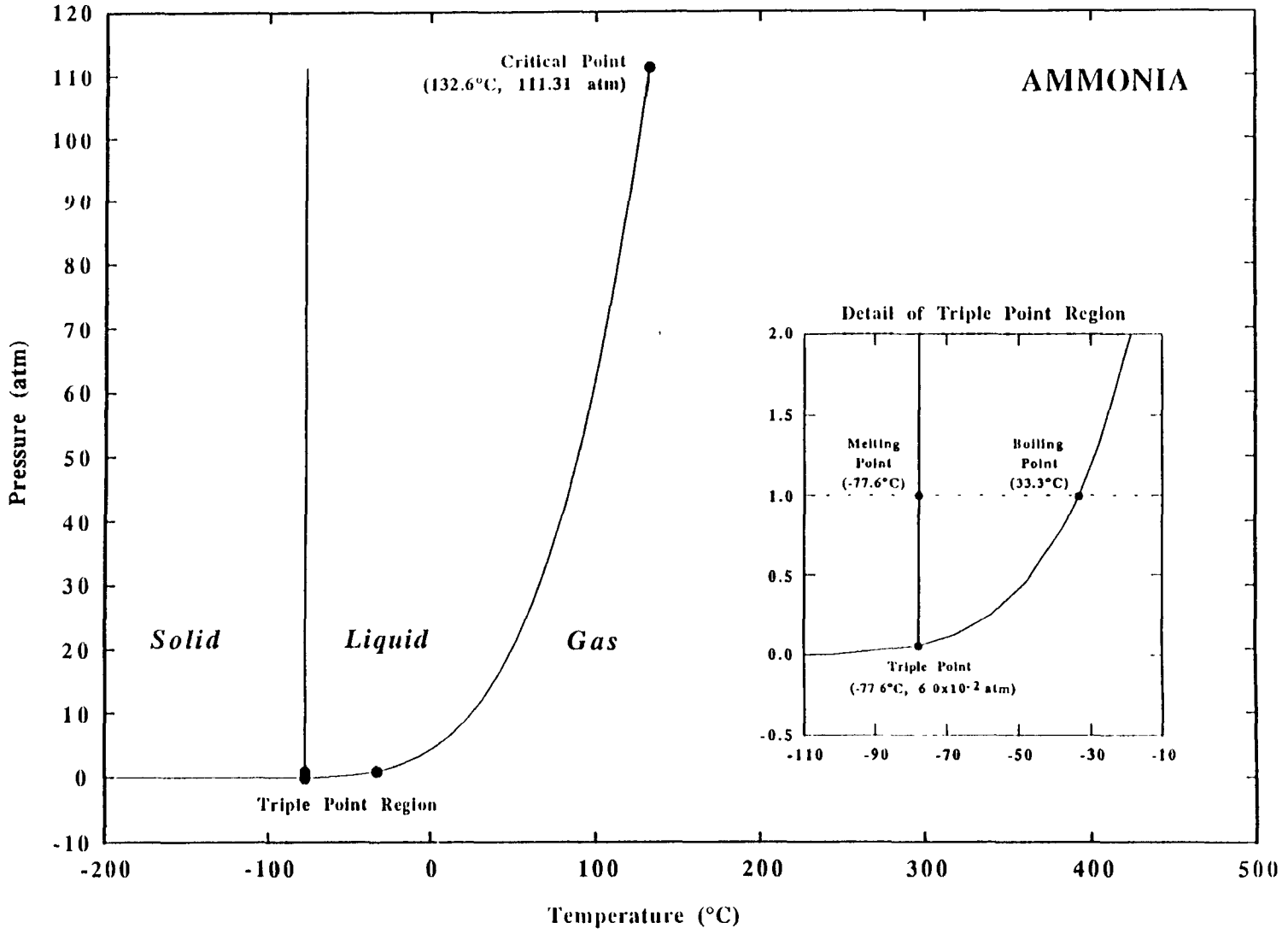
$$= 0.3170 \ (kg \ m/s^2) \ (kg \ s^2/kg \ m^2)^{\frac{1}{2}}$$

$$= 0.3170 \ kg/s$$

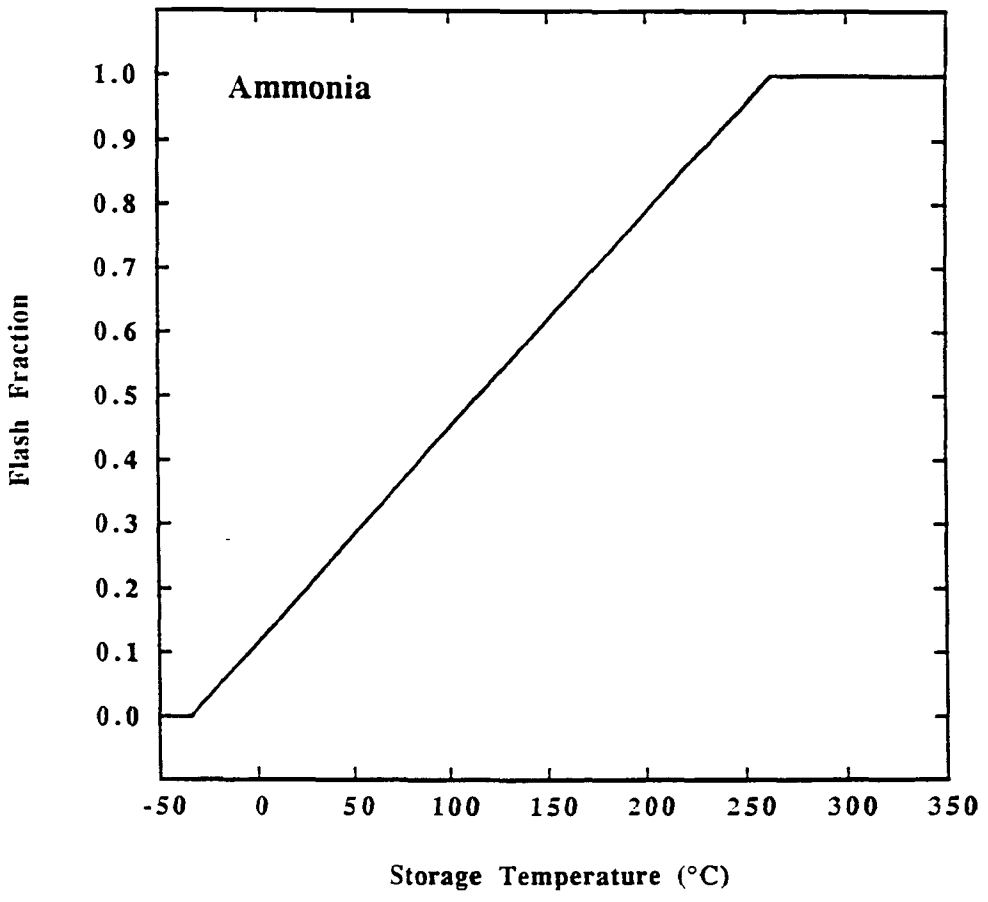
APPENDIX B

Triple Point Diagrams, Flash Diagrams, and Physical Property Data Tables for:

- Ammonia;
- Chlorine;
- Ethylene Oxide;
- Hydrogen Chloride;
- Hydrogen Fluoride; and
- Sulfur Dioxide.



