EPA-454/R-92-024

# WORKBOOK OF SCREENING TECHNIQUES FOR ASSESSING IMPACTS OF TOXIC AIR POLLUTANTS

## (REVISED)

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

December 1992

# PREFACE

This document supersedes the workbook version dated September 1988. Changes include: development of new methods for estimating emission rates; revisions to methods for esitmating emission rates to establish consistency with current guidance; addition of several new scenarios, especially those related to Superfund; and the addition of a new screening method based on the work of Britter and McQuaid to estimate the impact of aerosols and denser-than-air gases released from chemical spills. Ambient concentrations are now illustrated by using the TSCREEN model instead of hand calculations. Thus, users comparing the predicted maximum ground level concentrations with those shown in the earlier document will now find different, and more accurate, estimates.

# ACKNOWLEDGEMENTS

This report was prepared by Pacific Environmental Services, Inc., under EPA Contract No. 68D00124, with Mr. Jawad S. Touma as the Work Assignment Manager.

# TABLE OF CONTENTS

PREFACE . . . . . . . . . . . . . . . . . . . . . . . . . . . . iii

ACKNOWLEDGEMENTS . . . . . . . . . . . . . . . . . . . . . . . iv

1.0 INTRODUCTION . . . . . . . . . . . . . . . . . . . . . . . 1-1

2.0 SELECTION OF SCREENING TECHNIQUES FOR TOXIC AIR CONTAINMENTS . . . . . . . . . . . . . . . . . . . . . . . . . . . . 2-1
    2.1 Release Categorization . . . . . . . . . . . . . . . 2-1
    2.2 Limitations and Assumptions . . . . . . . . . . . . 2-1
    2.3 Scenario Selection . . . . . . . . . . . . . . . . . 2-3
    2.4 Determining Maximum Short-Term Ground Level Concentration . . . . . . . . . . . . . . . . . . 2-17
        2.4.1 Dispersion Models used in TSCREEN . . . . 2-17
        2.4.2 Dispersion Model Selection . . . . . . . . 2-17
    2.5 Considerations for Time-Varying and Time-Limited Releases . . . . . . . . . . . . . . . . . . . . 2-24
    2.6 Denser-Than-Air Materials . . . . . . . . . . . . 2-25
    2.7 Dispersion Screening Estimates for Denser-Than-Air Contaminants . . . . . . . . . . . . . . . . . . 2-26

3.0 SUPPORT DATA FOR SCREENING ESTIMATES . . . . . . . . . . 3-1
    3.1 Meteorological Data . . . . . . . . . . . . . . . . 3-1
        3.1.1 Wind Speed and Direction . . . . . . . . . . 3-1
        3.1.2 Stability and Turbulence . . . . . . . . . . 3-2
        3.1.3 Temperature . . . . . . . . . . . . . . . . . 3-3
        3.1.4 Atmospheric Pressure . . . . . . . . . . . . 3-3
    3.2 Chemical and Physical Parameters . . . . . . . . . 3-3

4.0 SCENARIOS AND TECHNIQUES FOR RELEASE AND EMISSIONS ESTIMATES . . . . . . . . . . . . . . . . . . . . . . . . 4-1
    4.1 Particulate Matter Release . . . . . . . . . . . . 4-2
        4.1.1 Releases from Stacks, Vents . . . . . . . . 4-2
        4.1.2 Continuous Fugitive/Windblown Dust Emissions . . . . . . . . . . . . . . . . . 4-11
        4.1.3 Ducting/Connector Failures . . . . . . . . 4-17
    4.2 Gaseous Release . . . . . . . . . . . . . . . . . . 4-23
        4.2.1 Continuous Flared Stack Emissions - Gaseous . . . . . . . . . . . . . . . . . . . . . 4-23
        4.2.2 Continuous Release from Stacks, Vents, Conventional Point Sources . . . . . . . . 4-28
        4.2.3 Continuous Gas Leaks from a Reservoir . . 4-34
        4.2.4 Instantaneous Gas Leaks from a Reservoir . 4-67
        4.2.5 Continuous Gas Leaks from a Pipe Attached to a Reservoir . . . . . . . . . . . . . . 4-69
        4.2.6 Instantaneous Gas Leaks from a Pipe Attached to a Reservoir . . . . . . . . . 4-87
        4.2.7 Continuous Multiple Fugitive Emissions . . 4-89
        4.2.8 Continuous Emissions from Land Treatment Facilities . . . . . . . . . . . . . . . . . 4-93
        4.2.9 Continuous Emissions from Municipal Solid Waste Landfills . . . . . . . . . . . . . . 4-97

4.2.10 Continuous Emissions of Pesticides . . . . 4-103
4.2.11 Instantaneous Discharges from Equipment Openings . . . . . . . . . . . . . . . . . 4-108
4.3 Liquid Release . . . . . . . . . . . . . . . . . 4-112
4.3.1 Continuous Evaporation from Surface Impoundments (Lagoons) . . . . . . . . . . 4-112
4.3.2 Continuous (Two-Phase) Release Rate Estimates: Saturated Liquid from Pressurized Storage . . . . . . . . . . . 4-116
4.3.3 Instantaneous (Two-Phase) Release Rate Estimates: Saturated Liquid from Pressurized Storage . . . . . . . . . . . 4-124
4.3.4 Continuous (Two-Phase) Release Rate Estimates: Subcooled Liquid from Pressurized Storage . . . . . . . . . . . 4-126
4.3.5 Instantaneous (Two-Phase) Release Rate Estimates: Subcooled Liquid from Pressurized Storage . . . . . . . . . . . 4-134
4.3.6 Continuous High Volatility Leaks . . . . . 4-136
4.3.7 Instantaneous High Volatility Leaks . . . 4-144
4.3.8 Continuous Low Volatility Liquids from Tanks and Pipes . . . . . . . . . . . . . . 4-146
4.3.9 Instantaneous Low Volatility Liquids from Tanks and Pipes . . . . . . . . . . . . . . 4-155
4.4 Superfund Releases . . . . . . . . . . . . . . . 4-162
4.4.1 Air Strippers . . . . . . . . . . . . . . 4-162

5.0 ATMOSPHERIC DISPERSION ESTIMATES . . . . . . . . . . . . 5-1
5.1 SCREEN . . . . . . . . . . . . . . . . . . . . . . 5-2
5.1.1 Point Sources . . . . . . . . . . . . . . . 5-2
5.1.2 Area Sources . . . . . . . . . . . . . . . 5-14
5.2 RVD . . . . . . . . . . . . . . . . . . . . . . 5-19
5.2.1 Inputs . . . . . . . . . . . . . . . . . . 5-19
5.2.2 Model Output . . . . . . . . . . . . . . . 5-21
5.3 PUFF . . . . . . . . . . . . . . . . . . . . . . 5-26
5.3.1 PUFF Model Discussion . . . . . . . . . . 5-26
5.3.2 Model Inputs . . . . . . . . . . . . . . . 5-28
5.3.4 Model Output . . . . . . . . . . . . . . . 5-30
5.4 Britter-McQuaid . . . . . . . . . . . . . . . . . 5-33
5.4.1 Method for Cold Contaminant Releases — Heat Transfer Effects . . . . . . . . . . . . . 5-34
5.4.2 Method for Contaminant Aerosol Releases . 5-34
5.4.3 Continuous (Plume) Releases . . . . . . . 5-36
5.4.4 Instantaneous (Puff) Releases . . . . . . 5-41
5.4.5 Assumptions in TSCREEN . . . . . . . . . . 5-45
5.4.6 Model Inputs . . . . . . . . . . . . . . . 5-46
5.4.7 Model Output . . . . . . . . . . . . . . . 5-47

REFERENCES . . . . . . . . . . . . . . . . . . . . . . . . R-1

APPENDIX A EMISSION FACTORS . . . . . . . . . . . . . . . A-1

APPENDIX B ESTIMATING SELECTED PHYSICAL PROPERTIES OF MIXTURES . . . . . . . . . . . . . . . . . . B-1

APPENDIX C SELECTED CONVERSION FACTORS . . . . . . . . C-1

APPENDIX D AVERAGING PERIOD CONCENTRATION ESTIMATES . . D-1

## 1.0 INTRODUCTION

This workbook provides a logical approach to the selection of appropriate screening techniques for estimating ambient concentrations due to various toxic/hazardous pollutant releases. Methods used in the workbook apply to situations where a release can be fairly well-defined, a condition typically associated with non-accidental toxic releases. The format of this workbook is built around a series of release scenarios which may be considered typical and representative of the means by which toxic chemicals become airborne. This document supersedes the earlier workbook (EPA, 1988a).

Screening techniques are simplified calculational procedures designed with sufficient conservatism to allow a determination of whether a source: 1) is clearly not an air quality threat or 2) poses a potential threat which should be examined with more sophisticated estimation techniques or measurements. Screening estimates obtained using this workbook represent maximum short-term ground level concentration estimates from a meteorological perspective. If the screening estimates demonstrate that during these conditions the ground level concentrations are not likely to be considered objectionable, further analysis of the source impact would not be necessary as part of the air quality review of the source. However, if screening demonstrates that a source may have an objectionable impact, more detailed analysis would be required using refined emissions and air quality models.

For each release scenario, the workbook describes the procedure to be used and provides an example illustration using the TSCREEN model. TSCREEN, a model for screening toxic air pollutant concentrations, is an IBM PC-based interactive model that implements the release scenarios and methods described in this workbook. TSCREEN allows the user to select a scenario, determine an emission rate, and then apply the appropriate dispersion model in a logical problem solving approach. The model consists of a front-end control program with many interactive menus and data entry screens. As much information as is logically and legibly possible is assembled onto unique data entry screens. All requests for input are written in clear text. Extensive help screens are provided to minimize numeric data entry errors, and default values are provided for some parameters. The user is able to return to previous screens and edit data previously entered. A chemical look-up database and an on-line calculator are also available. Once the nature of the release is determined, the user must specify the emission rate. For some scenarios, extensive references to EPA methods are provided, while for others, a specific method for calculating the emission rate is given. Density checks for the release are performed to determine which dispersion model is selected. Data necessary to execute that particular model is then requested in a logical format. Once the model is executed, the concentrations are calculated and then tabulated in a clear and legible manner, and an easy to read graph of concentration versus distance is provided. The printed text and graphical output can be sent to a variety of printers and plotters through built-in software; minimum user interface is required.

The front-end program in TSCREEN is written in the FoxPro™ programming language, a superset of the dBASE language family suitable for PC's running MS-DOS™. The primary purpose of a dBASE language is database manipulation, but is can also be used for general purpose programming. The reasons for using this system are: 1) a user interface which facilitates the debugging process, and as a result, reduces the development cost; 2) pull-down menus and windows which require minimal programming effort to create; 3) built-in functions for database manipulation, and as a result, much less code is required to create the chemical database in TSCREEN; 4) memory management capabilities that allow TSCREEN to run on machines with less random access memory (RAM); and 5) the ability to release most of the TSCREEN front-end program from memory before it executes the dispersion models. The main disadvantage of this system is the size of the files that a user needs to run. The system is distributed with two run-time libraries. These are files that contain the implementation of functions that are called by the program. One of these libraries is over 300 kilobytes (K) and the other is close to 1 megabyte (MB). TSCREEN is distributed through the EPA's Technology Transfer Network, SCRAM Bulletin Board System.

The workbook is organized into five sections and six supporting appendices. Section 2 discusses selection of screening techniques and the general approach to using the workbook. Users are advised to consult this section both for releases explicitly presented in the workbook and for less typical releases. This section also considers assumptions, limitations and conservatism of estimates. Section 3 describes the support data (i.e., meteorological data and chemical and physical parameters) needed for making estimates. Section 4 presents the inputs required for each scenario and the applicable methods for determining release (emission) rates. This section also includes an example showing the data entry screening and sample calculations for each scenario as used in TSCREEN. (Note: the values that TSCREEN produces may be slightly different than the values in the examples due to differences in rounding.) In this workbook 24 release scenarios have been selected to represent situations likely to be encountered. Section 5 describes the dispersion models that are referenced in this workbook and are embedded in TSCREEN.

Appendix A discusses currently available sources for obtaining emission factors that can be used for some of the scenarios. Appendix B provides a method for estimating selected physical properties for mixtures. Appendix C provides some useful unit conversion factors applicable to the workbook.

Appendix D provides some techniques for converting concentrations calculated by the models to different averaging times.

Methods used in this workbook should be applied with caution. Techniques for estimating emissions are evaluated and revised on a continuing basis by EPA. Thus the user should consult with EPA on the most recent emission models and emission factors. Meteorological methods presented in this workbook reflect guidance published elsewhere, and in particular the Guideline on Air Quality Models (Revised) (EPA, 1986) and its supplements. The Regional Modeling Contact should be consulted as to the present status of guidance on air quality modeling.

## 2.0 SELECTION OF SCREENING TECHNIQUES FOR TOXIC AIR CONTAMINANTS

This workbook attempts to account for many of the scenarios expected to produce toxic chemical releases to the atmosphere.

### 2.1 Release Categorization

Selection of appropriate technique for screening estimates requires categorization of the toxic chemical release of interest. There are three overlapping categories which should be considered when defining problems for screening:

1) Physical State - Gaseous releases to the atmosphere can, in general, be simulated using techniques developed for criteria air pollutants unless the gas is dense, is highly reactive, or rapidly deposits on surfaces. Additional source modeling must be performed if the release is liquid, aerosol or multi-phased to determine the state of the material as it disperses in air.

2) Process/Release Conditions - Knowledge of the circumstances under which chemicals are released helps to determine both state and dispersive characteristics. For example, location of a leak in a pressurized liquefied gas storage tank will determine if a release is liquid or gas and if source modeling is required prior to dispersion estimates.

3) Dispersive Characteristics - Techniques for pollutant dispersion estimates are categorized by terms such as instantaneous versus continuous, or point versus area or volume releases. To complete dispersion estimates, this final characterization is required at some point in concentration calculations.

The primary emphasis of this workbook is to serve as an accompanying guide to the TSCREEN program which implements screening techniques for estimating short-term, ground level concentrations of toxic chemicals released to the atmosphere. However, in order to do this, the workbook also provides assistance to the user in formulating the release conditions.

### 2.2 Limitations and Assumptions

Methods included in TSCREEN are intended to provide simplified screening estimates for situations which may represent extremely complex release scenarios. As such, the methods are limited in their applicability. Some of these limitations are as follows:

- Screening techniques provided are intended for use on small to mid-scale non-accidental releases.

- All techniques assume that the toxic air contaminant is non- reactive and non-depositing. Thus these screening methods are not applicable for reactive gases and particle depositions. For two-phase flows, all released liquid is assumed to travel downwind as an aerosol with insignificant (liquid) rain out near the source.

- Denser-than-air contaminant behavior is a consequence not only of the initial (depressurized) contaminant density but also of the contaminant release rate and the ambient wind speed; if denser-than-air contaminant behavior is not expected to be important, passive atmospheric dispersion modeling techniques should be applied. In TSCREEN Version 3.0, the determination of denser-than-air behavior is done based on the initial contaminant density comparison to ambient air.

- Conditions resulting in worst case concentrations cannot be uniquely defined where meteorological conditions affect source estimates. For example, in the case of evaporation, the highest emission rates are related to high wind speeds, which, however, result in more dilution and lower ambient concentrations.

- Time dependent emissions cannot be simulated with these simple screening technique. Techniques provided assume steady releases for a specified period.

- All release calculations assume ideal conditions for gas and liquid flows.

- The influence of obstructions such as buildings and topography on denser-than-air releases and releases close to the ground are not included.

- Complicated post-release thermodynamic behavior for denser-than-air releases is not accounted for in these screening techniques.

Because of the simplifying assumptions inherent in these screening methods, which are specifically aimed at decreasing the amount of information required from the user and decreasing the computation time and sophistication, more refined assessment techniques should be applied to a release scenario which is identified by these screening procedures as violating ambient air quality standards or other specified levels of concern. Refined techniques involve both refined release (emission) rate estimates as well as more refined atmospheric dispersion models. (See for example, "Guidance on the Application of Refined Dispersion Models for Air Toxics Releases" (EPA, 1991a).) As with any air quality assessment, the screening methods described here should be applied with due caution.

## 2.3 Scenario Selection

Release scenarios are grouped according to four categories: particulate matter, gases, liquids, and releases from Superfund sites as shown in Table 2-1. For some of the categories, there are additional subcategories. Figure 2-1 provides a graphical illustration of each release scenario. Descriptions on similar release scenarios are provided to help guide the user in selecting the correct release category. Once the correct release category has been selected, the user should proceed to the relevant section where further information on the release scenario is given. For each release scenario, methods for determining emission estimates are provided and then the appropriate dispersion model is selected to determine ambient concentrations.

## TABLE 2-1
## RELEASE SCENARIOS

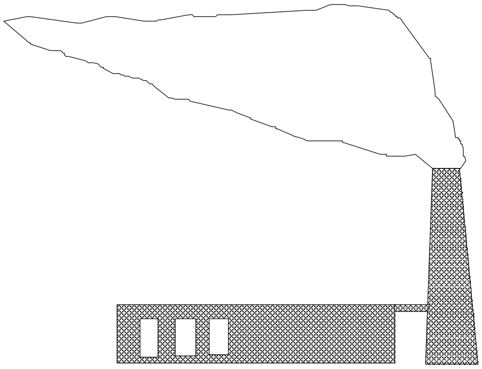
| Initial Form of Release | Release Type | Scenario Number | Modeling Category * |
|---|---|---|---|
| Particulate Matter | Continuous Particulate Release from Stack, Vents | 1.1 | CP |
| | Fugitive/Windblown Dust Emissions | 1.2 | CA |
| | Ducting/Connector Failures | 1.3 | IP |
| Gases | Flared Stack Emissions | 2.1 | CP |
| | Continuous Releases from Stacks, Vents, Point Sources | 2.2 | CP |
| | Continuous Leaks from Reservoir | 2.3 | CP |
| | Instantaneous Leak from Reservoir | 2.4 | IP |
| | Continuous Leaks from Pipe Attached to Reservoir | 2.5 | CP |
| | Instantaneous Leak from Pipe Attached to Reservoir | 2.6 | IP |
| | Gaseous Emissions from Multiple Fugitive Sources | 2.7 | CA |
| | Gaseous Emissions from Land Treatment Facilities | 2.8 | CA |
| | Emissions from Municipal Solid Waste Landfills | 2.9 | CA |
| | Emissions from Pesticides/Herbicide Applications | 2.10 | CA |
| | Discharges from Equipment Openings | 2.11 | IP |
| Liquid | Evaporation from Surface Impoundments (Lagoons) | 3.1 | CA |
| | Continuous 2-Phase Saturated Liquid from Pressurized Storage | 3.2 | CP |
| | Instantaneous 2-Phase Saturated Liquid from Pressurized Storage | 3.3 | IP |
| | Continuous 2-Phase Subcooled Liquid from Pressurized Storage | 3.4 | CP |
| | Instantaneous 2-Phase Subcooled Liquid from Pressurized Storage | 3.5 | IP |
| | Continuous High Volatility Liquid Leaks | 3.6 | CP |
| | Instantaneous High Volatility Liquid Leaks | 3.7 | IP |
| | Continuous Low Volatility Liquid Leaks | 3.8 | CA |
| | Instantaneous Low Volatility Liquid Leaks | 3.9 | IP |
| Superfund Sites | Air Stripper | 4.1 | CP |

* C - Continuous
P - Point
A - Area
I - Instantaneous

Table 2-1 shows that, for example, a continuous gaseous release from stacks, vents and point sources is given Scenario number 2.2. Figure 2-1 provides a graphical illustration and a brief description of this scenario. Figure 2-2 (Section 2.4) shows that this scenario is discussed in detail in Section 4.2.2 and that the SCREEN dispersion model is selected within TSCREEN to estimate ambient ground level concentrations for this scenario.

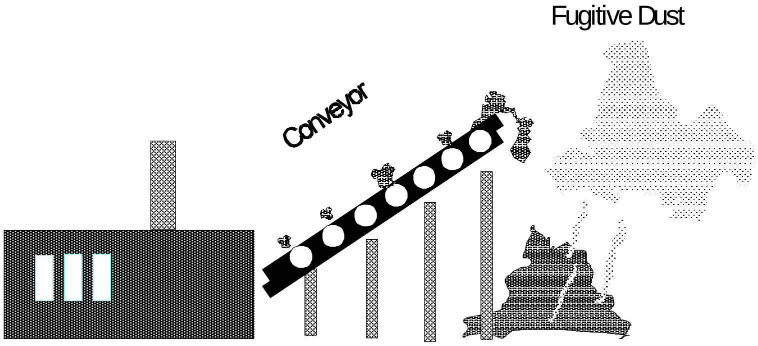
Figure 2-1. Schematic Illustrations of Scenarios

## Continuous Releases of Particulate Matter from Stacks, Vents -1.1



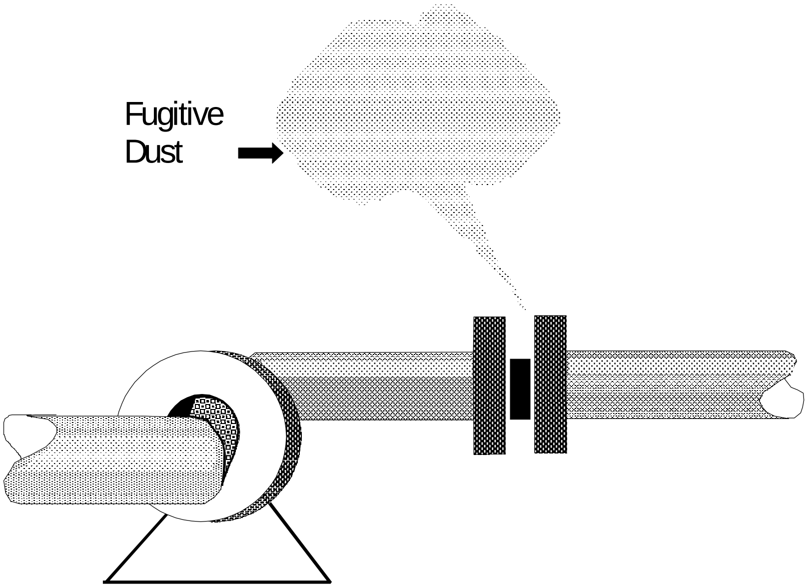
Similar Releases: Continuous emissions of particulate matter from vertical stacks and pipes or conventional point sources and some process vents when emission flow rates and temperature are known. Combustion sources and chemical reactors are typical emission sources that may emit such pollutants through stacks. These releases may also be due to a process failure such as a rupture disk release or failure of control equipment.

## Continuous Fugitive/Windblown Dust Emissions - 1.2



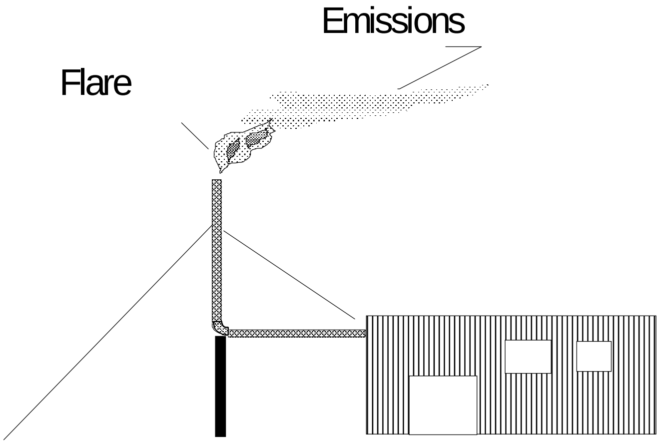
Similar Releases: Any fugitive dust from process losses, generated by mechanical action in material handling or windblown dust. Such emissions tend to originate from a surface or a collection of small poorly defined point sources.

## Particulate Releases from Ducting/Connector Failures - 1.3



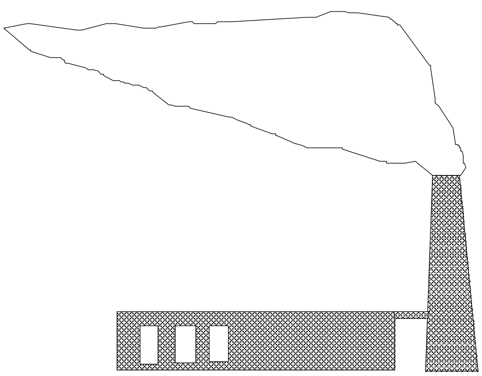
Similar Releases: Instantaneous bursts of particulates due to duct failure (e.g., pneumatic conveyor line failures), line disconnection, isolation joint failure, or other types of equipment openings.

## Continuous Flared Stack Emissions - 2.1



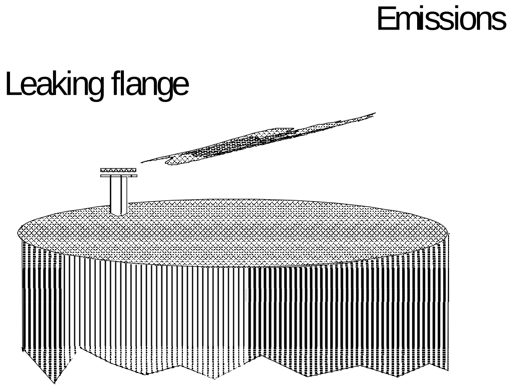
Similar Releases: Flares are used as a control device for a variety of sources. As such flares must comply with requirements specified in 40 CFR 60.18.

## Continuous Release from Stacks, Vents, Conventional Point Sources - 2.2



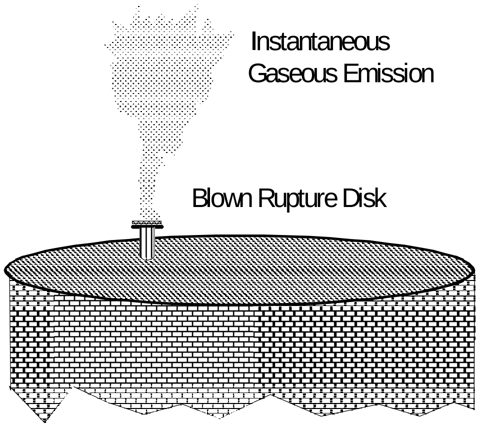
Similar Releases: Continuous emissions of a gas from vertical stacks and pipes or conventional point sources and some process vents when emission flow rates and temperature are known. Combustion sources and chemical reactors are typical emission sources that may emit such pollutants through stacks. These releases may also be due to a process failure such as a rupture disk release or failure of control equipment.

## Continuous Gaseous Leaks from Reservoir - 2.3



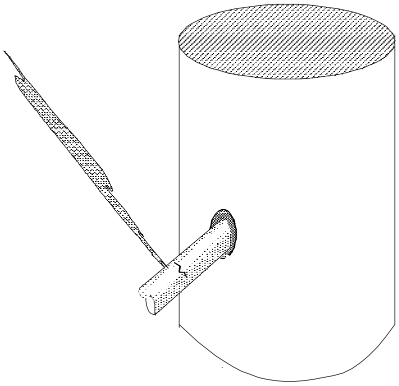
Similar Releases: Continuous release of a gas (at constant pressure and temperature) from a containment (reservoir) through a hole or opening. Possible applications include a gas leak from a tank, a (small) gas leak from a pipe, or gas discharge from a pressure relief valve mounted on a tank.

## Instantaneous Gaseous Leak from Reservoir - 2.4



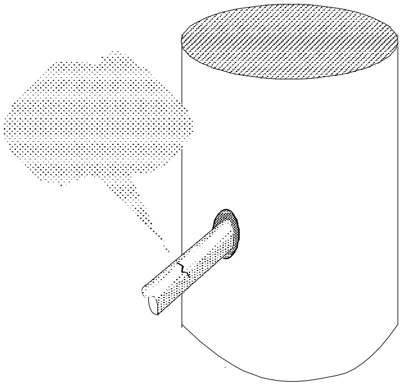
Similar Releases: Instantaneous release of a gas (at constant pressure and temperature) from a containment (reservoir) through a hole or opening. Possible applications include a gas leak from a tank, a (small) gas leak from a pipe, or gas discharge from a pressure relief valve mounted on a tank.

## Continuous Leaks from a Pipe Attached to a Reservoir - 2.5



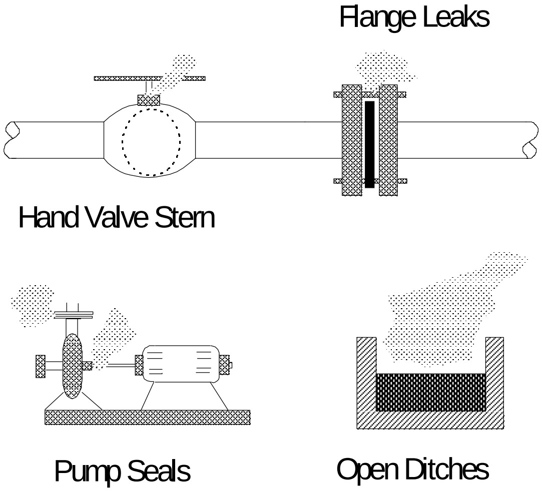
Similar Release: Continuous release of a gas (at constant pressure and temperature) from a containment (reservoir) through a long pipe.

## Instantaneous Leaks from a Pipe Attached to a Reservoir - 2.6



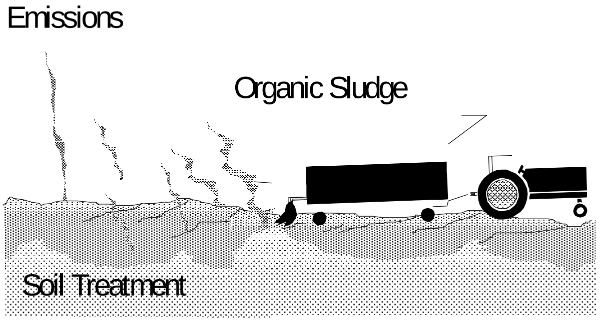
Similar Release: Instantaneous release of a gas (at constant pressure and temperature) from a containment (reservoir) through a long pipe.

## Continuous Multiple Fugitive Emissions - 2.7



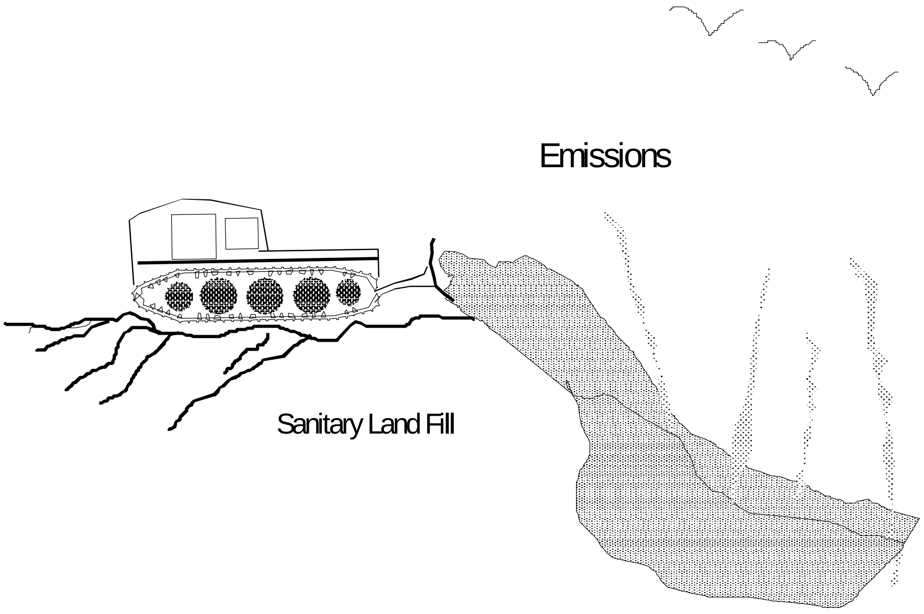
Similar Releases: Releases from any continuous area or volume source where the emissions are uniformly released over the area or the area represents a collection of small sources poorly defined in terms of location (e.g., multiple vents on large manufacturing buildings, fugitive VOC sources in refineries or chemical process manufacturing plants).

## Continuous Emissions from Land Treatment Facilities - 2.8



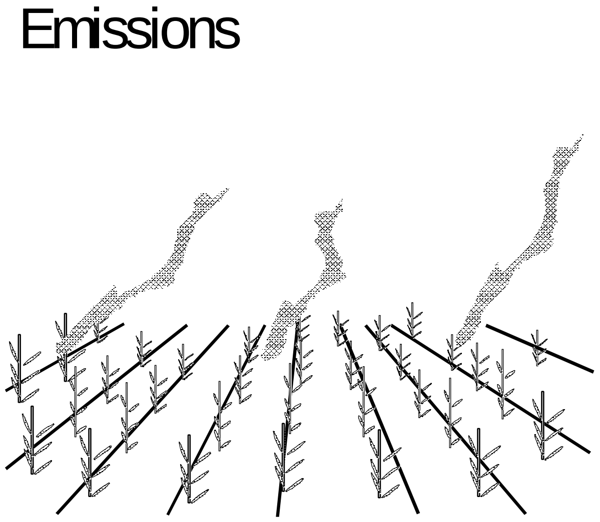
Similar Releases: Landfarms; ground level application of sludge (containing volatile organic material in oil) to soil surface.

## Continuous Emissions from Municipal Solid Waste Landfills - 2.9



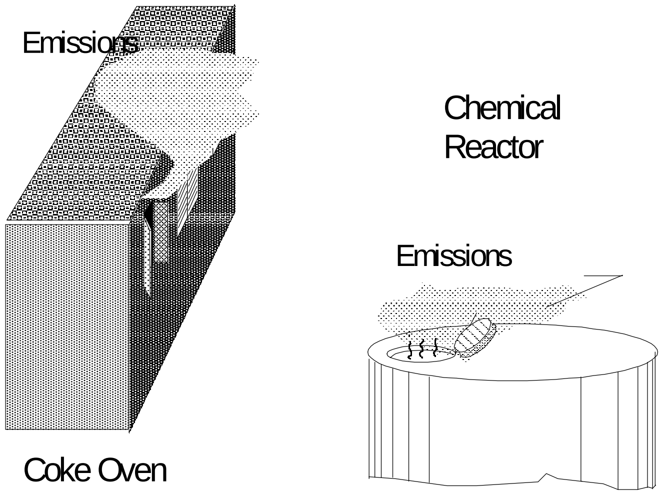
Similar Releases: None. Emission rates applicable to municipal solid waste landfills only.

### Continuous Emissions from Pesticides/Herbicide Applications - 2.10



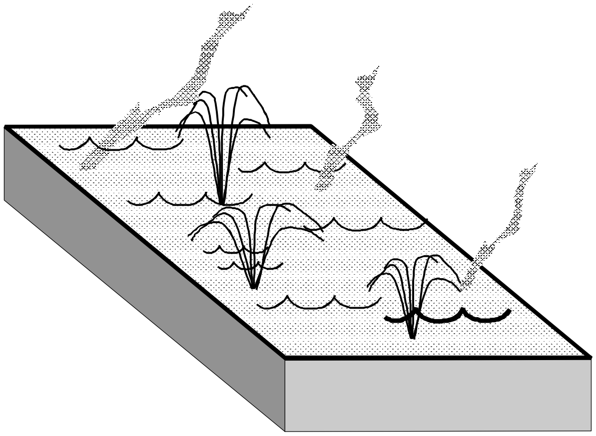
Similar Releases: Emissions resulting from the volatilization of pesticides or herbicides applied to open fields.

### Instantaneous Discharges from Equipment Openings - 2.11



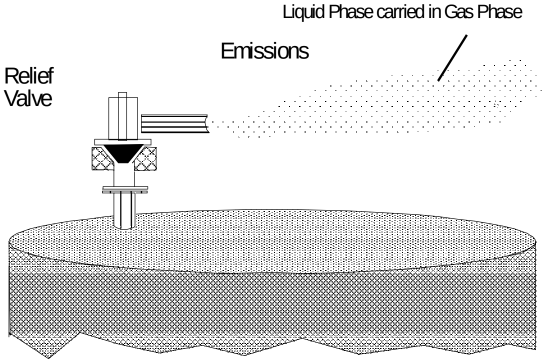
Similar Releases: Any puff or burst type release with short duration emissions resulting from the opening of equipment after processing (e.g., coke ovens or chemical reactors), from routine sampling of product processing or gaseous emissions from disconnected lines.

## Continuous Evaporation from Surface Impoundments (Lagoons) - 3.1



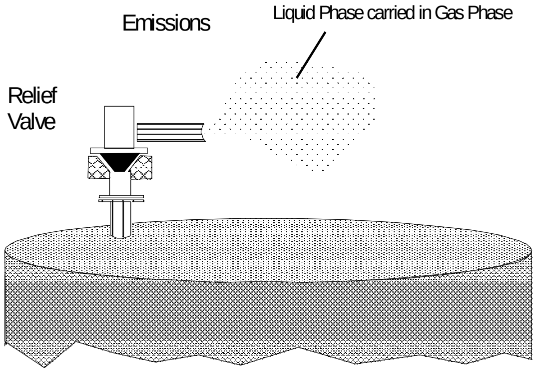
Similar Releases: Waste lagoons and other impoundments with emissions resulting from the evaporation of volatile chemicals from liquid mixtures with biological activity.

## Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2



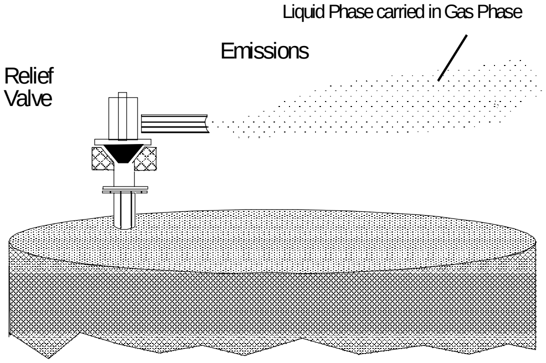
Similar Releases: Continuous release of a pressurized liquid stored under saturated conditions. The release occurs (at constant pressure and temperature) from the containment (reservoir) through a hole or opening; a provision is made for the effect of a pressure drop (piping) between the tank and the hole or opening. Possible applications include a saturated liquid leak from a pressurized tank or a saturated liquid leak from a pipe.

## Instantaneous 2-Phase Saturated Liquid from Pressurized Storage - 3.3



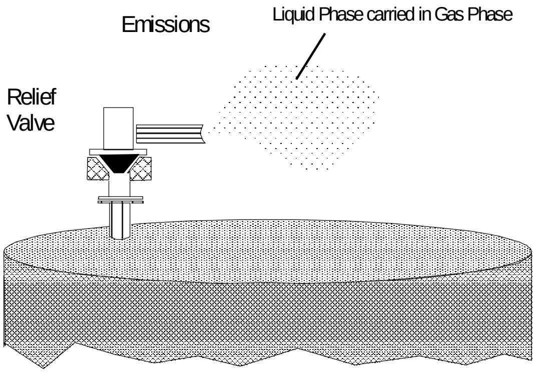
<u>Similar Releases:</u> Instantaneous release of a pressurized liquid stored under saturated conditions. The release occurs (at constant pressure and temperature) from the containment (reservoir) through a hole or opening; a provision is made for the effect of a pressure drop (piping) between the tank and the hole or opening. Possible applications include a saturated liquid leak from a pressurized tank or a saturated liquid leak from a pipe.