Triple Point Diagram for Ammonia



Flash Diagram for Ammonia

PHYSICAL PROPERTIES OF AMMONIA

CAS Registry Number	7664-41-7		
Chemical Formula	NH_3		
Toxicity Threshold Concentrations		Time (min)	Level (ppm)
	ERPG-1	60	25
	ERPG-2	60	200
	ERPG-3	60	1000
	IDLH	30	500
	STEL	15	35
Molecular Weight	17.030		
Normal Boiling Point	239.72 °K		
Vapor Density	0.708 kg/m^3 @ 293 °K, 1 atm		
Liquid Density	681.38 kg/m^3 @ 239.72 °K		
Liquid Specific Gravity (H_2O = 1)	0.638 @ 273 °K		
Vapor Specific Gravity (air = 1)	0.587		
Vapor Pressure Equation Log P_v = A - B/(T+C) where: P_v = vapor pressure, mmHg T = temperature, °C A = 7.3605, a constant B = 926.132, a constant C = 240.17, a constant	6320.9 mm Hg (8.32 atm) @ 20 °C		
Liquid Viscosity	0.000246 Pa-s @ 239.72 °K		
Liquid Surface Tension	0.0234 N/m @ 284 °K		
Solubility in Water	233.99 kg/m^3 @ 293 °K, 1 atm		
Heat Capacity at Constant Volume (Vapor)	1589.55 J/kg °K @ 273 °K		
Heat Capacity at Constant Pressure (Vapor)	2093.19 J/kg °K @ 273 °K		
Heat Capacity at Constant Pressure (Liquid)	4061.58 J/kg °K @ 240 °K		
Latent Heat of Vaporization	1367208 J/kg @ 240 °K		
Net Heating Value	18603850 J/kg		

Enthalpy Equation

$H = A + B_t + C_t^2$

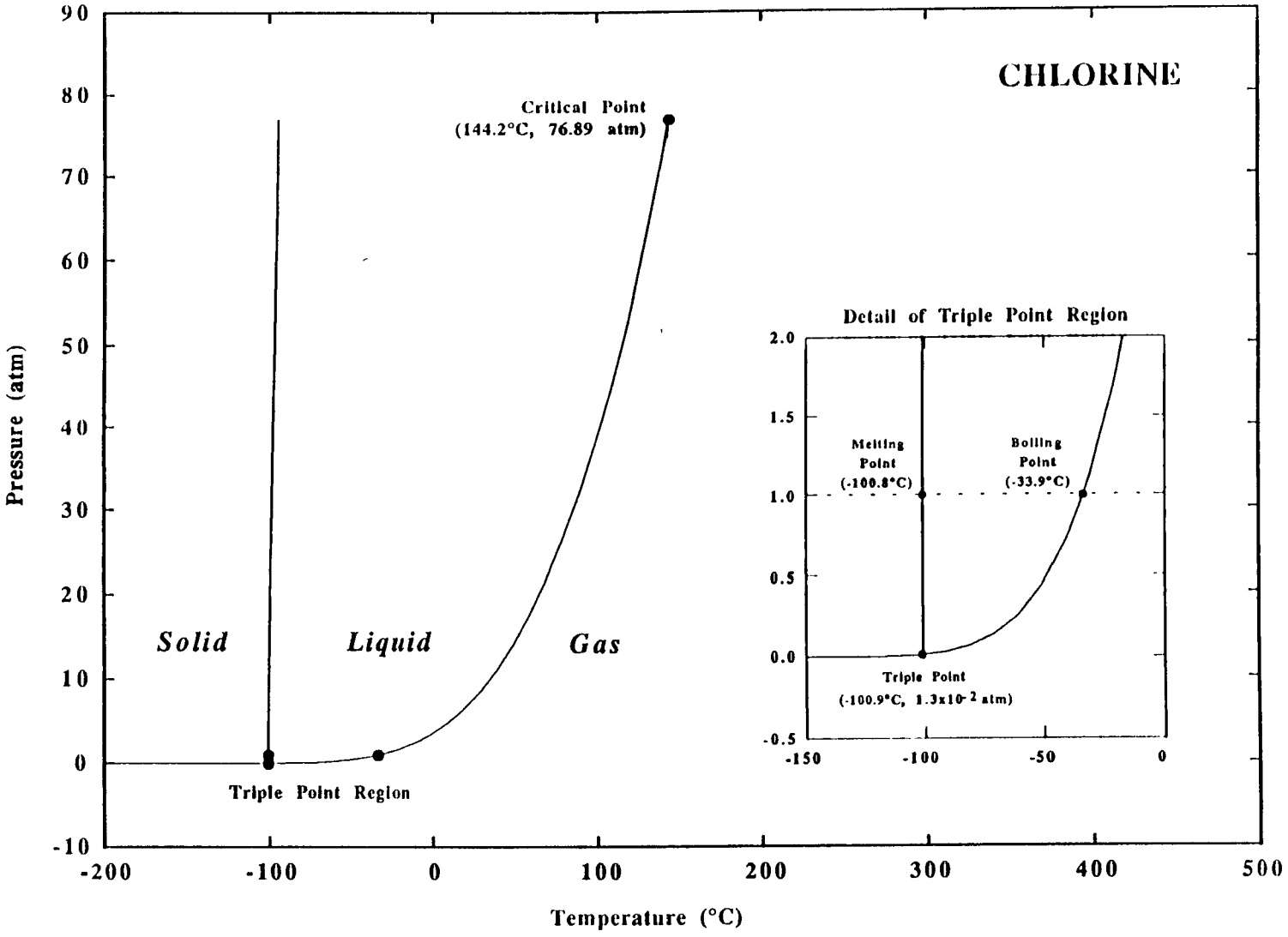
where: H = enthalpy, J/kg
t = temperature (°K); and
A, B, and C are constants for liquid and vapor enthalpies as follows:

	A	B	C
Liquid *		4672.5	-0.625
Vapor *		5138.333	-7.5

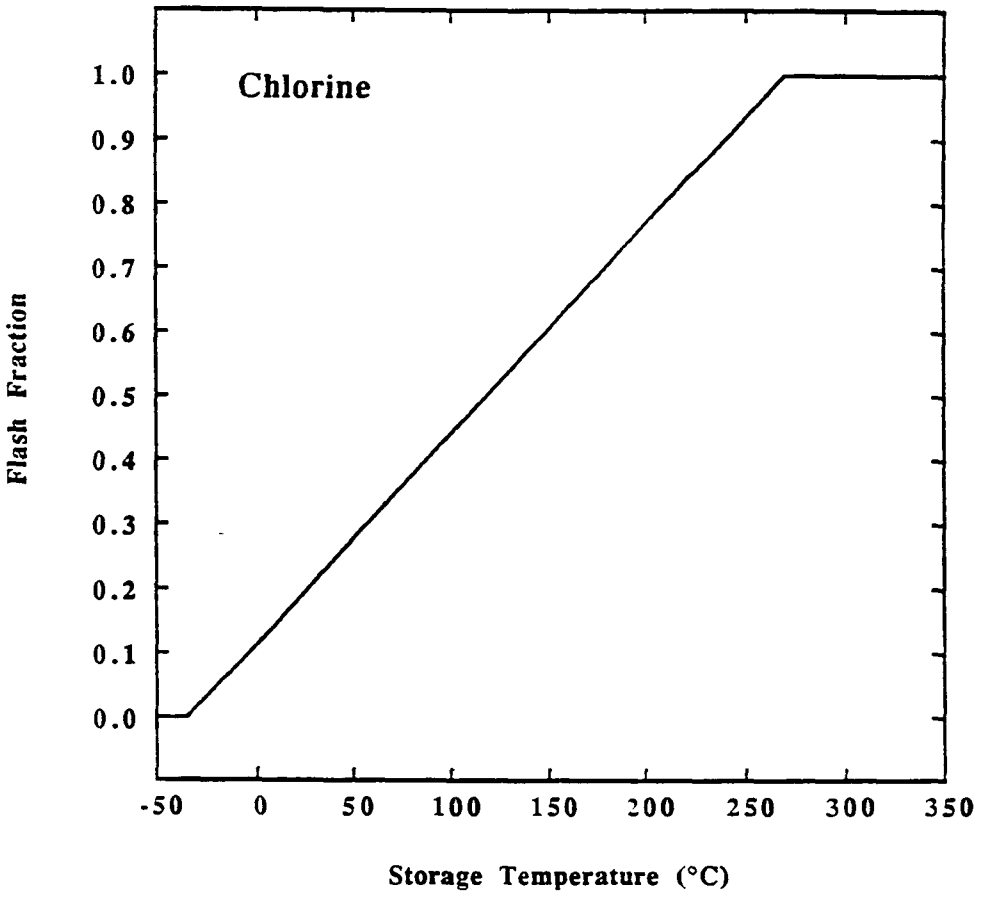
* Value of A depends on the selected reference state for the material. The numerical value of A does not affect release calculations since only enthalpy differences at various temperatures are applied to a single phase. To calculate enthalpy differences between phases, a reference state must be chosen to calculate A for each phase using the enthalpy equation.