## Continuous Subcooled Liquid from Pressurized Storage - 3.4



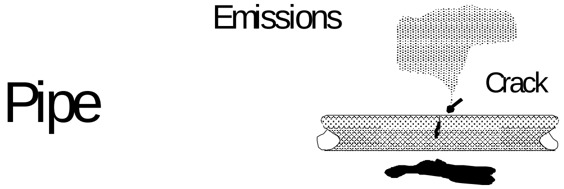
<u>Similar Releases:</u> Continuous release of pressurized liquid stored below its saturation pressure. The release occurs (at constant pressure and temperature) from a containment (reservoir) through a hole or opening; a provision is made for the effect of a pressure drop (piping) between the tank and the hole or opening. Possible applications include a subcooled liquid leak from a pressurized tank or a subcooled leak from a pipe.

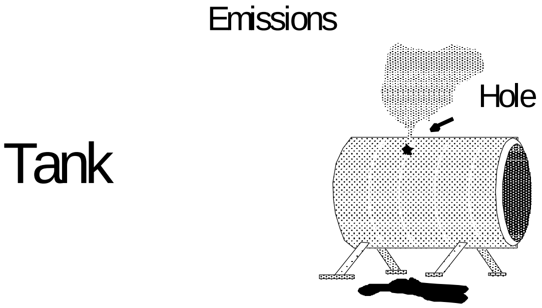
## Instantaneous Subcooled Liquid from Pressurized Storage - 3.5



Similar Releases: Instantaneous release of pressurized liquid stored below its saturation pressure. The release occurs (at constant pressure and temperature) from a containment (reservoir) through a hole or opening; a provision is made for the effect of a pressure drop (piping) between the tank and the hole or opening. Possible applications include a subcooled liquid leak from a pressurized tank or a subcooled leak from a pipe.

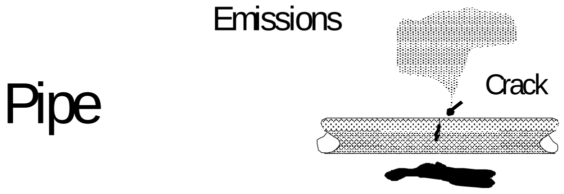
## Continuous High Volatility Liquid Leaks - 3.6

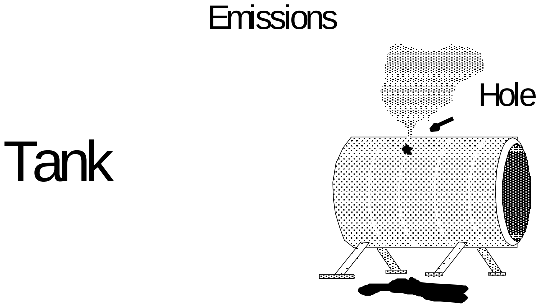




Similar Releases: Continuous release of high volatility liquid (at constant temperature and pressure) from a containment (reservoir) through a hole or opening. Possible applications include a (high volatility) liquid leak from a tank or a liquid leak from a pipe (when the ratio of the hole diameter to the pipe diameter is less than 0.2).

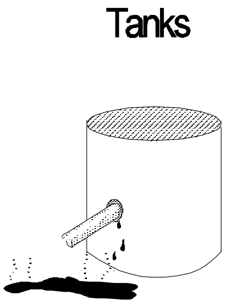
## Instantaneous High Volatility Liquid Leaks - 3.7

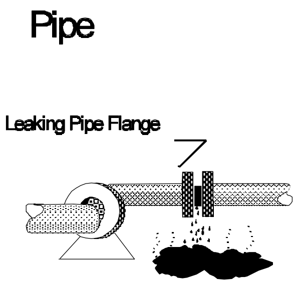




<u>Similar Releases:</u> Instantaneous release of high volatility liquid (at constant temperature and pressure) from a containment (reservoir) through a hole or opening. Possible applications include a (high volatility) liquid leak from a tank or a liquid leak from a pipe (when the ratio of the hole diameter to the pipe diameter is less than 0.2).

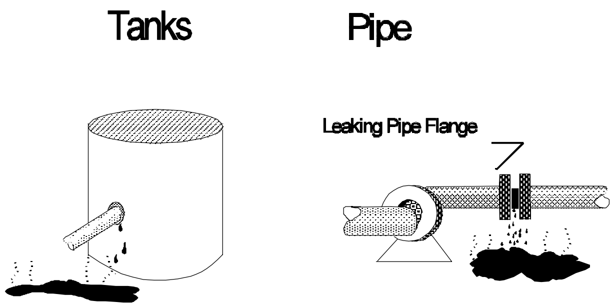
## Continuous Low Volatility Liquid Leaks - 3.8





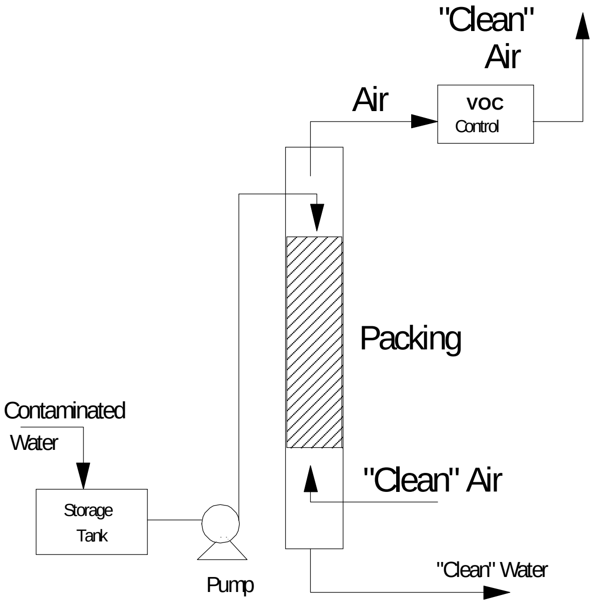
<u>Similar Releases:</u> Continuous release of liquid whose normal boiling point is above ambient temperature. A low volatility material stored at moderate to low pressure (and where the boiling point is above storage temperature) will typically be released as a liquid and form a pool or puddle on the ground. The (conservative) assumption is that the liquid evaporates at the same rate it is spilled (except when the liquid is confined by a bund dike from which liquid does not overflow). Possible applications include a (low volatility) liquid leak from a tank or a pipe.

## Instantaneous Low Volatility Liquid Leaks - 3.9



Similar Releases: Instantaneous release of liquid whose normal boiling point is above ambient temperature. A low volatility material stored at moderate to low pressure (and where the boiling point is above storage temperature) will typically be released as a liquid and form a pool or puddle on the ground. The (conservative) assumption is that the liquid evaporates at the same rate it is spilled (except when the liquid is confined by a bund dike from which liquid does not overflow). Possible applications include a (low volatility) liquid leak from a tank or a pipe.

## 4.1 Air Strippers



Similar Releases: None.

## 2.4 Determining Maximum Short-Term Ground Level Concentration

### 2.4.1 Dispersion Models used in TSCREEN

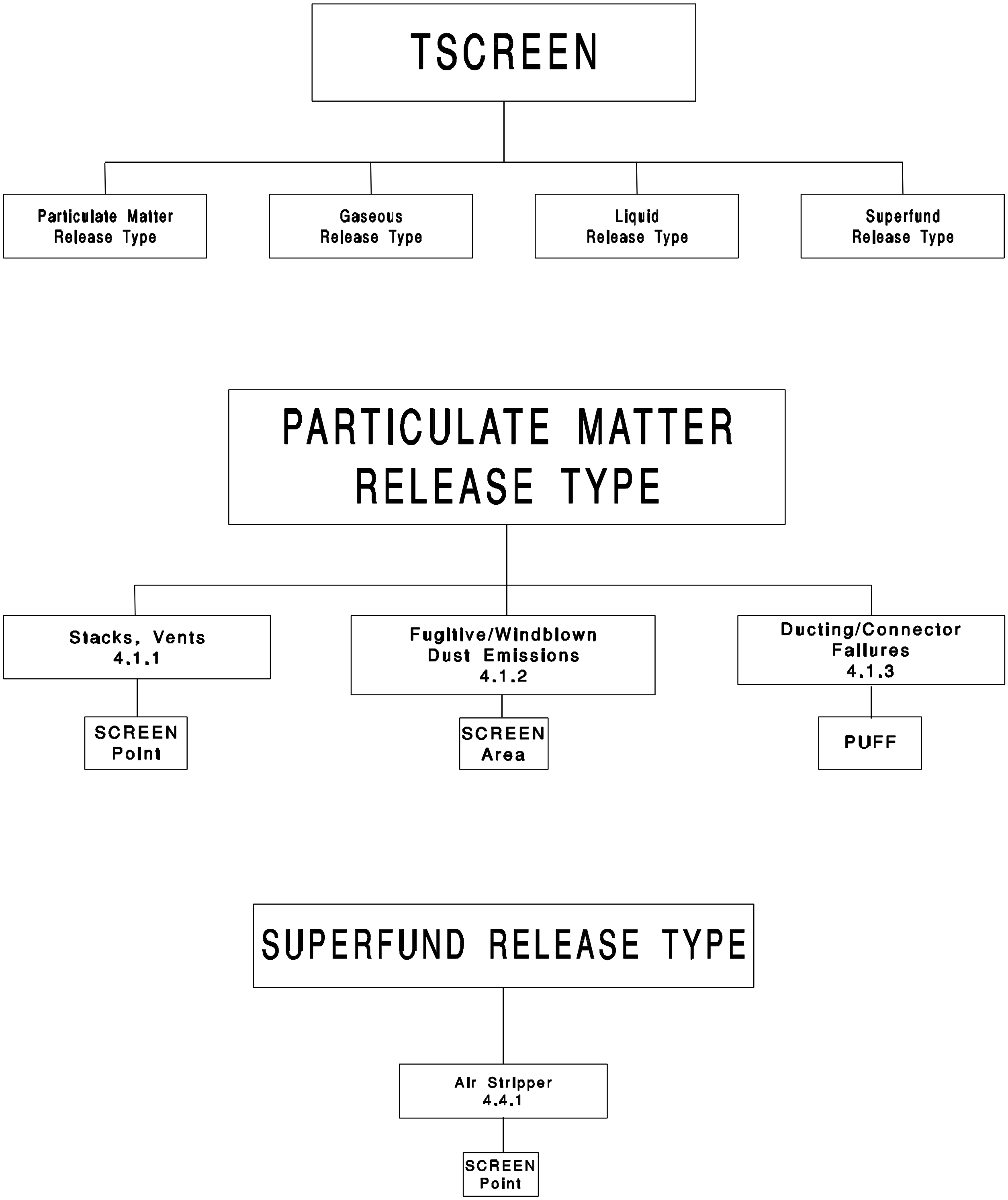
Maximum short-term ground level concentrations in TSCREEN are based on three current EPA screening models (SCREEN, RVD, and PUFF) and the Britter-McQuaid screening model. All four models are embedded in the TSCREEN model. SCREEN is a Gaussian dispersion model applicable to continuous releases of particulate matter and non-reactive, non-dense gases that are emitted from point, area, and flared sources. The SCREEN model implements most of the single source short-term procedures contained in the EPA screening procedures document (EPA, 1988c.) This includes providing estimated maximum ground-level concentrations and distances to the maximum based on a pre-selected range of meteorological conditions. In addition, SCREEN has the option of incorporating the effects of building downwash. The RVD model (EPA, 1989) provides short-term ambient concentration estimates for screening pollutant sources emitting denser-than-air gases and aerosols through vertically-directed jet releases. The model is based on empirical equations derived from wind tunnel tests and estimates the maximum ground level concentration at plume touchdown at up to 30 downwind receptor locations. The PUFF model (EPA, 1982) is used where the release is finite but smaller than the travel time (i.e., an instantaneous release.) This model is based on the Gaussian instantaneous puff equation and is applicable for neutrally buoyant non-reactive toxic air releases. The Britter-McQuaid model (1988) provides an estimate of dispersion of denser-than-air gases from area sources for continuous (plume) and instantaneous (puff) releases. Further discussion on model assumptions is given in Chapter 5.0.

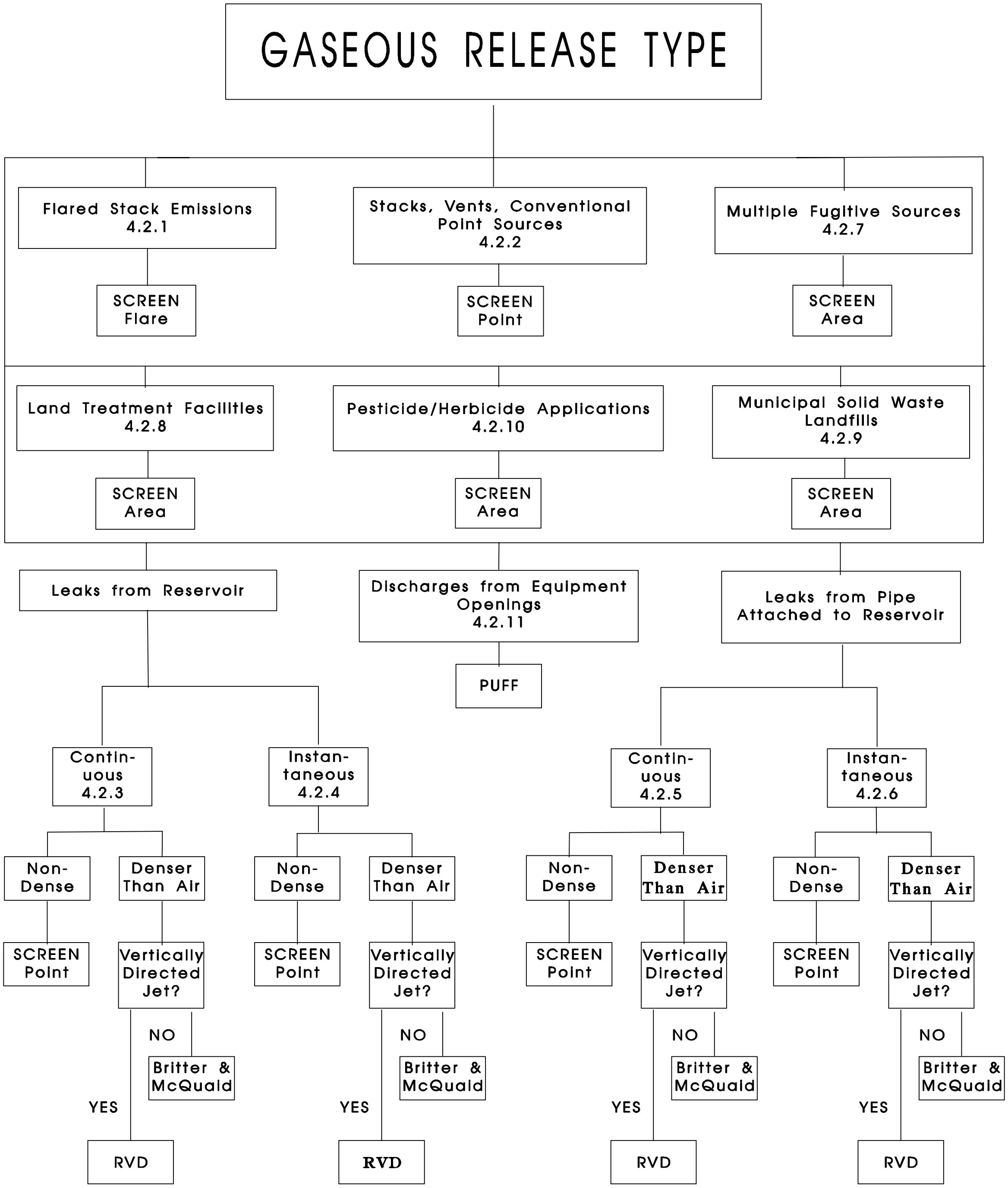
### 2.4.2 Dispersion Model Selection

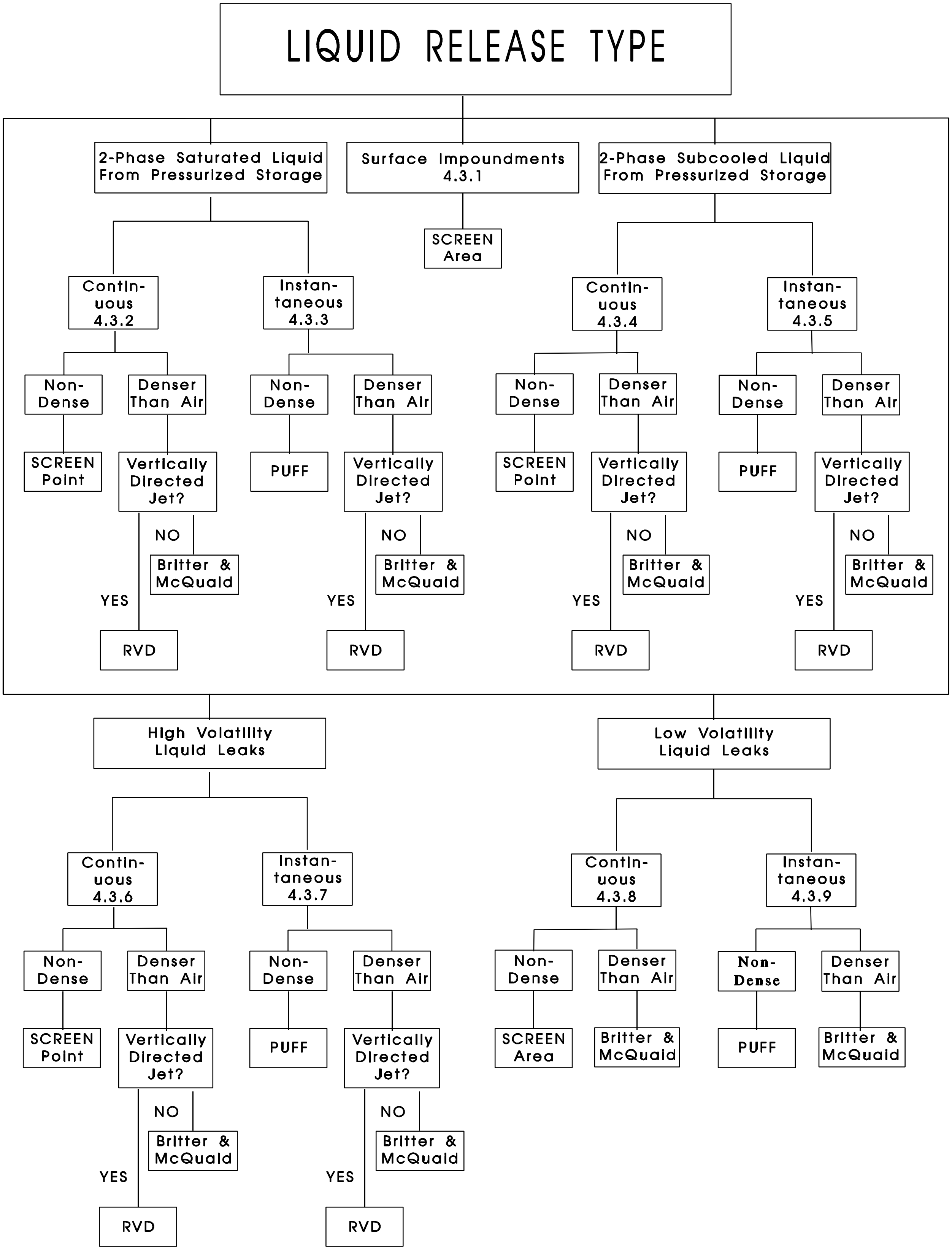
Figure 2-2 shows which screening model is associated with each scenario. In TSCREEN, ambient impacts of releases from pressurized storage vessels (and pipes) or liquid releases are evaluated using the following test. The release density $\rho_2$ (kg/m$^3$) is compared with ambient density, $\rho_{air}$ (kg/m$^3$). If the release density is more than ambient density (i.e., $\rho_2/\rho_{air} > 1$), then the release is considered denser-than-air. For denser-than-air releases (both continuous and instantaneous), TSCREEN uses the RVD model if the release is a vertically-directed jet and the Britter-McQuaid model for all other releases. For releases that are considered passive (i.e., $\rho_2/\rho_{air} \leq 1$), TSCREEN uses the SCREEN model for a continuous release and the PUFF model for an instantaneous release.

If the release density is greater than ambient density (i.e., $\rho_2/\rho_{air} > 1$), a further determination of the importance of denser-than-air behavior based on contaminant release rate and the ambient wind speed is made after calculating the Richardson number (see below). Since for many applications (e.g., planning analyses) the actual wind speed is not known, this method is not used in TSCREEN (version 3.0). The following shows how the user may approach the problem.

Figure 2-2. Model Selection




GASEOUS RELEASE TYPE
Flared Stack Emissions 4.2.1
SCREEN Flare
Stacks, Vents, Conventional Point Sources 4.2.2
SCREEN Point
Multiple Fugitive Sources 4.2.7
SCREEN Area
Land Treatment Facilities 4.2.8
SCREEN Area
Pesticide/Herbicide Applications 4.2.10
SCREEN Area
Municipal Solid Waste Landfills 4.2.9
SCREEN Area
Leaks from Reservoir
Discharges from Equipment Openings 4.2.11
PUFF
Leaks from Pipe Attached to Reservoir
Contin-uous 4.2.3
Instan-taneous 4.2.4
Contin-uous 4.2.5
Instan-taneous 4.2.6
Non-Dense
Denser Than Air
SCREEN Point
Vertically Directed Jet?
NO
Britter & McQuaid
YES
RVD


LIQUID RELEASE TYPE
2-Phase Saturated Liquid From Pressurized Storage
Surface Impoundments 4.3.1
2-Phase Subcooled Liquid From Pressurized Storage
SCREEN Area
Contin-uous 4.3.2
Instan-taneous 4.3.3
Contin-uous 4.3.4
Instan-taneous 4.3.5
Non-Dense
Denser Than Air
Non-Dense
Denser Than Air
Non-Dense
Denser Than Air
Non-Dense
Denser Than Air
SCREEN Point
Vertically Directed Jet?
PUFF
Vertically Directed Jet?
SCREEN Point
Vertically Directed Jet?
PUFF
Vertically Directed Jet?
NO
Britter & McQuaid
YES
RVD
NO
Britter & McQuaid
YES
RVD
NO
Britter & McQuaid
YES
RVD
NO
Britter & McQuaid
YES
RVD
High Volatility Liquid Leaks
Low Volatility Liquid Leaks
Contin-uous 4.3.6
Instan-taneous 4.3.7
Contin-uous 4.3.8
Instan-taneous 4.3.9
Non-Dense
Denser Than Air
Non-Dense
Denser Than Air
Non-Dense
Denser Than Air
Non-Dense
Denser Than Air
SCREEN Point
Vertically Directed Jet?
PUFF
Vertically Directed Jet?
SCREEN Area
Britter & McQuaid
PUFF
Britter & McQuaid
NO
Britter & McQuaid
YES
RVD
NO
Britter & McQuaid
YES
RVD

### 2.4.2.1 Continuous Release

1. Perform buoyancy check as a first check.

   A. Calculate the density of air using the following:

$$\rho_{air}\ '\ \frac{P_a\ M_a}{R\ T_a} \tag{2.4-1}$$

   where R = 8314 (J/kg-mole@EK). The molecular weight of air is assumed equal to 28.9 (kg/kmol), and atmospheric pressure is 101325 (Pa).

   B. If $D_2/D_{air} > 1$, then the buoyancy is negative; go to steps 2 or 3. Otherwise, buoyancy is neutral or positive and the SCREEN model for a point source should be used.

2. For a vertically directed jet release, the release Richardson number, Ri, is calculated using the following equation:

$$Ri\ '\ \left[ g \left( \frac{D_2}{D_{air}} \&1 \right) Q_m/u\ D_0\ \ D_2\ u_{10}^2\ \ (u_*/u_{10})^2 \right] \tag{2.4-2}$$

   where g is the acceleration of gravity ($m/s^2$), $D_2$ is the plume density ($kg/m^3$), $D_{air}$ is the ambient density ($kg/m^3$), $Q_m$ is the exhaust gas mass flow rate (kg/s), u is the wind velocity at the top of the stack (m/sec), $D_0$ is the stack diameter (m), $u_{10}$ is the wind velocity at 10m above the ground, $u_*/u_{10}$ is the ratio of friction velocity (m/s) to the wind speed at 10m (m/s). In version 2.0 of the RVD model, this ratio is assumed to equal 0.06 for all atmospheric stability classes. The value of u is calculated via the equation:

$$u\ '\ u_{10}\ \ (h_s/10)^p \tag{2.4-3}$$

   where $h_s$ is the stack height (m) and p is the wind speed profile exponent, which varies as a function of atmospheric stability. By using g = 9.81 $m/s^2$, u = 1 m/sec, $u_*/u_{10}$ = 0.06, $u_{10}$ = 1 m/s, the Richardson number is reduced to:

$$R\,i\ '\ 2{,}725\left(\frac{D_2}{D_{air}}\&1\right)\frac{Q_m}{D_1\ D_2} \qquad (2.4\text{-}4)$$

U = 1 m/sec was chosen as a screening method for determining denser-than-air effects. However, denser-than-air effects do not always correspond to largest hazard extent.

3. For other denser-than-air releases, Britter-McQuaid recommend that denser-than-air effects be ignored if:

$$U_r \Big/ \left(\frac{D_2\ \&\ D_a}{D_a}\right)\frac{g\ Q_m}{D_2\ D\ U_r^3}<0.005 \qquad (2.4\text{-}5)$$

where g is the acceleration of gravity (m/$s^2$), E is the release rate in kg/s, D is the (low-momentum) horizontal dimension of the source(m), $U_r$ is the wind speed at 10 m (m/s), $D_2$ is the discharge (depressurized) density of air (kg/$m^3$). See Section 5.0 for additional explanation.

Thus, if the wind speed during the release is known, then it can be inserted in the equation and a determination can be made whether a dense gas model should be used. Selections are summarized in the table below:

**TABLE 2-2**
**MODEL SELECTION FOR CONTINUOUS RELEASE**

| Continuous | Criteria | | Models |
|---|---|---|---|
| 1. Buoyancy Check | $D_2/D_{air} \leq 1$ | Passive | SCREEN |
| | $D_2/D_{air} > 1$ | (Go to '2. or 3.') | |
| 2. Vertically Directed Jet | Yes - Ri > 30 | Dense | RVD |
| | Ri < 30 | Nondense | SCREEN |
| | No - (Go to '3. Other') | | |
| 3. Other | Ri < $(1/6)^3$ | Dense | B-M |
| | Ri > $(1/6)^3$ | Passive | SCREEN |

### 2.4.2.2 Instantaneous Release

1. Perform buoyancy check as a first check.

   A. Calculate the density of air using equation 2.4-1.

B. If $D_2/D_{air} > 1$, then the buoyancy is negative; go to step 2 or 3. Otherwise, buoyancy is positive and the PUFF model will be used.

2. For a vertically directed jet release, calculate the release Richardson number as shown in equation 2.4-4.

3. For other denser-than-air releases, Britter-McQuaid recommend that denser-than-air effects be ignored if:

$$\left[\left(\frac{D_2 \ \& \ D_{air}}{D_{air}}\right) \frac{g\ (E_t/D_2)^{1/3}}{U_r^2}\right]^{1/2} \ \# \ 0.2 \tag{2.4-7}$$

where g is the acceleration of gravity (m/s$^2$), $D_2$ is the discharge density (kg/m$^3$), $D_{air}$ is the ambient density (kg/m$^3$), $E_t$ is the total amount of material released (kg), and $U_r$ is the wind speed at 10 m (m/s).

If denser-than-air effects are determined to be important, then the Britter-McQuaid model is used. Otherwise, the release is considered non-dense (passive) and the PUFF model applies. Selections are summarized in the table below:

**TABLE 2-3**
**MODEL SELECTION FOR INSTANTANEOUS RELEASE**

| Continuous | Criteria | | Models |
|---|---|---|---|
| 1. Buoyancy Check | $D_2/D_{air} \leq 1$ | Passive | PUFF |
| | $D_2/D_{air} > 1$ | (Go to '2. or 3.') | |
| 2. Vertically Directed Jet | Yes - Ri > 30 | Dense | RVD |
| | Ri < 30 | Nondense | PUFF |
| | No - (Go to '3. Other') | | |
| 3. Other | BM Criteria > 0.2 | Dense | B-M |
| | BM Criteria ≤ 0.2 | Passive | PUFF |

## 2.5 Considerations for Time-Varying and Time-Limited Releases

A release is considered time-varying if the release rate varies with time. Typically, this behavior might be expected because the reservoir pressure and temperature vary with time. As discussed in Chapter 4, reservoir pressure and temperature would be expected to vary with time if the release rate was very large in comparison with the reservoir volume. For these conditions, the release rate decreases with time so that the maximum release rate can be determined from initial reservoir (stagnation) conditions. Therefore, a screening method which uses the initial reservoir conditions would be expected to overestimate the release rate; this overestimation could be quite large depending on the situation.

A release is considered (only) time-limited if the release rate is constant over the duration of the release, but the release duration is short in comparison with other important time scales (e.g., the averaging time used to assess the toxicity, or the cloud travel time to a downwind position of interest). Typically, this behavior might be expected if, for example, an automatic shutoff system is assumed to stop the release after a specified (generally short) time period. The release rate for time-limited releases can still be estimated using the screening methods outlined in Chapter 4; the total amount of material released Q could then be estimated by $Q_m T_d$ where $Q_m$ is the release rate and $T_d$ is the release duration. (i.e., $Q = Q_m T_d$)

Finally, a release may be both time-varying and time-limited. As in the time-varying case, a screening method which uses the initial reservoir conditions can be used to (over) estimate the release rate, and the total amount released Q could again be estimated by $Q_m T_d$ where $Q_m$ is the release rate and $T_d$ is the release duration. Of course, the (estimated) total amount released can not exceed the amount of material on hand before the release.

## 2.6 <u>Denser-Than-Air Materials</u>

In this workbook, the discussion of gas leaks are for materials stored as a gas which remains entirely in the gas phase throughout the depressurization process. Two-phase leaks can result for materials which are stored under pressure and will depressurize when released to the atmosphere. This depressurization will then result in the formation of two contaminant phases (saturated liquid and vapor). Two-phase leaks occur for gases which cool so that condensation occurs during the depressurization process, and for high volatility liquids (liquids whose normal boiling point is below the ambient temperature) which are stored typically above ambient pressure. For screening purposes, a release from the liquid space is considered to form an aerosol when the liquid is stored at a temperature above its boiling point (and ambient pressure); this assumption becomes more unrealistic as the storage pressure approaches ambient pressure (or equivalently as the storage temperature approaches its boiling point).

A high volatility liquid is considered to be a material whose boiling point is below the ambient temperature; a high volatility material will be released as a liquid if the storage pressure is near ambient pressure whereas release from high pressure storage will result in aerosol formation; aerosol formation is assumed when the liquid is stored at a temperature above its (depressurized) boiling point. In contrast, a low volatility liquid is considered to be a material whose boiling point is above the ambient temperature; a low volatility material stored at moderate to low pressure (and where the boiling point is above the storage temperature) will typically be released as a liquid and form a pool or puddle on the ground. Releases of low volatility materials typically do not exhibit denser-than-air effects. Table 2-4 summarizes this information.

**TABLE 2-4**
**(DEPRESSURIZED) RELEASE PHASE FOR SCREENING PURPOSES***

| Storage Phase | (Depressurized) Release Phase |
|---|---|
| Gas | Gas<br>Aerosol possible (when $T_2 < T_b$) |
| High Volatility Liquid<br>($T_b < T_a$) | Liquid ($T_b \geq T_1$)<br>Aerosol($T_b < T_1$) |
| Low Volatility Liquid<br>($T_b \geq T_a$) | Liquid |

* where $T_a$ is ambient temperature, $T_b$ is the (ambient pressure) contaminant boiling point temperature, $T_1$ is the (initial) storage temperature, and $T_2$ is the depressurized release temperature.

In this workbook, two-phase leaks are assumed to occur for saturated liquids which are liquids stored at a (elevated) pressure equal to their vapor pressure for the storage temperature. Subcooled liquids are liquids stored at a pressure above their vapor pressure for the storage temperature.

## 2.7 Dispersion Screening Estimates for Denser-Than-Air Contaminants

A lot of effort has been focused over the past few years on estimating (by physical and mathematical models) the dispersion of denser-than-air contaminants in the atmosphere (as part of the overall concern of hazard assessment). Because physical models (wind tunnels) are not used directly for the purposes of a screening procedure as is desired for this discussion, direct use of physical models are not discussed here. Mathematical models (i.e., models which can be reduced to mathematical expressions) can be divided among three categories:

1. Complex models are typically based on the solution of the conservation equations of mass, momentum, and (thermal) energy;

they make no *a priori* assumptions about the distribution (shape) of the important dependent variables (such as contaminant concentration). Complex models (theoretically) have the capability of (rigorously) taking into account the effect of many complicating factors (such as the influence of obstacles); these capabilities are largely untested at present. Complex models typically are costly in terms of preparation time, computation time, and user sophistication; as such they are obviously unsuited for use in a screening program.

2. <u>Similarity models</u> are also based on the solution of the same conservation equations as complex models; however in contrast to complex models, similarity models make assumptions about the distribution (shape) of important dependent variables. Typically, similarity models do not take into account the influence of obstacles. However, many similarity models have been extensively compared to the large number of recent field test programs aimed at studying denser-than-air contaminants; some similarity models (e.g., DEGADIS) have been found to reproduce the range of the field results quite well. Unfortunately, this success comes at the (modest) cost of preparation time and user sophistication which may not entirely fit the mold of a screening program, but in fact, this "state-of-the-art" implies that proven similarity models should be the next tool applied if a screening program identifies a release scenario as a potential problem.

3. <u>Correlation models</u> are based on a dimensional analysis of the important parameters which influence the important dependent variables (e.g., distance to a given concentration level and area covered by a plume or puff) and on information gathered from field test results, laboratory results, and other mathematical models. The stated objective of a correlation-based model is to fit the observed data (on which it is based) within a certain factor (typically two). Because of the nature of a simple correlation, this approach is well suited for use in a screening program. The RVD and the Britter-McQuaid models are derived from correlations based on different wind tunnel experiments.

The screening techniques presented here are designed to identify release scenarios which may violate safety or health criteria. The simplifying assumptions inherent in these screening methods are specifically aimed at decreasing the amount of information required from the user and decreasing the computation time and sophistication. More refined assessment techniques should be applied to a release scenario which is identified by these screening procedures as violating safety or health criteria. As with any hazard assessment, these screening techniques should be applied with due caution.

Refined release rate estimates may involve more detailed analysis of the specifics of the release as well as application of more refined engineering methods (e.g., Lees (1980) and Perry et al. (1984)). Refined atmospheric dispersion models which account for denser-than-air contaminant behavior (such as DEGADIS; Spicer and Havens (1989)) can be applied. It should be noted that the screening assumptions inherent in the methods suggested by Britter and McQuaid (1989) and the RVD model (EPA, 1989) may become less justifiable for contaminants with more complicated thermodynamic behavior after release to the atmosphere -- particularly ammonia ($NH_3$), liquefied natural gas (LNG), and hydrogen fluoride (HF); more sophisticated atmospheric dispersion models may be used to account for such circumstances.

# 3.0 SUPPORT DATA FOR SCREENING ESTIMATES

Simulations of air toxic releases require information on the meteorological conditions at the time of release as well as physical and chemical parameters describing the materials being released.

## 3.1 Meteorological Data

Computational procedures for estimating concentrations require data on wind speed and direction, temperature and atmospheric pressure. These data are normally collected at National Weather Service stations and some military installations on an hourly basis. Stability and turbulence parameters can be estimated from cloud data as described below. A record of these is available from the National Climatic Data Center, Asheville, North Carolina and also from the EPA's SCRAM BBS. On-site meteorological data are sometimes recorded at air quality monitoring sites. Use of the on-site data with proper quality assurance procedures as described in On-site Meteorological Program Guidance for Regulatory Modeling Applications (EPA, 1987c) is preferred.

### 3.1.1 Wind Speed and Direction

Wind speed and direction data are required to estimate short-term peak concentrations. Wind speed is used to determine (1) plume dilution, (2) plume rise and (3) mass transfer in evaporation models. These factors, in turn, affect the magnitude of, and distance to, the maximum ground-level concentration.

Most wind data are collected near ground level. The wind speed at release height can be estimated by using the following power law equation:

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

where: u = the wind speed (m/s) at release height h (m),
$u_1$ = the wind speed at the anemometer height $z_1$ (m),
p = the stability-related exponent from Table 3-1.

## TABLE 3-1
## WIND PROFILE EXPONENT AS A FUNCTION OF ATMOSPHERIC STABILITY

| Stability Class | Rural Exponent | Urban Exponent |
|---|---|---|
| A | 0.07 | 0.15 |
| B | 0.07 | 0.15 |
| C | 0.10 | 0.20 |
| D | 0.15 | 0.25 |
| E | 0.35 | 0.30 |
| F | 0.55 | 0.30 |

The wind direction is an approximation for 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.

### 3.1.2 Stability and Turbulence

Stability categories, as depicted in Tables 3-1 and 3-2, are indicators of atmospheric turbulence. The stability category at any given time depends upon thermal turbulence (caused by heating of the air at ground level) and mechanical turbulence (a function of wind speed and surface roughness). Stability is generally estimated by a method given by Turner (1970), which requires information on solar elevation angle, cloud cover, cloud ceiling height, and wind speed (see Table 3-2).

## TABLE 3-2
## KEY TO STABILITY CATEGORIES

| Surface Wind Speed at Height of 10m (m/sec) | Day | | | Night* | |
|---|---|---|---|---|---|
| | Incoming Solar Radiation** (Insolation) | | | Thinly Overcast or ≥ 4/8 Low Cloud Cover | ≤ 3/8 Cloud Cover |
| | Strong | Moderate | Slight | | |
| <2 | A | A-B | B | F | F |
| 2-3 | A-B | B | C | E | F |
| 3-5 | B | B-C | C | D | E |
| 5-6 | C | C-D | D | D | D |
| >6 | C | D | D | D | D |

The neutral class (D) should be assumed for all overcast conditions during day or night.

* Night is defined as the period from one hour before sunset to one hour after sunrise.

** Appropriate insolation categories may be determined through the use of sky cover and solar elevation information as follows:

| Sky Cover (Opaque or Total) | Solar Elevation Angle > 60° | Solar Elevation Angle ≤ 60° But > 35° | Solar Elevation Angle ≤ 35° But > 15° |
|---|---|---|---|
| 4/8 or Less or Any Amount of High Thin Clouds | Strong | Moderate | Slight |
| 5/8 to 7/8 Middle Clouds (7000 feet to 16,000 foot base) | Moderate | Slight | Slight |
| 5/8 to 7/8 Low Clouds (less than 7000 foot base) | Slight | Slight | Slight |

The solar elevation angle is a function of the time of year and the time of day, and is presented in charts in the

Smithsonian Meteorological Tables (List, 1968). The hourly weather observations of the National Weather Service include cloud cover, cloud ceiling height, and wind speed. Methods for estimating atmospheric stability categories from on-site data are provided in EPA modeling guidelines.

Friction velocity ($u_*$) represents mechanical turbulence due to wind flow over the surface and is used in calculating the release Richardson number. Friction velocity is a function of stability, decreasing with increasing stability. An approximation of friction velocity under neutral stability conditions and assuming a roughness length of 1 cm is:

$$u_* = 0.06u$$

where u is the wind speed (m/s) at a height of 10 m.

### 3.1.3 Temperature

Ambient air temperature must be known in order to calculate the amount of rise of a buoyant plume and to calculate evaporation rates.