Additional properties useful in determining other properties from physical property correlations:

Critical Temperature	405.65 °K
Critical Pressure	11278000 Pa
Critical Density	234.99 kg/m^3
Energy of Molecular Interaction	276 °K
Effective Molecular Diameter	3.45 Angstroms



Triple Point Diagram for Chlorine



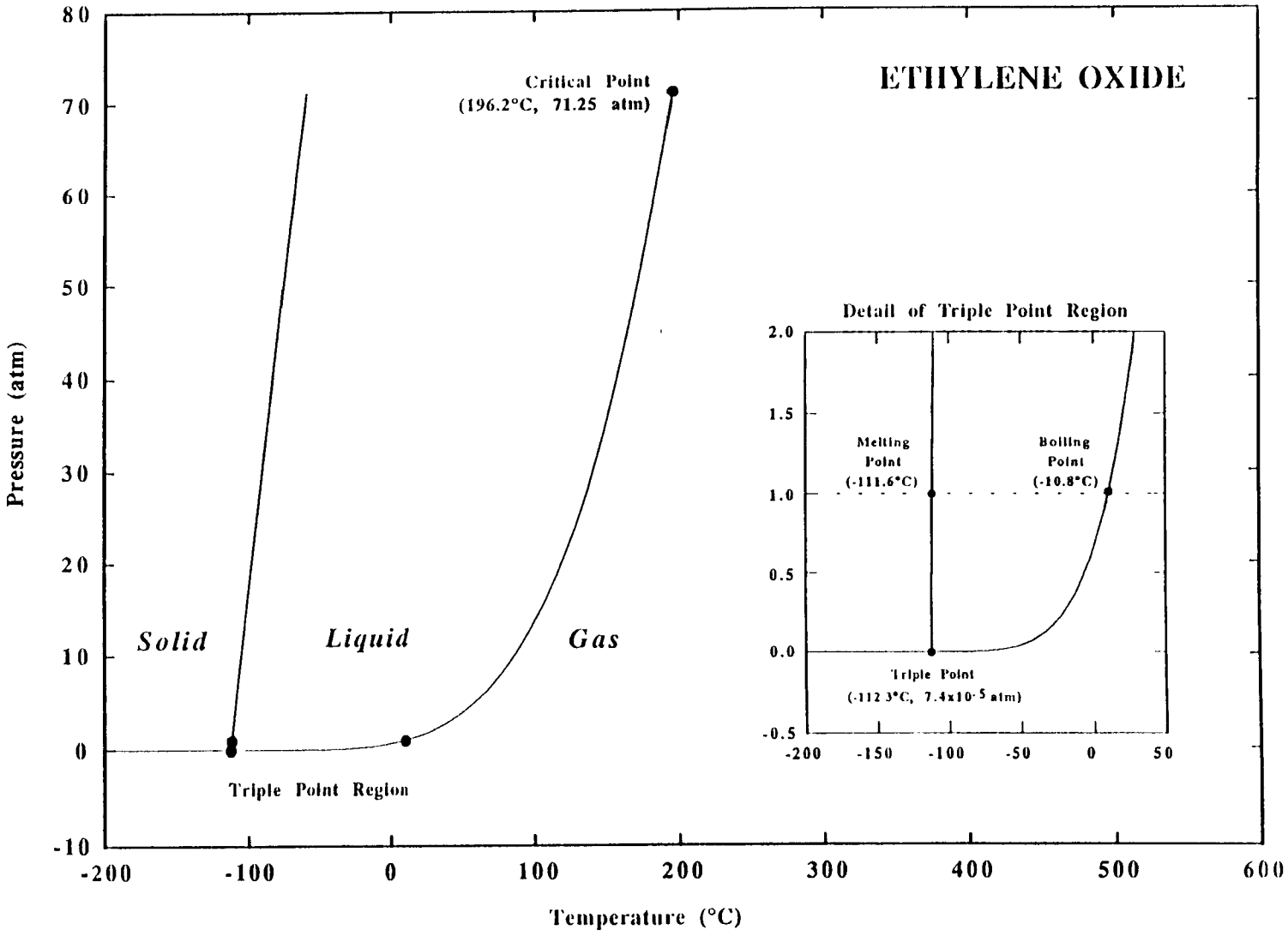
Flash Diagram for Chlorine

PHYSICAL PROPERTIES OF CHLORINE

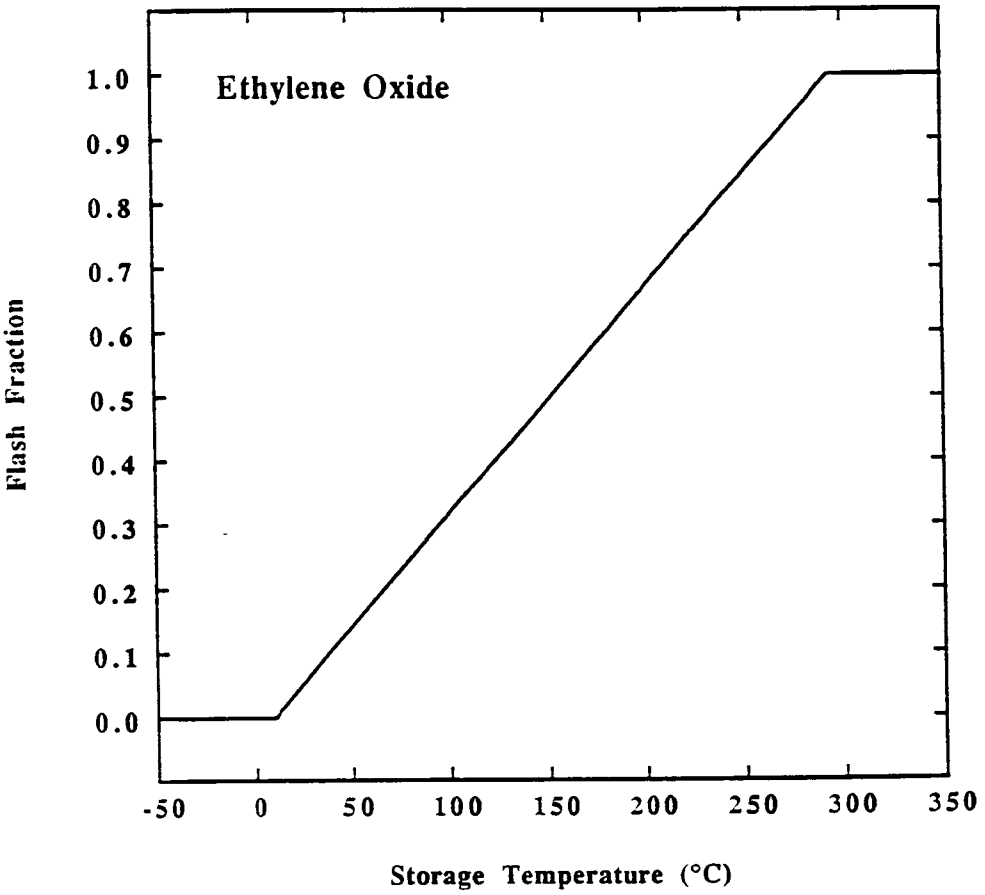
CAS Registry Number	7782-50-5
Chemical Formula	Cl_2
Toxicity Threshold Concentrations	Time (min) / Level (ppm) ERPG-1 60 1 ERPG-2 60 3 ERPG-3 60 20 IDLH 30 30 STEL 15 1
Molecular Weight	70.914
Normal Boiling Point	239.12 °K
Vapor Density	2.949 kg/m^3 @ 293 °K, 1 atm
Liquid Density	1562.19 kg/m^3 @ 239 °K
Liquid Specific Gravity (H_2O = 1)	1.47 @ 273 °K
Vapor Specific Gravity (air = 1)	2.45
Vapor Pressure Equation Log P_v = A - B/(T+C) where: P_v = vapor pressure, mmHg T = temperature, °C A = 6.9379, a constant B = 861.34, a constant C = 246.33, a constant	5055.8 mm Hg (6.65 atm) @ 20 °C
Liquid Viscosity	0.000489 Pa-s @ 239.09 °K
Liquid Surface Tension	0.0254 N/m @ 243 °K
Enthalpy Equation $H = A + B_t + C_t^2$ where: H = enthalpy, J/kg; t = temperature (°K); and A, B, and C are constants for liquid and vapor enthalpies as follows: A / B / C Liquid * / 821.3762 / 0.303672 Vapor * / 616.4956 / -0.43698	* Value of A depends on the selected reference state for the material. The numerical value of A does not affect release calculations since only enthalpy differences at various temperatures are applied to a single phase. To calculate enthalpy differences between phases, a reference state must be chosen to calculate A for each phase using the enthalpy equation.
Solubility in Water	3.744 kg/m^3 @ 293 °K, 1 atm
Heat Capacity at Constant Volume (Vapor)	355.81 J/kg°K @ 288 °K
Heat Capacity at Constant Pressure (Vapor)	481.49 J/kg°K @ 288 °K
Heat Capacity at Constant Pressure (Liquid)	927.13 J/kg°K @ 293.12 °K