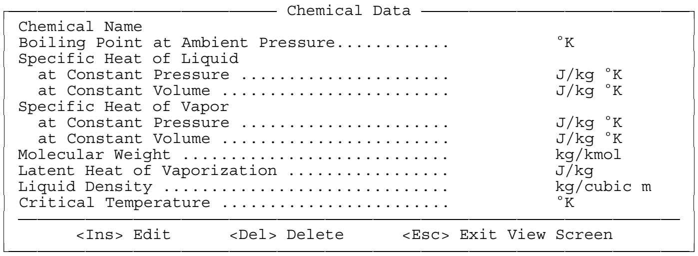
### 3.1.4 Atmospheric Pressure

Atmospheric pressure data are used in calculating gas and liquid release rates from storage and process vessels and pipes.

## 3.2 Chemical and Physical Parameters

Numerous chemical and physical properties of contaminants are required to perform some of the emission estimation techniques presented. TSCREEN includes a chemical database which contains values that can be automatically returned to data entry fields. For information on the use of the Chemical Database see Appendix D - Running TSCREEN. A list of the chemical properties from TSCREEN's Chemical Database is shown in Figure 3-1.

**Figure 3-1. TSCREEN's Chemical Database**



```
                          Chemical Data
Chemical Name
Boiling Point at Ambient Pressure............          °K
Specific Heat of Liquid
  at Constant Pressure .....................          J/kg °K
  at Constant Volume .......................          J/kg °K
Specific Heat of Vapor
  at Constant Pressure .....................          J/kg °K
  at Constant Volume .......................          J/kg °K
Molecular Weight ...........................          kg/kmol
Latent Heat of Vaporization ................          J/kg
Liquid Density .............................          kg/cubic m
Critical Temperature .......................          °K
-----------------------------------------------------------------
      <Ins> Edit      <Del> Delete      <Esc> Exit View Screen
```

The complexity and diversity of chemical and physical behavior of many air toxic substances make it critical that the correct input parameters are obtained. These parameters can be found in compendiums of physical and chemical characteristics. Three of the more comprehensive sources of information are listed in the reference section.

The user should be cautioned that a characteristic "constant" used in modeling may have different values depending on the reference from which the parameter was obtained.

## 4.0 SCENARIOS AND TECHNIQUES FOR RELEASE AND EMISSIONS ESTIMATES

Techniques for estimating air toxics emissions must be capable of treating a large variety of potential release scenarios. This section is intended to help the user identify the applicable release scenario, determine release and emission rates, and to guide the user through the scenario inputs into TSCREEN. Scenarios addressing various types of particulate, gaseous, and liquid releases are presented in this workbook. In addition there are scenarios typically found at Superfund sites. If the appropriate scenario choice is not obvious, consult the descriptions of similar releases that accompanies the graphical illustrations shown in Section 2.3 or the EPA Regional Modeling Contacts.

Since many various processes and sources have the potential for toxic chemical releases, the scenarios do not cover all possible release, emission, and dispersion combinations. In all applications, the characterization of emissions is a critical step which is best met through a complete and accurate measurement program. In practical applications, measured data are seldom available and the user is left to techniques such as those presented in this section, data from existing inventories, emission factors, or process specific material balance estimates.

Some of the numerous sources of existing data are permits and files, technical literature, and SARA Title III reporting forms. A new data source summarizing regulatory data is the National Air Toxics Information Clearinghouse (NATICH) and Data Base. Information on NATICH is available through the EPA Regional Air Toxics Contacts, Air/Superfund Coordinators and :

Pollution Assessment Branch (MD-12)
U.S. Environmental Protection Agency
Research Triangle Park, NC 27711
(919) 541-0850

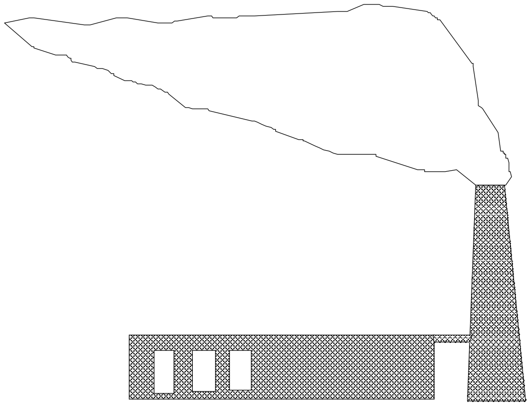
For some sources, mass balances are used to estimate releases when conservative assumptions concerning quantities of input and output streams are made. The amounts entering and/or leaving a process can be measured or estimated. A mass balance can then be performed on the process as a whole or on the subprocess. For processes where material reacts to form a product or is significantly changed, use of mass balance may be too difficult for estimating emissions and the use of emission factors may be more appropriate.

When measured or plant specific data are unavailable, the user is advised to review emission factors developed for specific processes. Appendix A provides a description of sources of emission factors. Emission factors represent average conditions and do not necessarily provide a conservative estimate of total emission rate.

## 4.1 Particulate Matter Release

A particulate matter release is a release of any solid material such as particulates, dust, or ash.

### 4.1.1 Releases from Stacks, Vents



Similar Releases: Continuous emissions of particulate matter from vertical stacks and pipes or conventional point sources and some process vents when emission flow rates and temperature are known. Combustion sources and chemical reactors are typical emission sources that may emit such pollutants through stacks. These releases may also be due to a process failure such as a rupture disk release or failure of control equipment.

Discussion:

Emission rates from such sources can be determined through source testing using EPA Reference Methods (40 CFR Part 60 Appendix A) or "Screening Methods for the Development of Air Toxics Emission Factors", EPA-450/4-91-021 or process calculations. If source-specific emissions are not available, representative emission factors can be substituted. Emission factors are available for individual toxic compounds (Appendix A). Otherwise, factors determined by compiling extensive source test results using EPA Reference Methods are reported in AP-42.

Since the input is source specific, there is no input section for this scenario. If this scenario is selected, TSCREEN directly accesses the SCREEN model input section for a point source. See Section 5.1.1 for a complete list of inputs.

Limitations and Assumptions:

- For screening, particulate deposition is assumed to be insignificant.

Input Information:

D diameter at release point (m)
V volumetric flow rate ($m^3/s$)

### 4.1.1.1 Procedure:

1. **Exit Velocity.** Calculate the exit velocity $V_s$ (m/s) through a stack as follows:

$$V_s = \frac{4\,V}{\pi\,D^2} \qquad (4.1.1\text{-}1)$$

### 4.1.1.2 Example: Cadmium emission

Discussion:

A facility emits 0.0029 tons per year of cadmium through a stack that is 16 meters above ground. The stack inside diameter is 0.1 meters, the stack exit temperature is 298 °K, and the volumetric flow rate is 0.14 $m^3/s$. The stack is adjacent to a square building with height and building dimensions equal to 19 m. The site is classified as rural, with complex terrain being present. Concentrations at a receptor located 25 meters from the stack is required.

The following information will be required to use the SCREEN model (see Section 5.1.1):

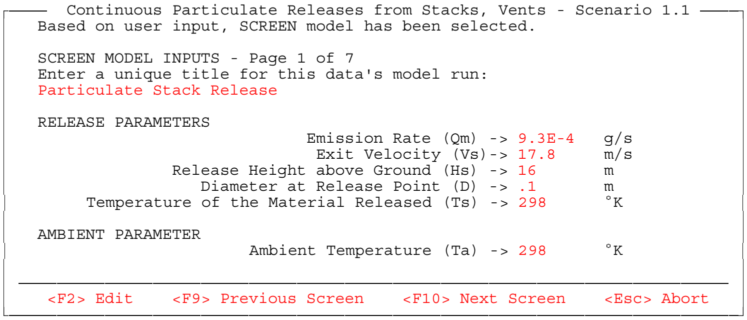
$B_{max}$ building maximum horizontal dimension (19 m)
$B_{min}$ building minimum horizontal dimension (19 m)
D diameter at release point (0.1 m)
$H_s$ release height above ground (16 m)
$H_b$ building height (19 m)
$Q_m$ emission rate (0.0029 tons per year is equal to $9.3 \times 10^{-4}$ g/s)
$T_s$ temperature of the material released (298 °K)
$T_a$ ambient temperature (298 °K)
V volumetric flow rate (0.14 $m^3/s$)

Procedure:

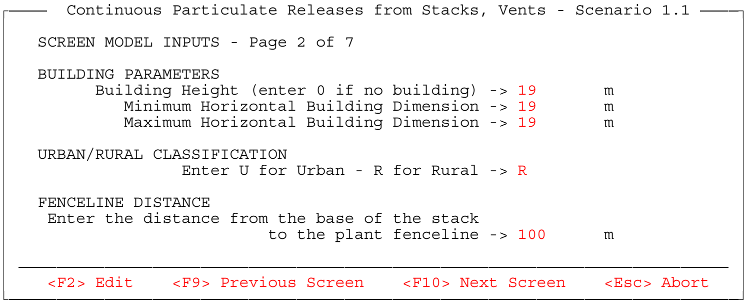
1. **Exit Velocity.** Calculate the stack gas exit velocity from Equation (4.1.1-1):

$$V_s = \frac{4 \cdot 0.14\ m^3/s}{3.14\ (.1)^2\ m^2} = 17.8\ m/s$$

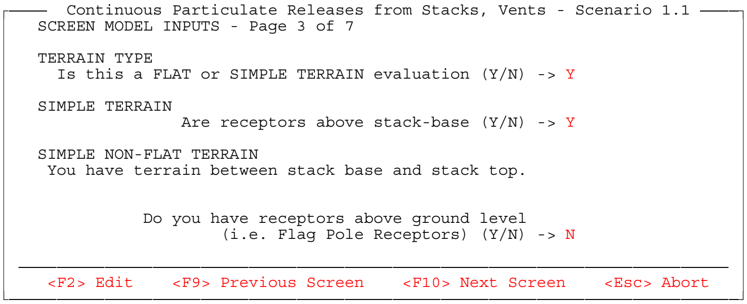
Data entry in the TSCREEN model for this example is shown below:



```
  Continuous Particulate Releases from Stacks, Vents - Scenario 1.1
 Based on user input, SCREEN model has been selected.

 SCREEN MODEL INPUTS - Page 1 of 7
 Enter a unique title for this data's model run:
 Particulate Stack Release

 RELEASE PARAMETERS
                            Emission Rate (Qm) -> 9.3E-4   g/s
                             Exit Velocity (Vs)-> 17.8     m/s
              Release Height above Ground (Hs) -> 16       m
                 Diameter at Release Point (D) -> .1       m
      Temperature of the Material Released (Ts) -> 298     °K

 AMBIENT PARAMETER
                      Ambient Temperature (Ta) -> 298      °K

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
  Continuous Particulate Releases from Stacks, Vents - Scenario 1.1

 SCREEN MODEL INPUTS - Page 2 of 7

 BUILDING PARAMETERS
       Building Height (enter 0 if no building) -> 19      m
          Minimum Horizontal Building Dimension -> 19      m
          Maximum Horizontal Building Dimension -> 19      m

 URBAN/RURAL CLASSIFICATION
                Enter U for Urban - R for Rural -> R

 FENCELINE DISTANCE
  Enter the distance from the base of the stack
                         to the plant fenceline -> 100     m

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
  Continuous Particulate Releases from Stacks, Vents - Scenario 1.1
 SCREEN MODEL INPUTS - Page 3 of 7

 TERRAIN TYPE
   Is this a FLAT or SIMPLE TERRAIN evaluation (Y/N) -> Y

 SIMPLE TERRAIN
                Are receptors above stack-base (Y/N) -> Y

 SIMPLE NON-FLAT TERRAIN
  You have terrain between stack base and stack top.


            Do you have receptors above ground level
                    (i.e. Flag Pole Receptors) (Y/N) -> N

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

2. In this example, there are receptors at or below stack top; therefore, "Y" is entered for the "terrain type" question.

3. In this example, there are receptors above stack base; therefore, "Y" is entered, for the "simple terrain" question.

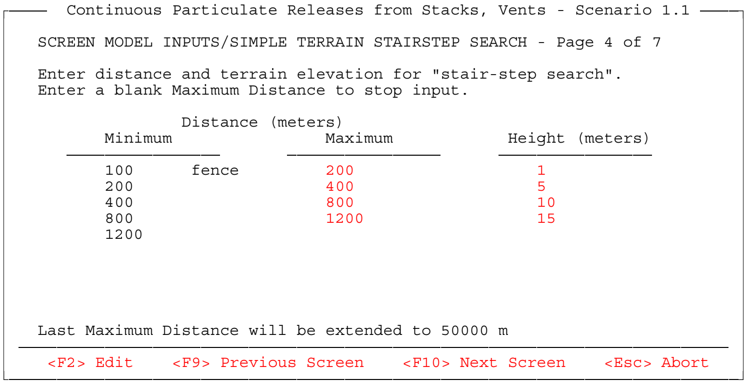
   Since "Y" was entered, proceed to step 5.

4. The question "Do you have specific locations where you would like pollution concentrations calculated (Y/N)" will be skipped at this point, but it will be asked after the user has finished entering terrain elevations on page 4 of 7.

5. In this example, receptors are at ground level; therefore, "N" is entered for the "flag pole receptor" question.

   Since "Y" was entered in Step 3, proceed to Step 7.

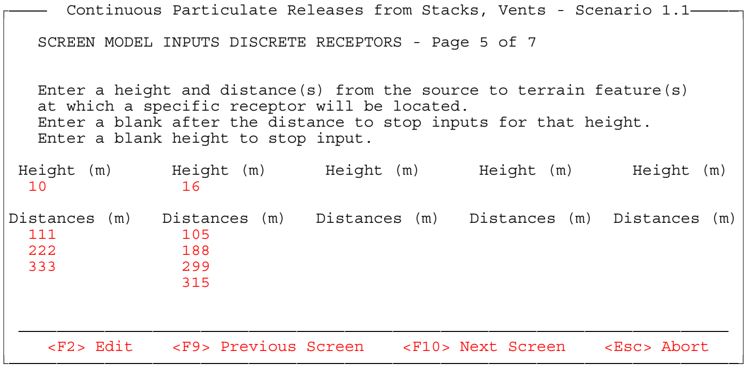
6. The prompt "You have completed simple terrain inputs. Do you want to continue with complex terrain (Y/N)" will be skipped at this point but will appear later.



```
Continuous Particulate Releases from Stacks, Vents - Scenario 1.1

SCREEN MODEL INPUTS/SIMPLE TERRAIN STAIRSTEP SEARCH - Page 4 of 7

Enter distance and terrain elevation for "stair-step search".
Enter a blank Maximum Distance to stop input.

               Distance (meters)
    Minimum                Maximum            Height (meters)

    100      fence         200                1
    200                    400                5
    400                    800                10
    800                    1200               15
    1200

Last Maximum Distance will be extended to 50000 m
```

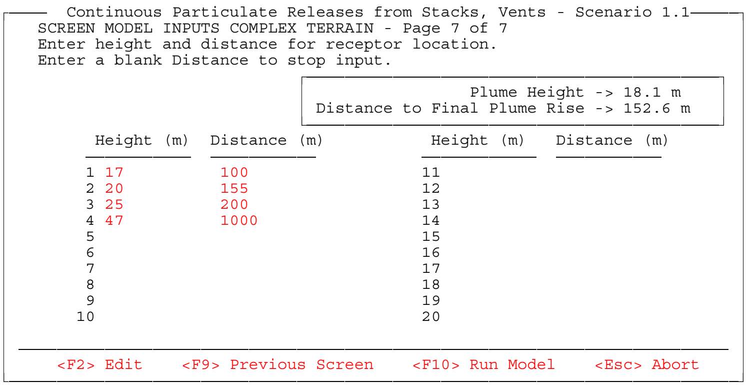
7. In this example, the terrain elevations for four distance ranges are shown above. After entries are complete a window will appear with the prompt listed in Step 4.

   In this example, there are specific locations of interest; therefore, proceed to Step 8.



```
Continuous Particulate Releases from Stacks, Vents - Scenario 1.1

SCREEN MODEL INPUTS DISCRETE RECEPTORS - Page 5 of 7

Enter a height and distance(s) from the source to terrain feature(s)
at which a specific receptor will be located.
Enter a blank after the distance to stop inputs for that height.
Enter a blank height to stop input.

 Height (m)      Height (m)      Height (m)      Height (m)      Height (m)
  10              16

Distances (m)   Distances (m)   Distances (m)   Distances (m)  Distances (m)
  111             105
  222             188
  333             299
                  315
```

8. In this example, the specific locations of interest are at distances associated with terrain heights shown in the figure above.



```
 Continuous Particulate Releases from Stacks, Vents - Scenario 1.1
   SCREEN MODEL INPUTS COMPLEX TERRAIN - Page 7 of 7
   Enter height and distance for receptor location.
   Enter a blank Distance to stop input.
                                                      Plume Height -> 18.1 m
                                       Distance to Final Plume Rise -> 152.6 m

         Height (m)  Distance (m)           Height (m)  Distance (m)

         1 17        100                    11
         2 20        155                    12
         3 25        200                    13
         4 47        1000                   14
         5                                  15
         6                                  16
         7                                  17
         8                                  18
         9                                  19
        10                                  20

     <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

9. In this example, terrain height for receptors above stack top and distances to those heights are shown in the figure above. The figure above shows that final plume height is 18.1 m and the distance to final plume rise is 152.6 m. This information is useful in determining at what elevation the plume will impact terrain and the user may wish to add other receptor heights at this elevation to ensure calculating the maximum concentration.

   After the complex terrain inputs have been entered, TSCREEN runs the SCREEN model for a point source.