PHYSICAL PROPERTIES OF CHLORINE (Continue

Latent Heat of Vaporization	287775 J/kg @ 239 °K
Net Heating Value	0 cal/gmole
Additional properties useful in determining other properties from physical property correlations:	
Critical Temperature	417.15 °K
Critical Pressure	7710800 Pa
Critical Density	572.98 kg/m^3
Energy of Molecular Interaction	275 °K
Effective Molecular Diameter	4.12 Angstroms



Triple Point Diagram for Ethylene Oxide



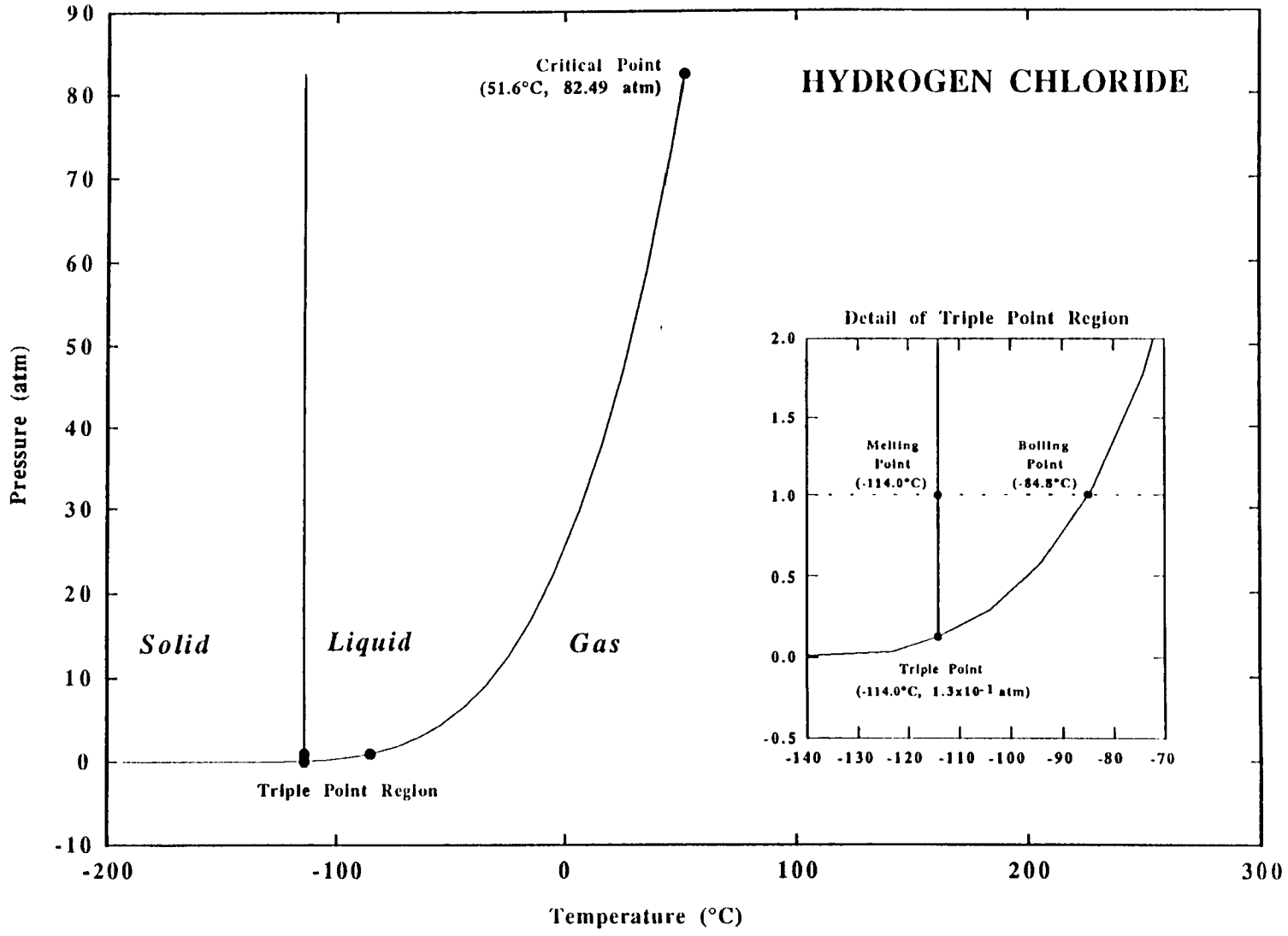
Flash Diagram for Ethylene Oxide

PHYSICAL PROPERTIES OF ETHYLENE OXIDE

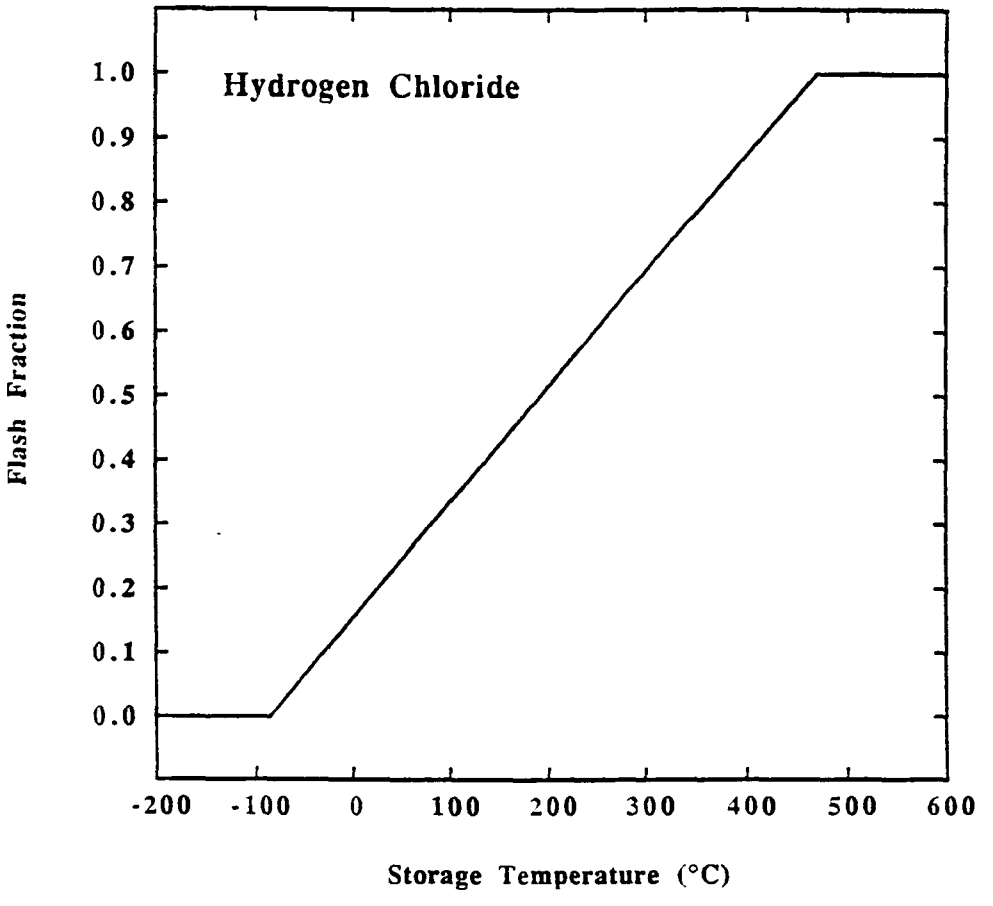
CAS Registry Number	75-21-8
Chemical Formula	C_2H_4O
Toxicity Threshold Concentrations	Time (min) / Level (ppm) ERPG-1 -- -- ERPG-2 -- -- ERPG-3 -- -- IDLH 30 800 STEL -- -- LEL = 3% UEL = 100%
Molecular Weight	44.053
Normal Boiling Point	283.85°K
Vapor Density	1.832 kg/m^3 @ 293°K, 1 atm
Liquid Density	882.67 kg/m^3 @ 283.85°K
Liquid Specific Gravity (H_2O = 1)	0.898 @ 273°K
Vapor Specific Gravity (air = 1)	1.52
Vapor Pressure Equation $\ln P_v = A + B/T + C\ln T + DT^E$ where: P_v = vapor pressure, Pa T = temperature, °K A = 96.820, a constant B = -5433.0, a constant C = -12.517, a constant D = 0.01608, a constant E = 1.00, a constant	145810 Pa (1.44 atm) @ 293°K (valid for T = 160.71°K to 469.15°K)
Liquid Viscosity	0.000269 Pa-s @ 293.15°K
Liquid Surface Tension	0.0244 N/m
Solubility in Water	0.1841 kg/m^3
Heat Capacity at Constant Volume (Vapor)	888.96 J/kg °K @ 293°K
Heat Capacity at Constant Pressure (Vapor)	1077.96 J/kg °K @ 293°K
Heat Capacity at Constant Pressure (Liquid)	1971.56 J/kg °K @ 283.85°K
Latent Heat of Vaporization	569000 J/kg @ 283.85°K
Net Heating Value	27648022 J/kg

PHYSICAL PROPERTIES OF ETHYLENE OXIDE (Continued)

Enthalpy Equation $H = A + B_t + C_t^2$ where: H = enthalpy, J/kg t = temperature (°K); and A, B, and C are constants for liquid and vapor enthalpies as follows: A B C Liquid* -25.25 4.73445 Vapor* -225.576 3.716791	* Value of A depends on the selected reference state for the material. The numerical value of A does not affect release calculations since only enthalpy differences at various temperatures are applied to a single phase. To calculate enthalpy differences between phases, a reference state must be chosen to calculate A for each phase using the enthalpy equation.
Additional properties useful in determining other properties from physical property correlations:	