The SCREEN model output is displayed below:

```
1                                                                    11-30-92
                                                                     15:05:25
  *** SCREEN-1.2 MODEL RUN ***
  *** VERSION DATED  90XXX ***

 Particulate Stack Release

 COMPLEX TERRAIN INPUTS:
    SOURCE TYPE           =    POINT
    EMISSION RATE (G/S) =    .9300E-03
    STACK HT (M)          =    16.00
    STACK DIAMETER (M)    =      .10
    STACK VELOCITY (M/S)=    17.80
    STACK GAS TEMP (K)   =   298.00
    AMBIENT AIR TEMP (K)=   298.00
    RECEPTOR HEIGHT (M) =      .00
    IOPT (1=URB,2=RUR)   =     2
1                                                                    11-30-92
                                                                     15:05:25
  *** SCREEN-1.2 MODEL RUN ***
  *** VERSION DATED  91/10 ***

 Particulate Stack Release

 SIMPLE TERRAIN INPUTS:
    SOURCE TYPE             =    POINT
    EMISSION RATE (G/S)     =    .9300E-03
    STACK HEIGHT (M)        =    16.00
    STK INSIDE DIAM (M)     =      .10
    STK EXIT VELOCITY (M/S)=  17.8000
    STK GAS EXIT TEMP (K)   =   298.00
    AMBIENT AIR TEMP (K)    =   298.00
    RECEPTOR HEIGHT (M)     =      .00
    IOPT (1=URB,2=RUR)      =     2
    BUILDING HEIGHT (M)     =    19.00
    MIN HORIZ BLDG DIM (M) =    19.00
    MAX HORIZ BLDG DIM (M) =    19.00


      ***************************************
      *** SUMMARY OF SCREEN MODEL RESULTS ***
      ***************************************

  CALCULATION         MAX CONC     DIST TO    TERRAIN
   PROCEDURE         (UG/M**3)     MAX (M)     HT (M)
 --------------     -----------   -------    -------
 SIMPLE TERRAIN       1.396          105.        16.
```

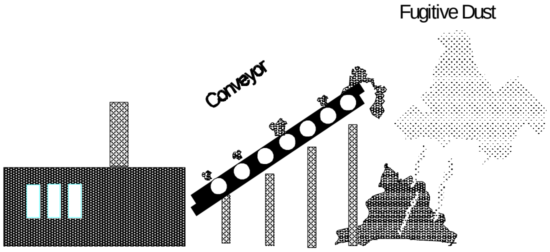
```
COMPLEX TERRAIN     3.204          100.       17. (24-HR CONC)

BUILDING CAVITY-1   1.717           28.       --  (DIST = CAVITY LENGTH)
BUILDING CAVITY-2   1.717           28.       --  (DIST = CAVITY LENGTH)


***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************


BUOY. FLUX =     .00 M**4/S**3;  MOM. FLUX =     .79 M**4/S**2.


FINAL STABLE PLUME HEIGHT (M) =   18.1
DISTANCE TO FINAL RISE (M)    =  152.6

                         *VALLEY 24-HR CALCS*   **SIMPLE TERRAIN 24-HR CALCS**
 TERR         MAX 24-HR              PLUME HT             PLUME HT
  HT    DIST    CONC        CONC    ABOVE STK    CONC    ABOVE STK    U10M UST
 (M)    (M)   (UG/M**3)   (UG/M**3)  BASE (M)  (UG/M**3)  HGT (M)  SC   (M/S)
----- ------- ----------  ----------  ------   ----------  ------  -- ---- ---
  17.    100.  3.204       .1377E-03    18.1    3.204         2.1   6  2.0  2.
  20.    155.  .4536E-02   .4536E-02    18.1    .0000          .0   0   .0   .
  25.    200.  .1232E-01   .1232E-01    18.1    .0000          .0   0   .0   .
  47.   1000.  .1047E-01   .1047E-01    18.1    .0000          .0   0   .0   .

BUOY. FLUX =     .00 M**4/S**3;  MOM. FLUX =     .79 M**4/S**2.

*** FULL METEOROLOGY ***

**********************************
*** SCREEN AUTOMATED DISTANCES ***
**********************************

*** TERRAIN HEIGHT OF    1. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

  DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
   (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
-------  ----------  ----  -----  -----  ------  ------  ------  ------  -----
   100.   .9131        3     1.0    1.0   320.0    15.1    12.5    15.3    SS
   200.   .5068        4     1.0    1.1   320.0    15.0    19.6    21.9    SS

MAXIMUM 1-HR CONCENTRATION AT OR BEYOND   100. M:
   100.   .9131        3     1.0    1.0   320.0    15.1    12.5    15.3    SS

**********************************
*** SCREEN AUTOMATED DISTANCES ***
**********************************

*** TERRAIN HEIGHT OF    5. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

  DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
   (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
-------  ----------  ----  -----  -----  ------  ------  ------  ------  -----
   200.   .5650        4     1.0    1.1   320.0    11.0    19.6    21.9    SS
   300.   .3969        6     1.0    1.3  5000.0    11.0    22.5    22.8    SS
   400.   .3410        6     1.0    1.3  5000.0    11.0    25.7    23.3    SS

MAXIMUM 1-HR CONCENTRATION AT OR BEYOND   200. M:
   200.   .5650        4     1.0    1.1   320.0    11.0    19.6    21.9    SS

**********************************
*** SCREEN AUTOMATED DISTANCES ***
**********************************

*** TERRAIN HEIGHT OF   10. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

  DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
   (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
-------  ----------  ----  -----  -----  ------  ------  ------  ------  -----
   400.   .3688        6     1.0    1.3  5000.0     6.0    25.7    23.3    SS
   500.   .3214        6     1.0    1.3  5000.0     6.0    28.9    23.9    SS
   600.   .2840        6     1.0    1.3  5000.0     6.0    32.0    24.4    SS
   700.   .2537        6     1.0    1.3  5000.0     6.0    35.1    24.9    SS
   800.   .2289        6     1.0    1.3  5000.0     6.0    38.2    25.4    SS

MAXIMUM 1-HR CONCENTRATION AT OR BEYOND   400. M:
   400.   .3688        6     1.0    1.3  5000.0     6.0    25.7    23.3    SS

**********************************
*** SCREEN AUTOMATED DISTANCES ***
**********************************

*** TERRAIN HEIGHT OF   15. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

  DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
   (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
-------  ----------  ----  -----  -----  ------  ------  ------  ------  -----
   800.   .2352        6     1.0    1.3  5000.0     1.0    38.2    25.4    SS
   900.   .2135        6     1.0    1.3  5000.0     1.0    41.2    26.0    SS
  1000.   .1952        6     1.0    1.3  5000.0     1.0    44.2    26.5    SS
  1100.   .1795        6     1.0    1.3  5000.0     1.0    47.2    27.0    SS
  1200.   .1697        6     1.0    1.3  5000.0     1.0    50.2    26.8    SS
  1300.   .1576        6     1.0    1.3  5000.0     1.0    53.2    27.3    SS
  1400.   .1472        6     1.0    1.3  5000.0     1.0    56.1    27.7    SS
  1500.   .1379        6     1.0    1.3  5000.0     1.0    59.0    28.1    SS
  1600.   .1296        6     1.0    1.3  5000.0     1.0    61.9    28.5    SS
  1700.   .1221        6     1.0    1.3  5000.0     1.0    64.8    28.9    SS
  1800.   .1154        6     1.0    1.3  5000.0     1.0    67.7    29.2    SS
  1900.   .1093        6     1.0    1.3  5000.0     1.0    70.5    29.6    SS
  2000.   .1038        6     1.0    1.3  5000.0     1.0    73.4    30.0    SS
  2100.   .9871E-01    6     1.0    1.3  5000.0     1.0    76.2    30.4    SS
  2200.   .9406E-01    6     1.0    1.3  5000.0     1.0    79.1    30.7    SS
  2300.   .8979E-01    6     1.0    1.3  5000.0     1.0    81.9    31.1    SS
  2400.   .8584E-01    6     1.0    1.3  5000.0     1.0    84.7    31.4    SS
```

```
  2500.   .8219E-01    6     1.0    1.3  5000.0     1.0    87.5    31.8    SS
  2600.   .7881E-01    6     1.0    1.3  5000.0     1.0    90.2    32.1    SS
  2700.   .7566E-01    6     1.0    1.3  5000.0     1.0    93.0    32.5    SS
  2800.   .7273E-01    6     1.0    1.3  5000.0     1.0    95.8    32.8    SS
  2900.   .6999E-01    6     1.0    1.3  5000.0     1.0    98.5    33.1    SS
  3000.   .6743E-01    6     1.0    1.3  5000.0     1.0   101.3    33.5    SS
  3500.   .5676E-01    6     1.0    1.3  5000.0     1.0   114.8    35.0    SS
  4000.   .4874E-01    6     1.0    1.3  5000.0     1.0   128.2    36.6    SS
  4500.   .4251E-01    6     1.0    1.3  5000.0     1.0   141.5    38.0    SS
  5000.   .3755E-01    6     1.0    1.3  5000.0     1.0   154.5    39.4    SS
  5500.   .3414E-01    6     1.0    1.3  5000.0     1.0   167.5    40.0    SS
  6000.   .3081E-01    6     1.0    1.3  5000.0     1.0   180.3    41.1    SS
  6500.   .2803E-01    6     1.0    1.3  5000.0     1.0   192.9    42.3    SS
  7000.   .2566E-01    6     1.0    1.3  5000.0     1.0   205.5    43.3    SS
  7500.   .2362E-01    6     1.0    1.3  5000.0     1.0   218.0    44.4    SS
  8000.   .2186E-01    6     1.0    1.3  5000.0     1.0   230.4    45.4    SS
  8500.   .2031E-01    6     1.0    1.3  5000.0     1.0   242.7    46.4    SS
  9000.   .1895E-01    6     1.0    1.3  5000.0     1.0   254.9    47.3    SS
  9500.   .1774E-01    6     1.0    1.3  5000.0     1.0   267.0    48.2    SS
 10000.   .1667E-01    6     1.0    1.3  5000.0     1.0   279.1    49.1    SS
 15000.   .1035E-01    6     1.0    1.3  5000.0     1.0   396.2    55.8    SS
 20000.   .7368E-02    6     1.0    1.3  5000.0     1.0   508.4    61.0    SS
 25000.   .5657E-02    6     1.0    1.3  5000.0     1.0   617.0    65.5    SS
 30000.   .4583E-02    6     1.0    1.3  5000.0     1.0   722.7    69.0    SS
 40000.   .3304E-02    6     1.0    1.3  5000.0     1.0   927.0    74.6    SS
 50000.   .2564E-02    6     1.0    1.3  5000.0     1.0  1124.0    79.3    SS

MAXIMUM 1-HR CONCENTRATION AT OR BEYOND   800. M:
   800.   .2352        6     1.0    1.3  5000.0     1.0    38.2    25.4    SS

 DIST    = DISTANCE FROM THE SOURCE
 CONC    = MAXIMUM GROUND LEVEL CONCENTRATION
 STAB    = ATMOSPHERIC STABILITY CLASS (1=A, 2=B, 3=C, 4=D, 5=E, 6=F)
 U10M    = WIND SPEED AT THE 10-M LEVEL
 USTK    = WIND SPEED AT STACK HEIGHT
 MIX HT  = MIXING HEIGHT
 PLUME HT= PLUME CENTERLINE HEIGHT
 SIGMA Y = LATERAL DISPERSION PARAMETER
 SIGMA Z = VERTICAL DISPERSION PARAMETER
 DWASH   = BUILDING DOWNWASH:
           DWASH=   MEANS NO CALC MADE (CONC = 0.0)
           DWASH=NO MEANS NO BUILDING DOWNWASH USED
           DWASH=HS MEANS HUBER-SNYDER DOWNWASH USED
           DWASH=SS MEANS SCHULMAN-SCIRE DOWNWASH USED
           DWASH=NA MEANS DOWNWASH NOT APPLICABLE, X<3*LB

*********************************
*** SCREEN DISCRETE DISTANCES ***
*********************************

*** TERRAIN HEIGHT OF   10. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

  DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
   (M)    (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
-------  ----------   ----  -----  -----  ------  ------  ------  ------  -----
   111.   1.230        4     1.0    1.1   320.0     6.0    13.0    16.0    SS
   222.   .5581        4     1.0    1.1   320.0     6.0    21.2    22.5    SS
   333.   .4084        6     1.0    1.3  5000.0     6.0    23.6    22.9    SS

*********************************
*** SCREEN DISCRETE DISTANCES ***
*********************************

*** TERRAIN HEIGHT OF   16. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

  DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
   (M)    (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
-------  ----------   ----  -----  -----  ------  ------  ------  ------  -----
   105.   1.396        4     1.0    1.1   320.0      .0    12.6    15.7    SS
   188.   .7250        4     1.0    1.1   320.0      .0    18.2    20.9    SS
   299.   .4471        6     1.0    1.3  5000.0      .0    22.5    22.7    SS
   315.   .4353        6     1.0    1.3  5000.0      .0    23.0    22.8    SS

 DWASH=   MEANS NO CALC MADE (CONC = 0.0)
 DWASH=NO MEANS NO BUILDING DOWNWASH USED
 DWASH=HS MEANS HUBER-SNYDER DOWNWASH USED
 DWASH=SS MEANS SCHULMAN-SCIRE DOWNWASH USED
 DWASH=NA MEANS DOWNWASH NOT APPLICABLE, X<3*LB

 *********************************************
 *  SUMMARY OF TERRAIN HEIGHTS ENTERED FOR  *
 *    SIMPLE ELEVATED TERRAIN PROCEDURE      *
 *********************************************

      TERRAIN        DISTANCE RANGE (M)
       HT (M)       MINIMUM     MAXIMUM
      -------      --------    --------
           1.          100.        200.
           5.          200.        400.
          10.          400.        800.
          15.          800.      50000.
          10.          111.          --
          10.          222.          --
          10.          333.          --
          16.          105.          --
          16.          188.          --
          16.          299.          --
          16.          315.          --

 *** CAVITY CALCULATION - 1 ***       *** CAVITY CALCULATION - 2 ***
  CONC (UG/M**3)     =    1.717        CONC (UG/M**3)     =    1.717
  CRIT WS @10M (M/S) =     1.00        CRIT WS @10M (M/S) =     1.00
  CRIT WS @ HS (M/S) =     1.10        CRIT WS @ HS (M/S) =     1.10
  DILUTION WS (M/S)  =     1.00        DILUTION WS (M/S)  =     1.00
  CAVITY HT (M)      =    27.28        CAVITY HT (M)      =    27.28
  CAVITY LENGTH (M)  =    27.97        CAVITY LENGTH (M)  =    27.97
  ALONGWIND DIM (M)  =    19.00        ALONGWIND DIM (M)  =    19.00
```

```
**********************************
*** END OF SCREEN MODEL OUTPUT ***
**********************************
```

At 25 m from the stack, the receptor is in the cavity region and the maximum concentration is 1.72 µg/$m^3$. The maximum concentration, however, is 2.21 µg/$m^3$ at a distance of 105 m from the source in complex terrain 16 m above stack base.

### 4.1.2 Continuous Fugitive/Windblown Dust Emissions



Similar Releases: Any fugitive dust from process losses, generated by mechanical action in material handling or windblown dust. Such emissions tend to originate from a surface or a collection of small poorly defined point sources.

Discussion:

These fugitive dust releases are generalized area emissions originating from a surface or collection of small, poorly quantified point sources. Emissions are either user-specified or calculated with representative emission factors. Emission factors for fugitive dust emissions are typically found in AP-42 and are assumed to be independent of wind speed for this workbook. Toxic components can be determined using the methods described in Appendix A, item 4. This example demonstrates calculation of particulate emissions from storage piles and use of particulate matter profiles to study a specific chemical.

Limitations and Assumptions:

- Worst case emission estimates are wind speed dependent.
- For screening, particle desposition is assumed to be insignificant.

Input Information:

s percent silt content (%)
p number of days per year with more than 25 mm of precipitation (dimensionless)
w percent of time wind speed exceeds 5.4 m/s (%)
m pollutant percent of total mass (%)
D diameter of storage pile (m)

4.1.2.1 Procedure:

1. **Emission Rate.** Calculate emission rate for wind blown dust ($Q_m$) (g/s):

   A. **Emission Factor.** Calculate the aggregate storage emission factor for wind blown dust:

$$E\,(\text{kg/dy/hectare}) = 1.9\,(s/1.5)\,\frac{(365-p)}{235}\,(w/15) \qquad (4.1.2\text{-}1)$$

   B. **Area.** Calculate the area (A) ($m^2$) of the storage pile:

$$A\,(m^2) = \pi\left(\frac{D\,(m)}{2}\right)^2 \qquad (4.1.2\text{-}2)$$

   C. **Convert.** Convert the emission factor (E) in kg/dy/hectare to g/s-$m^2$:

$$E\,(\text{g/s-m}^2) = \frac{E\,(\text{kg/dy/hectare})\;1000\,(\text{g/kg})}{86400\,(\text{s/dy})\;1000\,(\text{m}^2\text{/hectare})}$$

   D. **Emission Rate.** Calculation of emission rate ($Q_m$) in g/s.

$$Q_m\,(\text{g/s}) = E\,(\text{g/s-m}^2)\,\frac{m\,(\%)}{100}\,A\,(m^2) \qquad (4.1.2\text{-}3)$$

2. Run the SCREEN model for an area source. For an explanation of inputs for the SCREEN model for an area source, see Section 5.1.2.

4.1.2.2 Example: Emission from Pile of Flyash

Discussion:

Concentration estimates at the fenceline (100 m) are required for arsenic emissions resulting from wind erosion from a circular pile of flyash (3 m high, and 10 m in diameter) at a secondary lead smelter blast furnace. Since the emissions factor is not directly applicable, conservative assumptions are made that the silt content is 50 percent, no days have precipitation in excess of 25 mm and that 20 percent of wind exceeds 5.4 m/s.

The following information will be required:

s percent silt content (50 %)
p number of days per year with more than 25 mm of precipitation (0)
w percent of time wind speed exceeds 5.4 m/s (20 %)

m percent of pollutant in total mass (.3 %)
D diameter of storage pile (10 m)

Procedure:

1. **Emission Rate.** Emissions factors for aggregate storage are available in AP-42 as are particulate matter profiles (Appendix A). For this example, the profiles indicate that arsenic makes up 0.3 percent of fine particles (less than 2.5 microns) emissions mass.

   A. **Emission Factor.** Calculate the aggregate storage emission factor for wind blown dust from Equation (4.1.2-1):

$$E\,(\mathrm{kg/dy/hectare}) = 1.9\,(50/1.5)\,\frac{(365-0)}{235}\,(20/15) = 131.2$$

   B. **Area.** Calculate area (A)($m^2$) of the storage pile from Equation (4.1.2-2):

$$A = 3.14159\left(\frac{10}{2}\right)^2 = 78.5\,(m^2)$$

   C. **Convert.** Convert emission factor (E) in kg/dy/hectare to g/s-$m^2$:

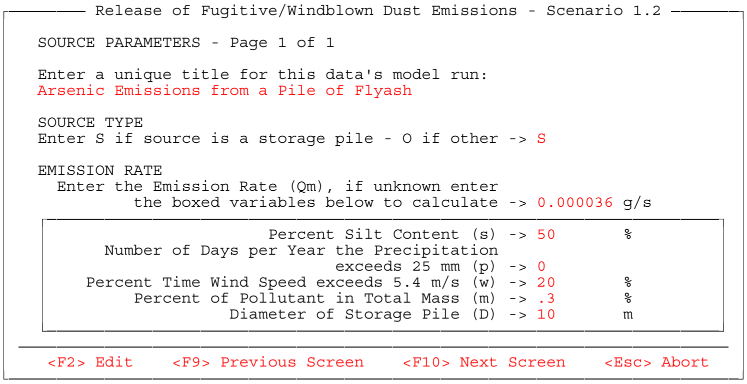
$$E = \frac{131.5\,(\mathrm{kg/dy/hectare})\;1000\,(\mathrm{g/kg})}{86400\,(\mathrm{s/dy})\;1000\,(m^2/\mathrm{hectare})} = 0.00015\,(\mathrm{g/s}-m^2)$$

   D. **Emission Rate.** Since 0.3 % of this mass is arsenic, calculate emission rate ($Q_m$) in g/s from Equation (4.1.2-3).