Critical Temperature	469.15 °K
Critical Pressure	7194100 Pa
Critical Density	313.99 kg/m^3
Energy of Molecular Interaction	326 °K
Effective Molecular Diameter	4.35 Angstroms



Triple Point Diagram for Hydrogen Chloride



Flash Diagram for Hydrogen Chloride

PHYSICAL PROPERTIES OF HYDROGEN CHLORIDE

CAS Registry Number	7647-01-0
Chemical Formula	HCl
Toxicity Threshold Concentrations	Time (min) / Level (ppm) ERPG-1: 60 / 3 ERPG-2: 60 / 20 ERPG-3: 60 / 100 IDLH: 30 / 100 STEL: -- / --
Molecular Weight	36.461
Normal Boiling Point	188.15 °K
Vapor Density	1.516 kg/m^3 @ 293 °K, 1 atm
Liquid Density	1194.20 kg/m^3 @ 188.15 °K
Liquid Specific Gravity (H_2O = 1)	0.916 @ 273 °K
Vapor Specific Gravity (air = 1)	1.26
Vapor Pressure Equation $L_nP_v = A + B/T + (CL_nT + DT^E)$ where: Pv = vapor pressure, Pa T = temperature, °K A = 105.16, a constant B = -3748.4, a constant C = -15.214, a constant D = 0.031737, a constant E = 1.00, a constant	4187527 Pa (41.33 atm) @ 293 °K (valid for T = 158.97 °K to 324.65 °K)
Liquid Viscosity	0.000084 Pa-s @ 293.15 °K
Liquid Surface Tension	0.0041 N/m @ 293 °K
Solubility in Water	6.70 kg/m^3
Heat Capacity at Constant Volume (Vapor)	571.46 J/kg °K @ 273 °K
Heat Capacity at Constant Pressure (Vapor)	799.81 J/kg °K @ 273 °K
Heat Capacity at Constant Pressure (Liquid)	1655.85 J/kg °K @ 163 °K
Latent Heat of Vaporization	442708 J/kg @ 188 °K
Net Heating Value	784436 J/kg

PHYSICAL PROPERTIES OF HYDROGEN CHLORIDE (Continued)

Enthalpy Equation $H = A + B_t + C_t^2$ where: H = enthalpy, J/kg; t = temperature (°K); and A, B, and C are constants for liquid and vapor enthalpies as follows: A / B / C Liquid* / 1297.277 / 2.468391 Vapor* / 798.9364 / 6.1×10^{-8}	* Value of A depends on the selected reference state for the material. The numerical value of A does not affect release calculations since only enthalpy differences at various temperatures are applied to a single phase. To calculate enthalpy differences between phases, a reference state must be chosen to calculate A for each phase using the enthalpy equation.
Additional properties useful in determining other properties from physical property correlations:	
Critical Temperature	324.65 °K
Critical Pressure	8308700 Pa
Critical Density	450.02 kg/m^3
Energy of Molecular Interaction	216 °K
Effective Molecular Diameter	6.4 Angstroms

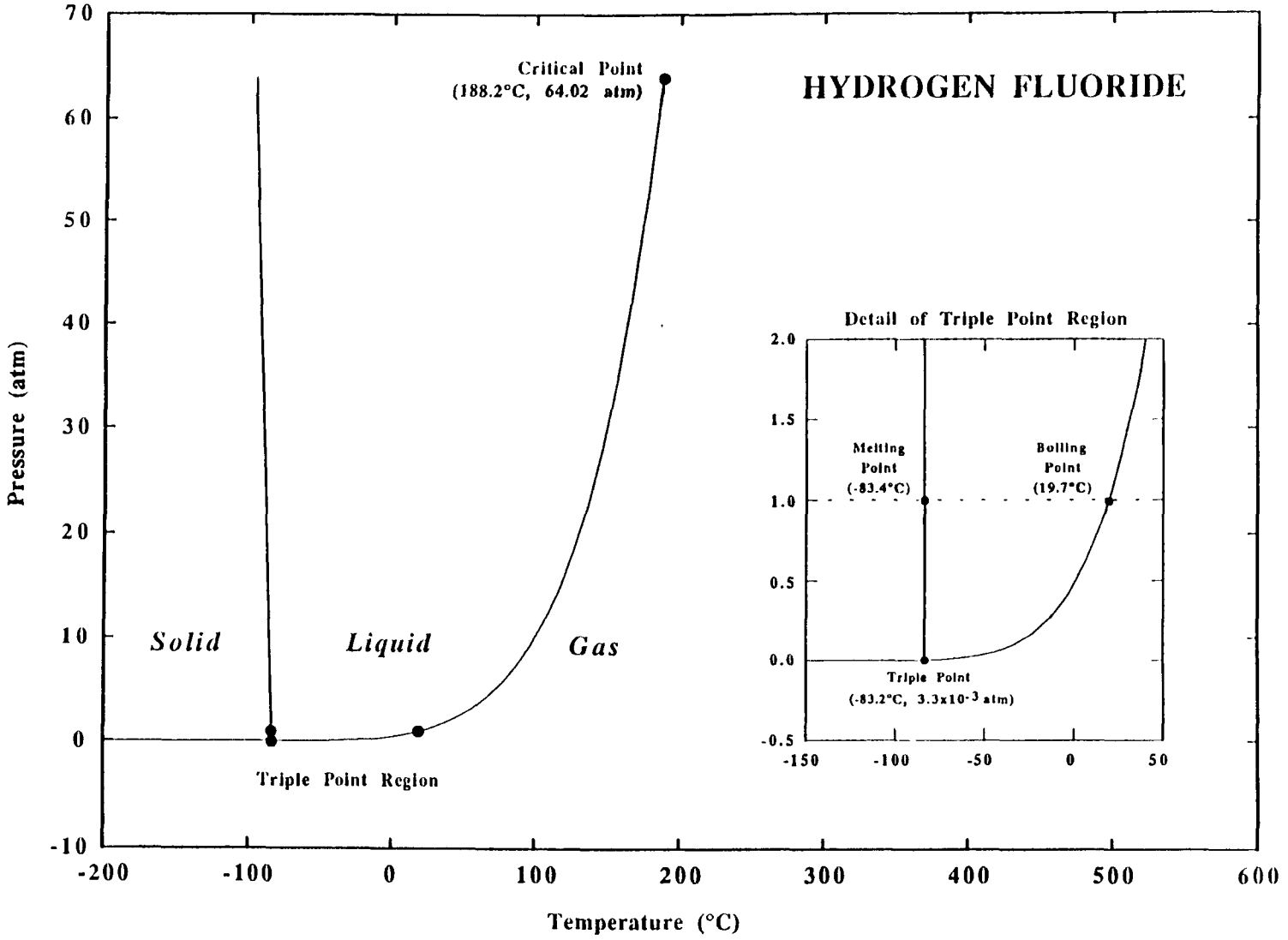
PHYSICAL PROPERTIES OF 30 WT% HYDROCHLORIC ACID

CAS Registry Number	7647-01-0
Chemical Formula	HCl
Toxicity Threshold Concentrations	Time (min) / Level (ppm) ERPG-1: 60 / 3 ERPG-2: 60 / 20 ERPG-3: 60 / 100 IDLH: 30 / 100 STEL: -- / -
Molecular Weight	21.24
Normal Boiling Point	370.2 °K
Vapor Density	1.516 kg/m^3 @ 298 °K, 1 atm
Liquid Density	993.3 kg/m^3 @ 370.2 °K
Liquid Specific Gravity (H_2O = 1)	0.985 @ 273 °K
Vapor Specific Gravity (air = 1)	1.26
Vapor Pressure Equation (HCl over 30% Hydrochloric Acid) Log P_v = A - B/T where: P_v = vapor pressure, mmHg T = temperature, °K A = 9.8763, a constant B = 2593, a constant	Vapor Pressures from the equation represent the partial pressures of anhydrous HCl over a 30% hydrochloric acid solution.
Vapor Pressure Equation (Water over 30% Hydrochloric Acid) Log P_v = A - B/T where: P_v = vapor pressure, mmHg T = temperature, °K A = 9.00117, a constant B = 2422, a constant	Vapor pressures from the equation represent the partial pressures of water over a 30% hydrochloric acid solution.
Liquid Viscosity	0.00048 Pa-s
Liquid Surface Tension	0.0808 N/m @ 370.2 °K
Solubility in Water	
Heat Capacity at Constant Volume (Vapor)	980.98 J/kg °K @ 273 °K
Heat Capacity at Constant Pressure (Vapor)	1372.97 J/kg °K @ 273 °K
Heat Capacity at Constant Pressure (Liquid)	3475.26 J/kg °K @ 273 °K
Latent Heat of Vaporization	2354863 J/kg @ 370.2 °K
Net Heating Value	1346578 J/kg

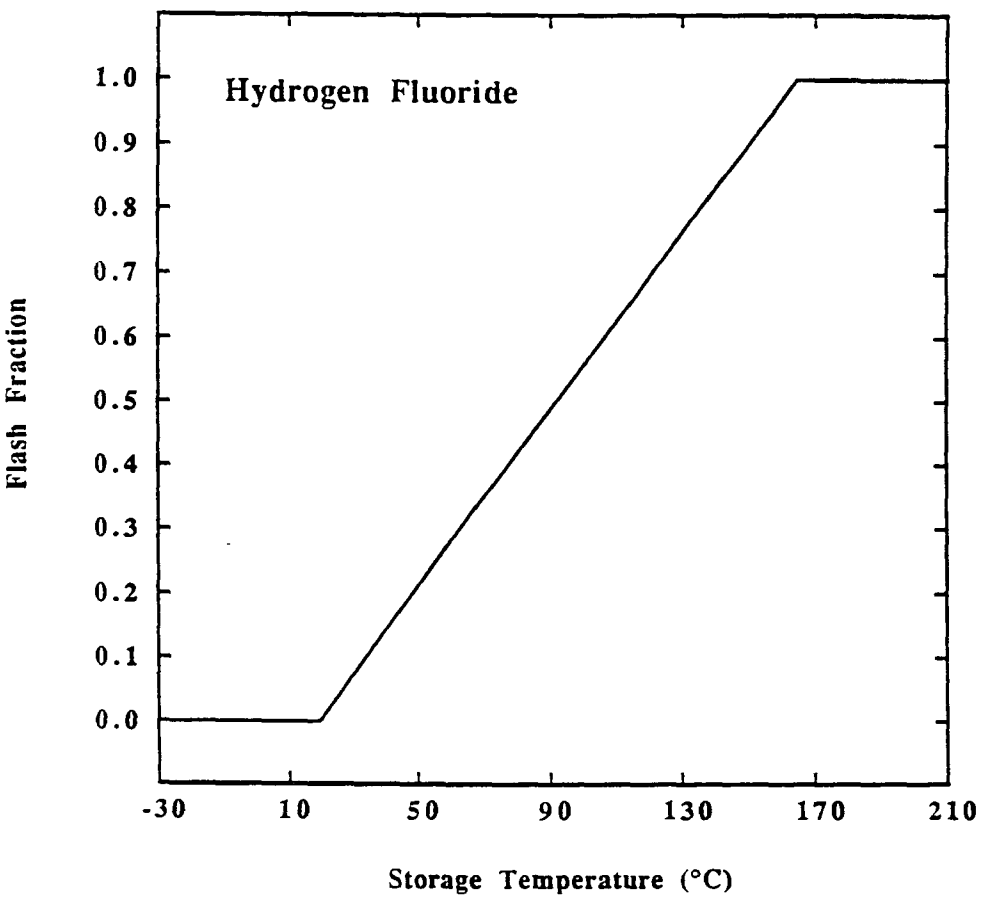
PHYSICAL PROPERTIES OF 30 WT% HYDROCHLORIC ACID (Continued)

Enthalpy Equation $H = A + B_t + C_t^2$ where: H = enthalpy, J/kg t = temperature (°K); and A, B, and C are constants for liquid and vapor enthalpies as follows: A / B / C Liquid* / 3475.256 / -8.0×10^{-8} Vapor* / 798.9364 / 6.1×10^{-8}	* Value of A depends on the selected reference state for the material. The numerical value of A does not affect release calculations since only enthalpy differences at various temperatures are applied to a single phase. To calculate enthalpy differences between phases, a reference state must bechosen to calculate A for each phase using the enthalpy equation.