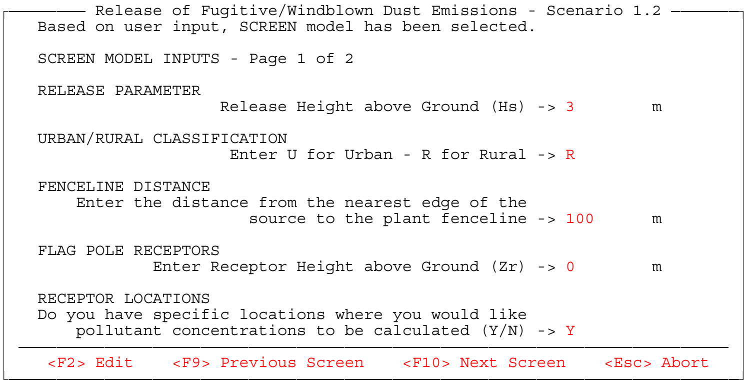
$$Q_m = 0.00015\,(\mathrm{g/s}-m^2)\cdot\frac{0.3\,(\%)}{100}\cdot 78.5\,(m^2) = 0.000036\,(\mathrm{g/s})$$

2. TSCREEN will run the SCREEN model for an area source.

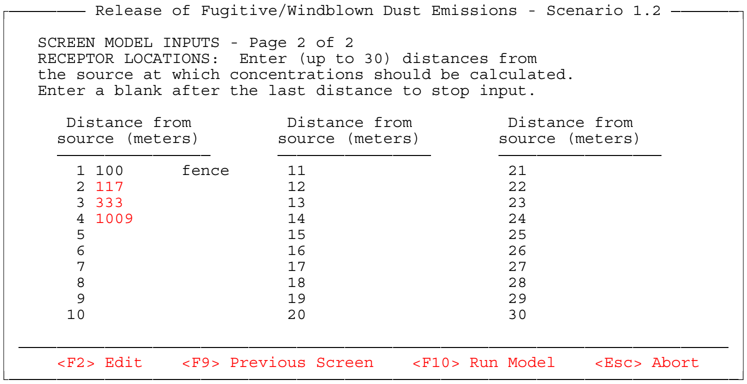
Data entry in the TSCREEN model for this example is shown below:



```
 Release of Fugitive/Windblown Dust Emissions - Scenario 1.2

SOURCE PARAMETERS - Page 1 of 1

Enter a unique title for this data's model run:
Arsenic Emissions from a Pile of Flyash

SOURCE TYPE
Enter S if source is a storage pile - O if other -> S

EMISSION RATE
  Enter the Emission Rate (Qm), if unknown enter
          the boxed variables below to calculate -> 0.000036 g/s

                       Percent Silt Content (s) -> 50       %
       Number of Days per Year the Precipitation
                             exceeds 25 mm (p) -> 0
     Percent Time Wind Speed exceeds 5.4 m/s (w) -> 20       %
          Percent of Pollutant in Total Mass (m) -> .3       %
                    Diameter of Storage Pile (D) -> 10       m

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Release of Fugitive/Windblown Dust Emissions - Scenario 1.2
Based on user input, SCREEN model has been selected.

SCREEN MODEL INPUTS - Page 1 of 2

RELEASE PARAMETER
                   Release Height above Ground (Hs) -> 3        m

URBAN/RURAL CLASSIFICATION
                    Enter U for Urban - R for Rural -> R

FENCELINE DISTANCE
    Enter the distance from the nearest edge of the
                      source to the plant fenceline -> 100      m

FLAG POLE RECEPTORS
              Enter Receptor Height above Ground (Zr) -> 0        m

RECEPTOR LOCATIONS
Do you have specific locations where you would like
    pollutant concentrations to be calculated (Y/N) -> Y

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Release of Fugitive/Windblown Dust Emissions - Scenario 1.2

SCREEN MODEL INPUTS - Page 2 of 2
RECEPTOR LOCATIONS:  Enter (up to 30) distances from
the source at which concentrations should be calculated.
Enter a blank after the last distance to stop input.

   Distance from          Distance from          Distance from
  source (meters)        source (meters)        source (meters)
  _______________        _______________        _______________

    1 100     fence        11                     21
    2 117                  12                     22
    3 333                  13                     23
    4 1009                 14                     24
    5                      15                     25
    6                      16                     26
    7                      17                     27
    8                      18                     28
    9                      19                     29
   10                      20                     30

    <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

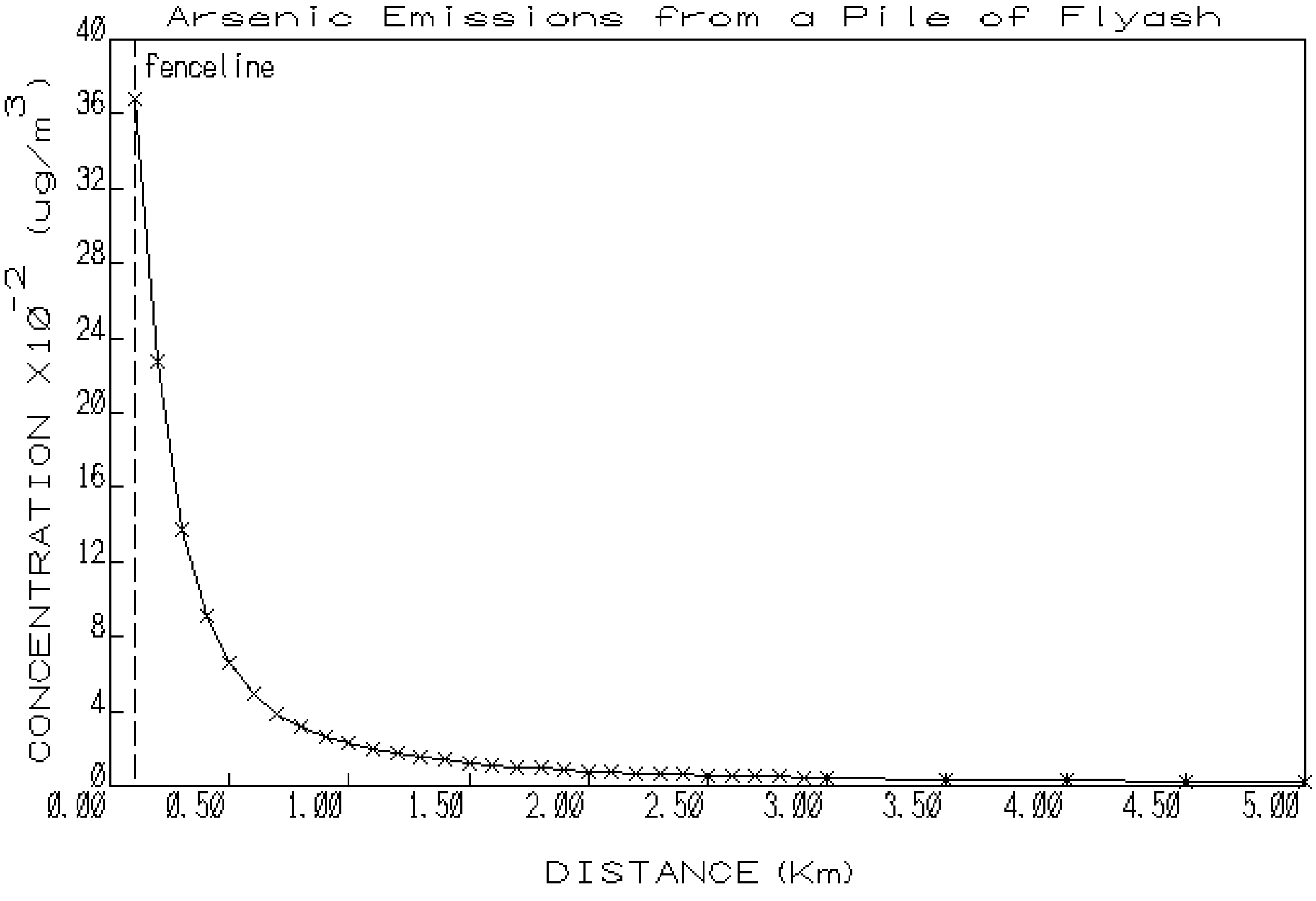
A summary of the SCREEN model's output is displayed below:

```
1                                                                  03-03-92
                                                                   10:04:59
  *** SCREEN-1.2 MODEL RUN ***
  *** VERSION DATED  90XXX ***

 Arsenic Emissions from a Pile of Flyash

 SIMPLE TERRAIN INPUTS:
    SOURCE TYPE            =      AREA
    EMISSION RATE (G/S)    =     .3600E-04
    SOURCE HEIGHT (M)      =      3.00
    LENGTH OF SIDE (M)     =      8.86
    RECEPTOR HEIGHT (M)    =       .00
    IOPT (1=URB,2=RUR)     =      2


      ***************************************
      *** SUMMARY OF SCREEN MODEL RESULTS ***
      ***************************************

  CALCULATION         MAX CONC     DIST TO    TERRAIN
   PROCEDURE         (UG/M**3)     MAX (M)     HT (M)
 --------------     -----------    -------    -------
 SIMPLE TERRAIN       .3677          100.         0.
```

```
***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
.
.
.
```

---

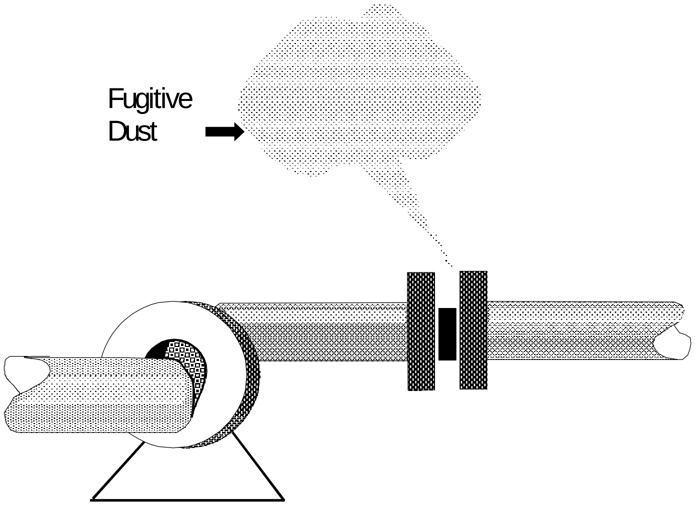
The following is a graphic representation of the model output. This graph plots concentration vs. distance. The plot of the SCREEN model's data contains only points for the automated distance array used by the model.



Maximum concentration 3.677E-001 ug/cubic m at 0.100 Km (Automated Distances)

Press any key to continue

### 4.1.3 Ducting/Connector Failures



Similar Releases: Instantaneous bursts of particulate matter due to duct failure (e.g., pneumatic conveyor line failures), line disconnection, isolation joint failure, or other types of equipment openings.

Discussion:

Limited information on powder releases from duct failures is available in the technical literature. Crude estimates of release amounts can be made based on transfer line rates and time for equipment shutdown and equipment capacity. If possible, the user should attempt to estimate the initial cloud dimension resulting from dilution due to the mechanical action of the release. If initial dilution cannot be estimated by the user, conservative concentration estimates can be obtained using an instantaneous point source simulation with the PUFF model. There is no release rate input section for this scenario. For this scenario, TSCREEN goes directly to the PUFF model input section. See Section 5.3 for a complete list of inputs.

Limitations and Assumptions:

- For screening, particle deposition is assumed to be insignificant.

Input Information:

$Q$ total amount of material released (g)
$H_s$ release height above ground (m)
$\sigma_y$ initial laterial dispersion (m)
$\sigma_z$ initial vertical dispersion (m)

### 4.1.3.1 Example: Failure of a Pneumatic Conveyor System

Discussion:

A failure of a pneumatic conveyor system carrying 3,3-dichlorobenzidine powder from a spray dryer lasted 5 minutes. Estimates are required for 15-minute average concentrations at receptors downwind at or beyond the 100 m fenceline. The release height is 10 m, the conveyance rate is 2 kg/s and the duct diameter is 0.305 m.

The example represents a class of possible releases from various types of gas-solid conveyance systems or reactor failures. Common causes of this type of release are duct failure due to abrasion or failure of flexible connectors. Short duration events can be simulated as instantaneous passively dispersing puffs (i.e., all mass was released instantaneously (within a few minutes)). The effect of this assumption is a conservative estimate of the ambient concentration. In general, powders emitted by this type of release will consist of relatively large particles (greater than 10 μ) which would be subject to gravitational fallout.

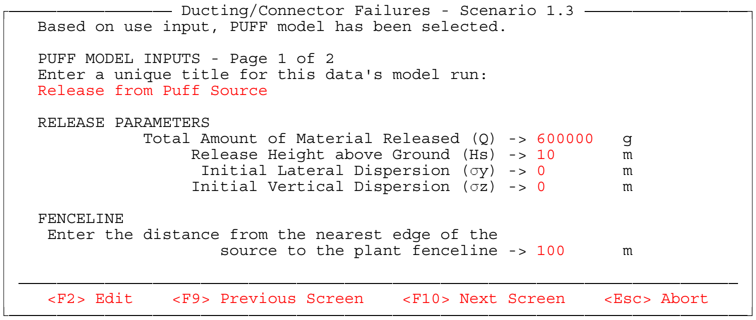
Procedure:

1. The release scenario would result in an initially high rate of emissions which decreases rapidly as line pressure decreases, as in a pipeline blowdown. A point source is assumed because there was no indication of initial dilution dimensions in the problem. The total emissions (Q) is:

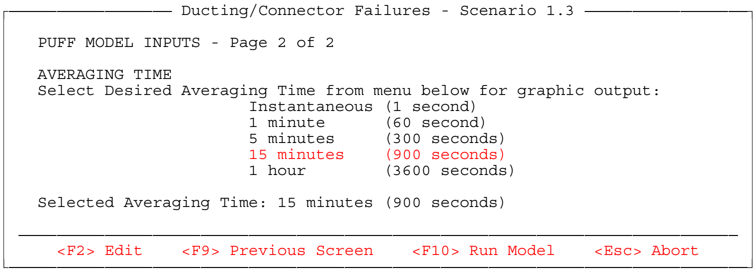
$$Q = 5(\text{min})\ 60(\text{s/min})\ 2(\text{kg/s})\ 1000(\text{g/kg}) = 600{,}000(\text{g})$$

2. The release height is 10 m above ground, the initial lateral and vertical dispersion parameters are 0 m, and the fenceline distance is 100 m.

Data entry in the TSCREEN model for this example is shown below:



```
──────────── Ducting/Connector Failures - Scenario 1.3 ────────────
  Based on use input, PUFF model has been selected.

  PUFF MODEL INPUTS - Page 1 of 2
  Enter a unique title for this data's model run:
  Release from Puff Source

  RELEASE PARAMETERS
              Total Amount of Material Released (Q) -> 600000   g
                   Release Height above Ground (Hs) -> 10       m
                    Initial Lateral Dispersion (σy) -> 0        m
                   Initial Vertical Dispersion (σz) -> 0        m

  FENCELINE
   Enter the distance from the nearest edge of the
                     source to the plant fenceline -> 100      m

 ─────────────────────────────────────────────────────────────────
   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Ducting/Connector Failures - Scenario 1.3

PUFF MODEL INPUTS - Page 2 of 2

AVERAGING TIME
Select Desired Averaging Time from menu below for graphic output:
                      Instantaneous (1 second)
                      1 minute      (60 second)
                      5 minutes     (300 seconds)
                      15 minutes    (900 seconds)
                      1 hour        (3600 seconds)

Selected Averaging Time: 15 minutes (900 seconds)
```

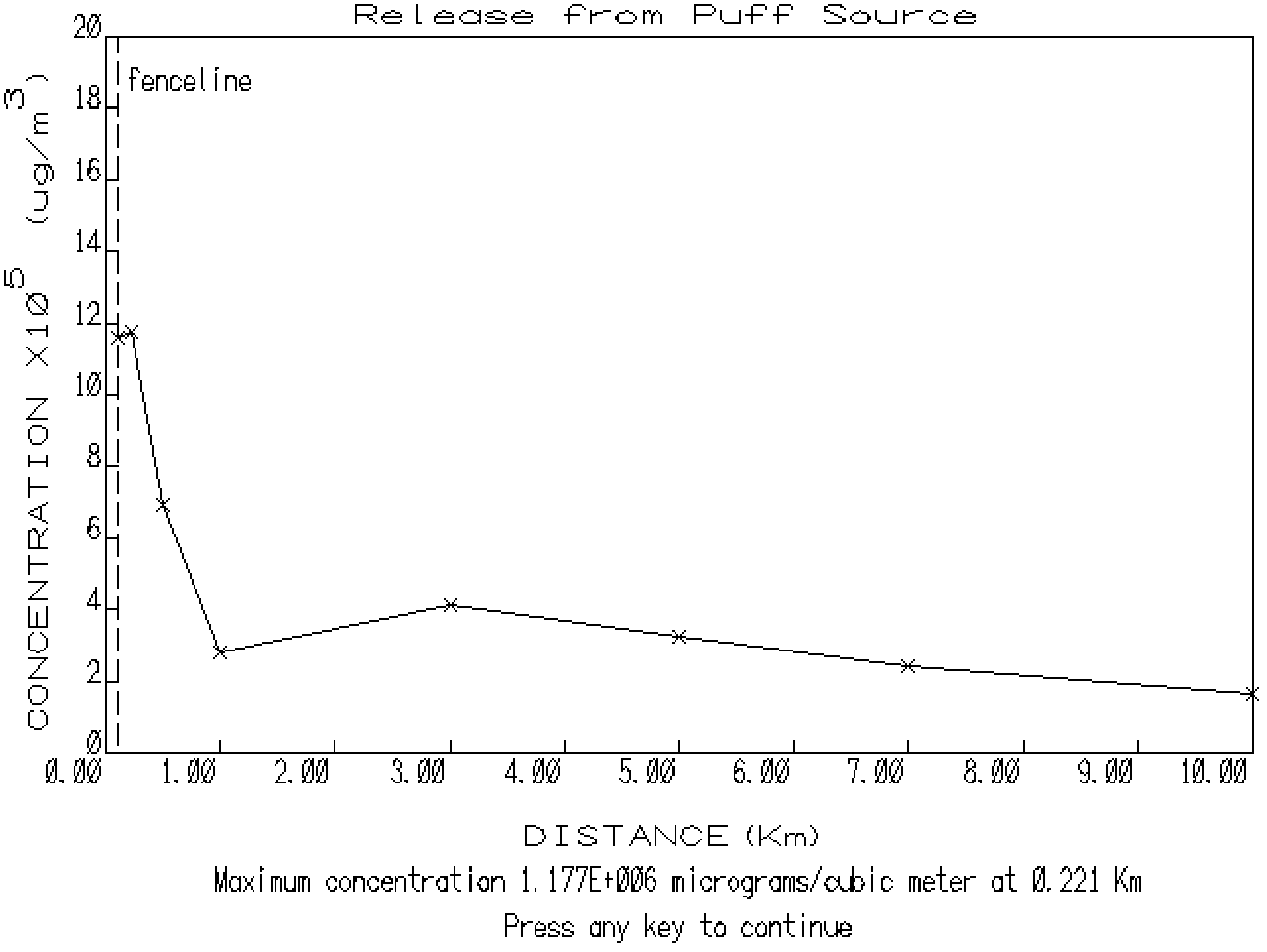
The PUFF model's output is shown below:

```
============================================================================================================

 Release from Puff Source

    TOTAL AMOUNT OF MATERIAL RELEASED (G):   .6000E+06
          RELEASE HEIGHT ABOVE GROUND (M):   10.00
 INITIAL LATERAL DISPERSION SIGMA (Y) (M):   .0000
INITIAL VERTICAL DISPERSION SIGMA (Z) (M):   .0000

 ******************************************************
 ***         SUMMARY OF PUFF MODEL RESULTS          ***
 ******************************************************

THE MAXIMUM CONCENTRATION AND THE DISTANCE TO MAXIMUM
CONCENTRATION FOR DISTANCES BEYOND FENCELINE    .100 (KM).
FOR NEAR SURFACE RELEASE MAXIMUM CONCENTRATION WILL OCCUR AT
THE FENCELINE.

    AVERAGING           MAXIMUM             DISTANCE TO         STABILITY
    TIME (MIN)     CONCENTRATION (G/M**3)   MAX. CONC. (KM)     CLASS

 INSTANTANEOUS             5.734E+01            .161               N
       1                   1.764E+01            .221               N
       5                   3.530E+00            .221               N
*      15                  1.177E+00            .221               N
       60                  2.941E-01            .221               N

 ******************************************************
 **   REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS  **
 ******************************************************


 *********************************
 ***      PUFF DISTANCES      ***
 *********************************

 THE MAXIMUM CONCENTRATION AS A FUNCTION OF DOWNWIND DISTANCE
 AND THE CONDITIONS THAT PRODUCED THE MAXIMUM AT THAT DISTANCE.