Additional properties useful in determining other properties from physical property correlations:	
Critical Temperature	572.74 °K
Critical Pressure	20405355 Pa
Critical Density	366.52 kg/m^3
Energy of Molecular Interaction	433.37 °K
Effective Molecular Diameter	4.367 Angstroms



Triple Point Diagram for Hydrogen Fluoride



Flash Diagram for Hydrogen Fluoride

PHYSICAL PROPERTIES OF HYDROGEN FLUORIDE

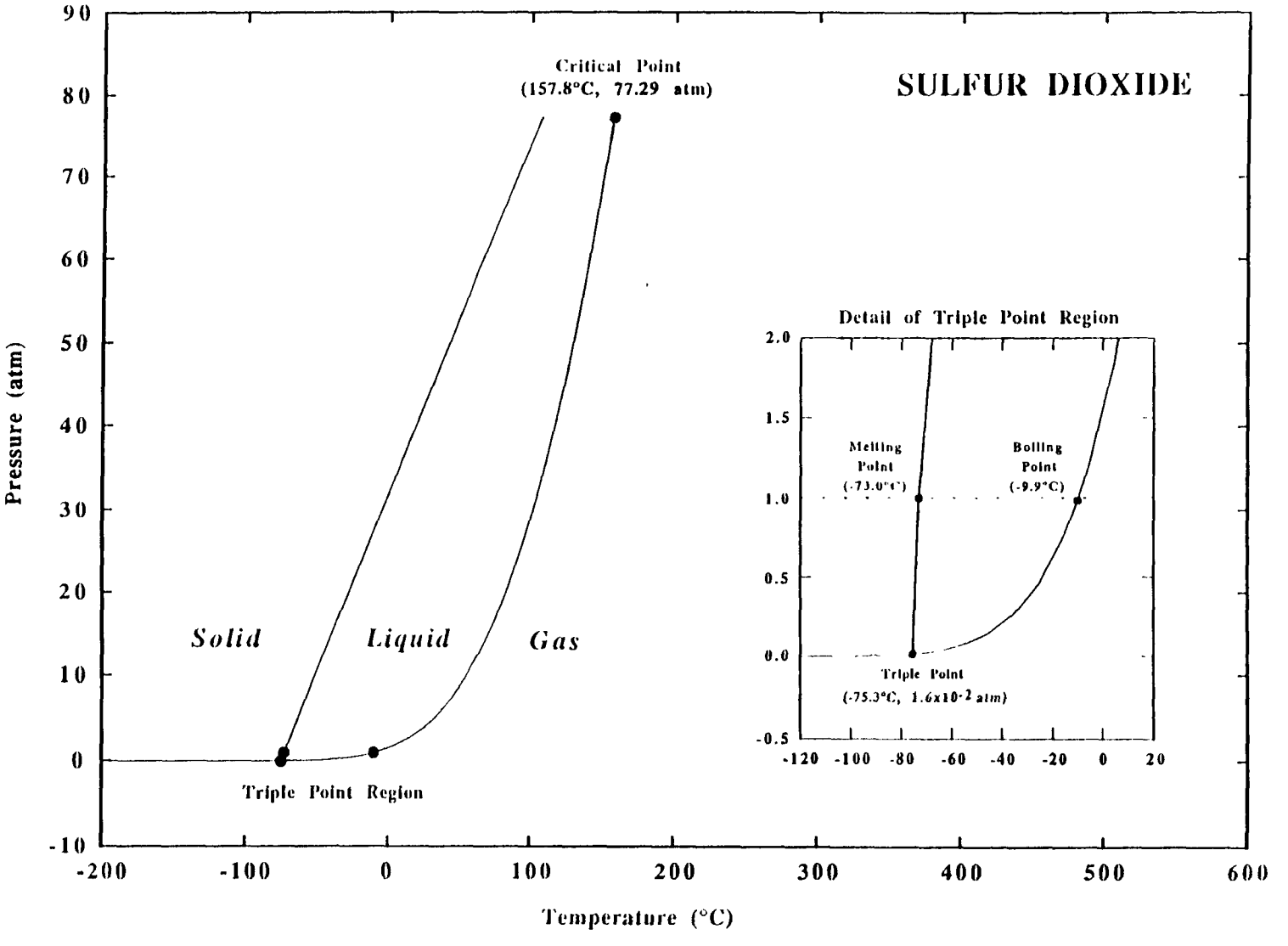
CAS Registry Number	7664-39-3		
Chemical Formula	HF		
Toxicity Threshold Concentrations		Time (min)	Level (ppm)
	ERPG-1	60	5
	ERPG-2	60	20
	ERPG-3	60	50
	IDLH	30	30
	STEL	15	6
Molecular Weight	20.006		
Normal Boiling Point	292.67 °K		
Vapor Density	0.832 kg/m^3 @ 293°K, 1 atm		
Liquid Density	955.18 kg/m^3 @ 292.67		
Liquid Specific Gravity (H_2O = 1)	1.004 @ 273°K		
Vapor Specific Gravity (air = 1)	0.69		
Vapor Pressure Equation Log P_v = A - B/(T+C) where: P_v = vapor pressure, mmHg T = temperature, ° C A = 7.6810, a constant B = 1475.60, a constant C = 287.88, a constant	773.08 mmHg (1.02 atm) @ 20°C		
Liquid Viscosity	0.000256 Pa-s @ 273 °K		
Liquid Surface Tension	0.0088 N/m @ 273 °K		
Solubility in Water	Complete		
Heat Capacity at Constant Volume (Vapor)	1041.49 J/kg °K @ 293 °K		
Heat Capacity at Constant Pressure (Vapor)	1455.57 J/kg °K @ 293 °K		
Heat Capacity at Constant Pressure (Liquid)	2559.79 J/kg °K @ 293 °K		
Latent Heat of Vaporization	376440 J/kg @ 293 °K		
Net Heating Value	7579626 J/kg		

PHYSICAL PROPERTIES OF HYDROGEN FLUORIDE (Continued)

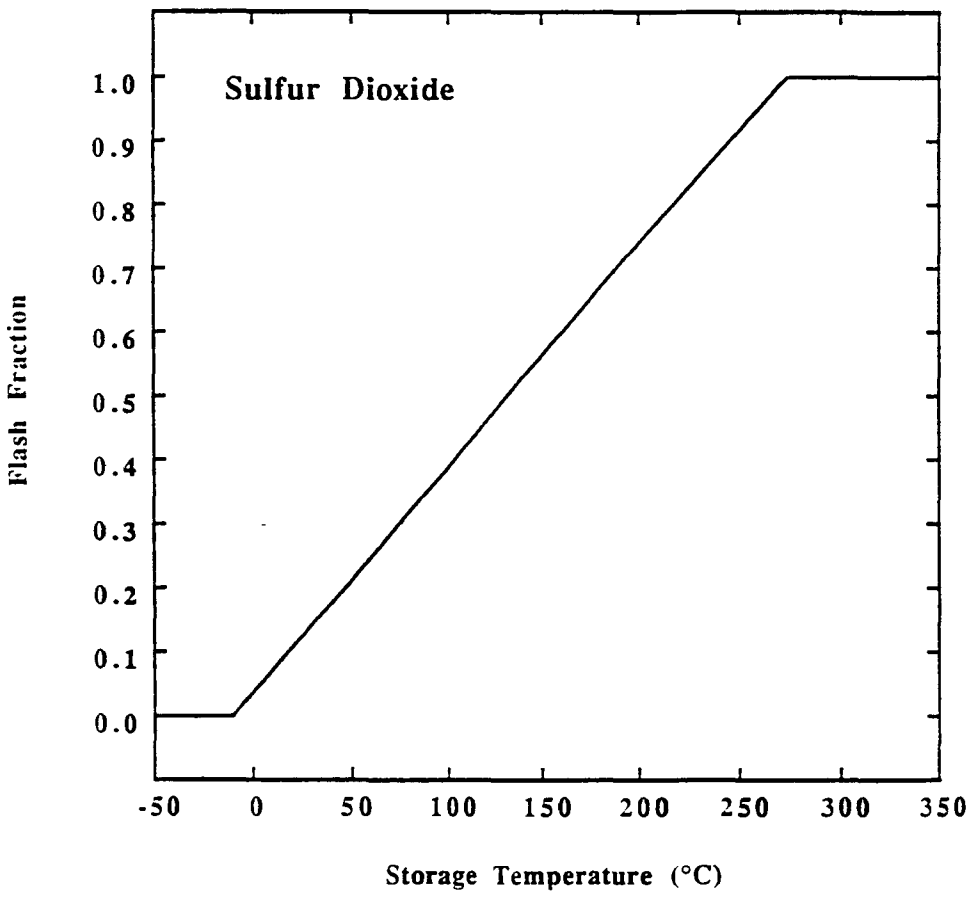
Enthalpy Equation: $H = A + B_t + C_t^2$ where: H = enthalpy, J/kg t = temperature (°K); and A, B, and C are constants for liquid and vapor enthalpies as follows: A / B / C Liquid* / 1238.668 / 4.264261 Vapor* / 1456.623 / -7.1×10^{-9}	* Value of A depends on the selected reference state for the material. The numerical value of A does not affect release calculations since only enthalpy differences at various temperatures are applied to a single phase. To calculate enthalpy differences between phases, a reference state must be chosen to calculate A for each phase using the enthalpy equation.
Additional properties useful in determining other properties from physical property correlations:	
Critical Temperature	461.15 °K
Critical Pressure	6484800 Pa
Critical Density	289.94 kg/m^3
Energy of Molecular Interaction	337 °K
Effective Molecular Diameter	3.24 Angstroms

HYDROGEN FLUORIDE APPARENT MOLECULAR WEIGHT AS A FUNCTION OF TEMPERATURE AND MOLAR FRACTION CONCENTRATION.

Temp(°C) / f_i	1.0	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1
20	51.59	48.58	43.78	39.53	35.47	31.56	27.03	23.78	21.53	20.32
30	36.22	33.45	30.51	27.20	24.65	22.91	21.65	20.68	20.37	20.03
40	25.26	23.66	22.50	21.51	20.88	20.53	20.36	20.15	20.02	20.01
50	21.06	20.65	20.53	20.32	20.18	20.09	20.02	20.01	20.01	20.01
60	20.17	20.10	20.05	20.01	20.01	20.01	20.01	20.01	20.01	20.01
70	20.01	20.01	20.01	20.01	20.01	20.01	20.01	20.01	20.01	20.01



Triple Point Diagram for Sulfur Dioxide



Flash Diagram for Sulfur Dioxide

PHYSICAL PROPERTIES OF SULFUR DIOXIDE

CAS Registry Number	7446-09-5
Chemical Formula	SO_2
Toxicity Threshold Concentrations	Time (min) / Level (ppm) ERPG-1: 60 / 0.3 ERPG-2: 60 / 3 ERPG-3: 60 / 15 IDLH: 30 / 100 STEL: 15 / 5
Molecular Weight	64.06
Normal Boiling Point	263.13 °K
Vapor Density	2.664 kg/m^3 @ 293°K, 1 atm
Liquid Density	1460.42 kg/m^3 @ 263.13 °K
Liquid Specific Gravity (H_2O = 1)	1.436 @ 273°K
Vapor Specific Gravity (air = 1)	2.21
Vapor Pressure Equation Log P_v = A - B/(T+C) where: P_v = vapor pressure, mmHg T = temperature, °C A = 7.2823, a constant B = 999.900, a constant C = 237.190, a constant	2480.3 mmHg (3.26 atm) @ 20°C
Liquid Viscosity	0.000431 Pa-s @ 263.13 °K, 0.97 atm
Liquid Surface Tension	0.0286 N/m @ 263 °K
Solubility in Water	13.875 kg/m^3 @ 293 °K, 1 atm
Heat Capacity at Constant Volume (Vapor)	493.77 J/kg °K @ 298 °K
Heat Capacity at Constant Pressure (Vapor)	623.09 J/kg °K @ 298 °K
Heat Capacity at Constant Pressure (Liquid)	1386.32 J/kg °K @ 293 °K
Latent Heat of Vaporization	388747 J/kg @ 263 °K
Net Heating Value	0 J/kg
Enthalpy Equation $H = A + B_t + C_t^2$ where: H = enthalpy, J/kg; t = temperature (°K); and A, B, and C are constants for liquid and vapor enthalpies as follows: A / B / C Liquid*: -110.556 / 3.0556 Vapor*: 1566.667 / -2.00	* Value of A depends on the selected reference state for the material. The numerical value of A does not affect release calculations since only enthalpy differences at various temperatures are applied to a single phase. To claculate enthalpy differences between phases, a reference state must be chosen to calculate A for each phase using the enthalpy equation.

PHYSICAL PROPERTIES OF SULFUR DIOXIDE (Continued)

Additional properties useful in determining other properties from physical property correlations:	
Critical Temperature	430.75 °K
Critical Pressure	7884100 Pa
Critical Density	527.07 kg/m^3
Energy of Molecular Interaction	303 °K
Effective Molecular Diameter	4.29 Angstroms

TECHNICAL REPORT DATA
(Please read Instructions on reverse before completing)

1. REPORT NO EPA-454/R-93-002	2	3. RECIPIENT'S ACCESSION NO
4. TITLE AND SUBTITLE Guidance on the Application of Refined Dispersion Models for Hazardous/Toxic Air Releases		5. REPORT DATE May 1993 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Radian Corporation 8501 N. Mopac Blvd. Austin, TX 78759		10. PROGRAM ELEMENT NO 11. CONTRACT/GRANT NO. EPA Contract No. 68-D00125 WA51
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency Office of Air Quality Planning and Standards, TSD Research Triangle Park, NC 27711		13. TYPE OF REPORT AND PERIOD COVERED Final Report 14. SPONSORING AGENCY CODE

15. SUPPLEMENTARY NOTES
This document revises EPA-450/4-91-007
Technical Representative: Jawad S. Touma

16. ABSTRACT

This document provides general guidance on characterizing hazardous air pollutant releases and shows how to apply appropriate dispersion models. The document: 1) helps determine likely or reasonable storage conditions for specific conditions for which a release might occur; 2) helps determine release classes; 3) defines the steps to be taken when determining if a release should be considered a dense gas release; 3) defines the methods used to determine the input variables used by refined models in the public domain; 4) points out the implications and effects of various choices for input information; 5) shows by example, the calculation of the input variables used by the models; 6) describes the output available from these models; and 7) discusses how to determine the input that gives the worst-case impact conditions. Because many chemicals may form dense gas clouds upon release, and refined dispersion models that can simulate these releases are complex, particular attention is paid to models that can address these types of release.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution Hazardous Waste Assessment Toxic Air Pollutants Dense Gas Air Quality Dispersion Model TSCREEN Model	Dispersion Modeling Meteorology Air Pollution Control	13B
18. DISTRIBUTION STATEMENT Release Unlimited	19. SECURITY CLASS (Report) Unclassified	21. NO. OF PAGES 464
	20. SECURITY CLASS (Page) Unclassified	22. PRICE

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