 MIXING HEIGHT (M)   320.
 WIND SPEED (M/SEC)    1.0

 AVERAGING                         DOWNWIND DISTANCE (KM)
 TIME (MIN)   MAXIMUM CONCENTRATION (G/M**3) AT VARIOUS DOWNWIND DISTANCES.
                  STABILITY CLASS THAT PRODUCED THE MAX. LISTED BELOW
             0.01      0.03      0.05      0.07       0.1       0.5
 ===========================================================================
 INST.   3.997E+01 3.376E+02 1.748E+02 9.261E+01 4.288E+01 1.359E+01
               U         U         U         U         U         N
 1       2.005E+00 4.531E+01 3.745E+01 2.701E+01 1.732E+01 9.327E+00
               U         U         U         U         U         N
 5       4.009E-01 9.062E+00 7.490E+00 5.403E+00 3.472E+00 2.073E+00
               U         U         U         U         U         N
*15      1.336E-01 3.021E+00 2.497E+00 1.801E+00 1.157E+00 6.910E-01
               U         U         U         U         U         N
 60      3.341E-02 7.551E-01 6.242E-01 4.502E-01 2.893E-01 1.728E-01
               U         U         U         U         U         N



 AVERAGING                         DOWNWIND DISTANCE (KM)
 TIME (MIN)   MAXIMUM CONCENTRATION (G/M**3) AT VARIOUS DOWNWIND DISTANCES.
                  STABILITY CLASS THAT PRODUCED THE MAX. LISTED BELOW
             1.0       3.0       5.0       7.0      10.0      30.0
 ===========================================================================
 INST.   3.239E+00 5.931E+00 2.976E+00 1.637E+00 8.060E-01 7.088E-02
               S         S         S         S         S         S
 1       2.610E+00 4.759E+00 2.709E+00 1.554E+00 7.837E-01 7.061E-02
               N         S         S         S         S         S
 5       8.487E-01 1.232E+00 9.742E-01 7.200E-01 4.701E-01 6.436E-02
               N         S         S         S         S         S
*15      2.829E-01 4.108E-01 3.248E-01 2.411E-01 1.630E-01 3.736E-02
               N         S         S         S         S         S
 60      7.072E-02 1.027E-01 8.119E-02 6.027E-02 4.076E-02 9.529E-03
               N         S         S         S         S         S

 STABILITY CLASSES
 U = UNSTABLE
 N = NEUTRAL
 S = STABLE
```

```
 * INDICATES AVERAGING TIME THAT WAS SELECTED FOR PLOTTING

********************************
*** END OF PUFF MODEL OUTPUT ***
********************************
```

---

The following is a graph of the PUFF model output. The data that are plotted are for the averaging time that the user selected from the second page of the PUFF model inputs. These data are marked with an asterisk (*) above.



Maximum concentration 1.177E+006 micrograms/cubic meter at 0.221 Km

Press any key to continue

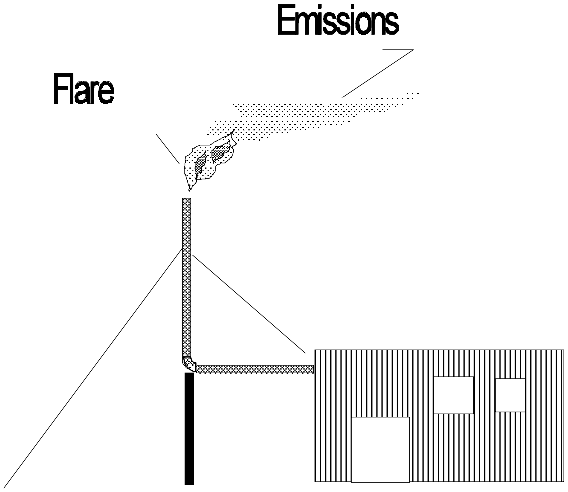
This is a plot of maximum concentration regardless of meterological conditions. For example close to the source unstable conditions produce the maximum concentrations. Beyond 3 km stable conditions produce the maximum concentration.

The output of the PUFF model consists of four parts. Part 1 summarizes the input parameters by the user. These values shoud be checked to insure accurate entry. Part 2 of the model output is a table that provides the maximum concentration and the distance to maximum concentration for different averaging times. In this table the minimum distance for concentration calculations is the fenceline. For near surface releases, highest concentrations will always occur at the fenceline. Part 3 of the output is an extended table showing the maximum concentration versus downwind distance (beyond fenceline) for four averaging times and the atmospheric stability conditions that produced the maximum. For a surface release, stable atmospheric conditions produce maximum concentrations for all downwind distances and averaging times. With increasing puff release height the atmospheric stability conditions which produce the maximum surface concentrations change. In this example, where the release hiehgt is 10 m, unstable atmospheric conditions produce the maximum concentrations near the source. It is the values from this table that are used to produce the plot of maximum concentration versus downwind distance shown in the fourth part of the output of the PUFF model. The plot, however, only displays the averaging time selected by the user.

## 4.2 Gaseous Release

A gaseous release is a release of any matter in vapor form such as sulfur dioxide, volatile organics, etc.

### 4.2.1 Continuous Flared Stack Emissions - Gaseous



Similar Releases: Flares are used as control devices for a variety of sources. As such, flares must comply with requirements specified in 40 CFR 60.18. Once emissions are vented through the flare, a minimum 98% reduction of all combustible components of the original emission must be achieved.

Discussion:

Flare problems are done in two parts, an emission calculation and dispersion modeling. Toxic emissions for permitted flares are reduced to 2% of the potential emissions based on a required control efficiency of 98%. Flare problems are similar to stack examples except that there are buoyancy flux reductions associated with radiative heat losses and a need to account for flame length in estimating plume height.

Flares are used as a control device for a variety of sources. As such, flares must comply with requirements specified in 40 CFR 60.18 if the flare is subject to the requirements of Part 60 (New Source Performance Standards) or Part 61 (National Emission Standards for Hazardous Air Pollutants). Not all flares are subject to these requirements. Properly designed and operated flares should be able to meet a 98% control requirement, however, the actual control efficiency will depend on whether the flare is steam or air assisted, whether the gases are combusted, whether an auxiliary fuel is used for combustion of low heat content gases, etc. Refer to AP-42 (EPA, 1985) Section 11.5, "Industrial Flares", when estimates of flare emissions are needed. There is no release rate input section for this scenario. For this scenario, TSCREEN goes immediately to the SCREEN model input section for a flare source. See Section 5.1.1 for a complete list of SCREEN model inputs.

Limitations and Assumptions:

- Approximately 45% of the total heat release is assumed to be radiated as sensible heat.

Input Information:

$H_r$ total heat release rate (J/s)
$H_s$ physical stack height above ground (m)
$H_{s1}$ effective release height before plume rise (m)
$M_w$ molecular weight of material released (g/g-mole)
V volumetric flow rate to the flare ($m^3$/s)
vol volume fraction of pollutant (%)
$f_i$ volume fraction of each component of the flare input gas
$H_i$ net heating value of each component (J/g-mole)

### 4.2.1.1 Procedure:

1. **Emission Rate ($Q_m$).** Calculate the emission rate in g/s:

$$Q_m(g/s) = \frac{(Vol(\%)/100)\ V(m^3/s)\ M_w(g/g\text{-}mole)\ 0.02}{0.0224(m^3/g\text{-}mole)} \qquad (4.2.1\text{-}1)$$

2. **Total Heat Release Rate ($H_r$) (m).** Calculate the total heat release rate from the flare gas combustion (Lahey & Davis, 1984):

$$H_r = 44.64\ V \sum_{i=1}^{n} f_i\ H_i \qquad (4.2.1\text{-}2)$$

where the value 44.6 is derived for air as:

$$\frac{\rho_{air}(g/m^3)}{M_w(g/g\text{-}mole)} = \frac{1292.}{28.97} = 44.6(g\text{-}mole/m^3)$$

and the summation is over the n components of the flare input gas stream.

3. **Effective Release Height above Ground ($H_{s1}$).** Calculate the effective release height by adding the flare height to the stack height, as follows (Beychok, 1979):

$$H_{s1} = H_s + 4.56\times10^{-3}\left(\frac{H_r}{4.1868}\right)^{0.478} \qquad (4.2.1\text{-}3)$$

where 4.1868 is a conversion factor (Joules to calories). Plume rise for the combusted gas is calculated in the SCREEN model for this effective release height (EPA, 1988c).

### 4.2.1.2 Example: Flare Emission

Discussion:

A gas is sent to an elevated flare to be burned. For simplicity, it is assumed that the flare is a permitted one. The gas is a mixture with one toxic component. The gas stream is made up of 50% methane, 9.8% ethane, and 40% carbon dioxide and .2% benzene. Maximum one-hour concentrations are required for benzene assuming 98% reduction efficiency of the flare. There is a cubical building, 19 m in height, next to this flare. The fenceline is 100 m from the flare.

The following input information will be required:

| | |
|---|---|
| $H_r$ | total heat release rate ($3.84\times10^7$ J/s) |
| $H_s$ | physical stack height above ground (32 m) |
| $H_{s1}$ | effective release height (m) |
| $M_w$ | molecular weight of material (78.1 g/g-mole) |
| V | volumetric flow rate (6.58 $m^3$/s) |
| vol | volume fraction of pollutant in feed gas (0.2 %) |

Procedure:

1. **Emission Rate ($Q_m$).** Calculate the emission rate in g/s. Determine the emission rate of benzene from the volume fraction, molar volume, flow rate, and molecular weight. The volume of benzene is the volume fraction of pollutant (vol) times material flow rate (V). Mass emission rate ($Q_m$) after controls is given by determining the number of moles in the benzene fraction and multiplying by the molecular weight (the gas is assumed to be at standard conditions considering the control efficiency) from Equation (4.2.1-1):

$$Q_m(g/s) = \frac{.002 \cdot 6.58(m^3/s) \cdot 78.1(g/g\text{-}mole) \cdot 0.02}{0.0224(m^3/g\text{-}mole)} = 0.918(g/s)$$

2. **Total Heat Release Rate ($H_r$) (m).** The user calculates the total heat release ($H_r$) from the flare from Equation (4.2.1-2). In this example, carbon dioxide is not combustible and is assumed not to affect flame heat. Total heat generated by the flame is determined using mole

fractions, molar flow rate, and heats of combustion for methane, ethane, and benzene (see references for physical constants).

$$H_r(J/s) = (44.64 \text{ g-mole/m}^3)\ 6.58 \text{ m}^3/s\ [0.5(8.0286\times10^5 \text{ J/g-mole}) + 0.098\ (1.4288\times10^6 \text{ J/g-mole}) + 0.002\ (3.2696\times10^6 \text{ J/g-mole})]$$

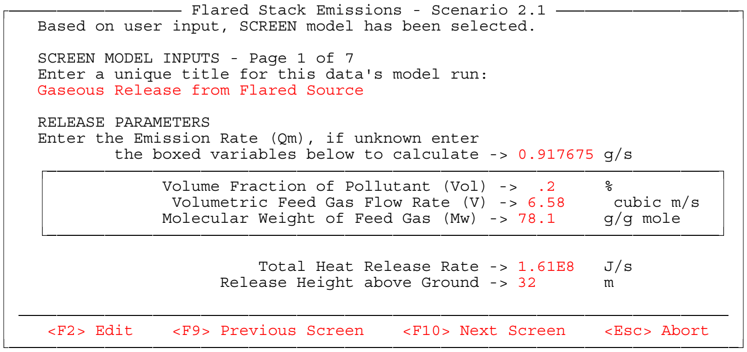
$$= 1.61 \times 10^8\ (J/s)\ (\text{or } 3.84\times10^7\ (cal/s))$$

3. **Effective Release Height above Ground ($H_{s1}$).** The effective release height is calculated from Equation (4.2.1-3):

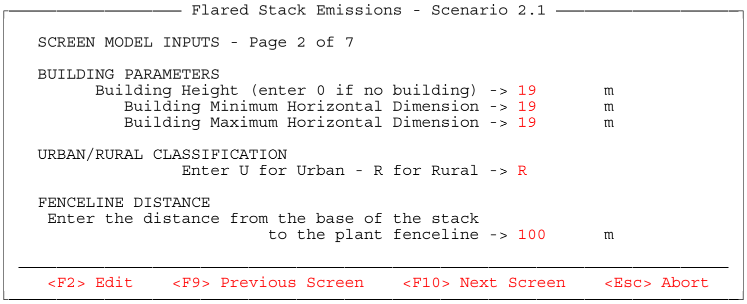
$$H_{s1} = 32 + 4.56\times10^{-3} \bullet \left(\frac{1.61\times10^8}{4.1868}\right)^{.478} = 51.26 \text{ m}$$

Dispersion calculations for this scenario are made using the SCREEN model for a flare.

Data entry in the TSCREEN model for this example is shown below:



```
                Flared Stack Emissions - Scenario 2.1
  Based on user input, SCREEN model has been selected.

  SCREEN MODEL INPUTS - Page 1 of 7
  Enter a unique title for this data's model run:
  Gaseous Release from Flared Source

  RELEASE PARAMETERS
  Enter the Emission Rate (Qm), if unknown enter
          the boxed variables below to calculate -> 0.917675 g/s

              Volume Fraction of Pollutant (Vol) ->  .2       %
               Volumetric Feed Gas Flow Rate (V) -> 6.58      cubic m/s
              Molecular Weight of Feed Gas (Mw)  -> 78.1      g/g mole

                        Total Heat Release Rate -> 1.61E8    J/s
                    Release Height above Ground -> 32        m

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
                Flared Stack Emissions - Scenario 2.1

  SCREEN MODEL INPUTS - Page 2 of 7

  BUILDING PARAMETERS
        Building Height (enter 0 if no building) -> 19        m
           Building Minimum Horizontal Dimension -> 19        m
           Building Maximum Horizontal Dimension -> 19        m

  URBAN/RURAL CLASSIFICATION
                 Enter U for Urban - R for Rural -> R

  FENCELINE DISTANCE
   Enter the distance from the base of the stack
                          to the plant fenceline -> 100       m

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

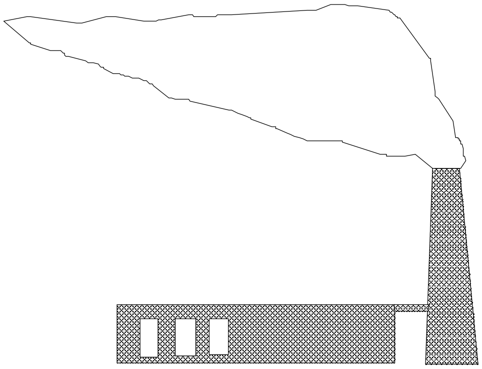
A summary of the SCREEN model's output for this example is shown below.

---

```
  *** SCREEN-1.2 MODEL RUN ***
  *** VERSION DATED  90XXX ***

 Release from Flare Source

 SIMPLE TERRAIN INPUTS:
    SOURCE TYPE            =    FLARE
    EMISSION RATE (G/S)    =    .9177
    FLARE STACK HEIGHT (M) =    32.00
    TOT HEAT RLS (CAL/S)   =    .3840E+08
    RECEPTOR HEIGHT (M)    =      .00
    IOPT (1=URB,2=RUR)     =     2
    EFF RELEASE HEIGHT (M) =    51.24
    BUILDING HEIGHT (M)    =    19.00
```

```
    MIN HORIZ BLDG DIM (M) =    19.00
    MAX HORIZ BLDG DIM (M) =    19.00


      ***************************************
      *** SUMMARY OF SCREEN MODEL RESULTS ***
      ***************************************

  CALCULATION        MAX CONC    DIST TO   TERRAIN
   PROCEDURE        (UG/M**3)    MAX (M)    HT (M)
 --------------    -----------   -------   -------
 SIMPLE TERRAIN      .5505        1243.       15.


 ***************************************************
 ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
 ***************************************************
.
.
.
```

### 4.2.2 Continuous Release from Stacks, Vents, Conventional Point Sources



Similar Releases: Continuous emissions of gases from building vents, vertical stacks and pipes or conventional point sources when emission flow rates and temperature are known. These results may also be due to a process failure such as a rupture disk release or failure of control equipment.

Discussion:

Continuous emissions of gases from stacks are analyzed in this scenario. Emission factors are available for individual toxic compounds for some processes (Appendix A, items 1, 2, and 3). In other cases, total VOC emission rates can be obtained from AP-42. To determine toxic components of these emissions, see Appendix A item 4.

Limitations and Assumptions:

- Release behaves as an ideal gas
- Release is neutrally buoyant

Input Information:

| | |
|---|---|
| $D_o$ | diameter at release point (m) |
| $M_s$ | mean molecular weight (g/g-mole) |
| R | gas constant (8314 Pa•$m^3$/kg-mole•°K or 8314 J/kg-mole•°K) |
| $Q_m$ | total material emission rate (g/s) |
| $T_a$ | ambient temperature (°K) |
| $T_s$ | temperature of material released (°K) |
| V | volumetric flow rate ($m^3$/s) |
| $H_s$ | release height above ground (m) |

4.2.2.1 Procedure:

1. **Density Check.** The user should choose to perform a density check if the release material is thought to be denser-than-air. TSCREEN will help the user determine if the release is buoyant (passive gas) or denser-than-air. If the release is thought to be buoyant (e.g., a very hot plume from an incinerator, power plant, furnace, etc.), then a density check need not be performed. To perform a density check, proceed to step 2. Otherwise, proceed to step 4.

2. **Buoyancy Check.**

   A. **Mean Molecular Weight ($M_s$).** Determine the mean molecular weight of the gas stream using the method described in Appendix B:

$$M_s = \left( \sum_{i=1}^{n} (m_i \ / \ M_i) \right)^{-1} \qquad (4.2.2\text{-}1)$$

   where:
   $m_i$ = mass fraction of each component
   $M_i$ = molecular weight of each component (g/g-mole)

   B. **Discharge Density.** Calculate the discharge density $\rho_2$ (g/m$^3$) using the ideal gas law:

$$\rho_2 = \frac{P_a \, M_s}{R \, T_s} \qquad (4.2.2\text{-}2)$$

   where $P_a$ is the ambient pressure (assumed to equal 101325Pa).

   C. **Density of Air .** Calculate the density of air $\rho_{air}$ (kg/m$^3$) using the ideal gas law:

$$\rho_{air} = \frac{P_a \, M_a}{R \, T_a} \qquad (4.2.2\text{-}3)$$

   where $P_a$ is the ambient pressure (assumed to equal 101325Pa), and $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kg-mole).

   D. **Perform Buoyancy Check.**

   If $\dfrac{\rho_2}{\rho_{air}} > 1$

buoyancy is negative and the release is denser-than-air. If buoyancy is negative proceed to step 3. Otherwise, buoyancy is positive and the release is assumed to be passive (i.e., not denser-than-air). If buoyancy is positive proceed to step 4.

3. **Richardson Number.** Perform release Richardson number (Ri) check:

$$Ri = 2725 \frac{\left( \frac{\rho_2}{\rho_{air}} - 1 \right) Q_m}{1000 \cdot D_o \, \rho_2} \qquad (4.2.2\text{-}4)$$

where 1000 is used to convert the densities from $kg/m^3$ to $g/m^3$. Emission rates ($Q_m$) must be calculated from process parameters or determined from representative emission factors. If there are emission factors, then convert to emission rate by multiplying by production rate:

$$\begin{matrix}\text{AP-42} \\ \text{emission factor}\end{matrix} \left( \frac{\text{lb}}{1000 \text{ ft}^2} \right) \cdot \begin{matrix}\text{production} \\ \text{rate}\end{matrix} \left( \frac{1000\text{ft}^2}{\text{hr}} \right) = \begin{matrix}\text{emission} \\ \text{rate}\end{matrix} \left( \frac{\text{lb}}{\text{hr}} \right)$$

$$\text{emission rate (g/s)} = \text{emission rate (lb/hr)} \cdot \text{conversion factor}$$

See Section 2.4 for a discussion of the Richardson number. If Ri is ≥ 30 then the release is passive. Otherwise, the release is dense.

4. **Exit Velocity.** Determine stack gas exit velocity ($V_s$) (m/s):

$$V_s = \frac{4 \, V}{\pi \, D_o^2} \qquad (4.2.2\text{-}5)$$

where: V = volumetric flow rate ($m^3/s$)

5. If the release is passive, then TSCREEN runs the SCREEN model for a point source. If the release is dense, use Scenario 2.3 - Continuous Gaseous Leaks from Holes in Tanks, Pipes, Relief Valves.

### 4.2.2.2 Example: Hydrogen Cyanide (HCN) release

Discussion:

Hydrogen Cyanide (HCN) is released from a vent stack at a rate of 0.2 tons/day. The stack is 16 meters above ground, has an inside diameter of 0.1 meter, the stack exit temperature is 298 °K and the volumetric flow rate is 0.14 $m^3/s$. The stack is adjacent to a square building with height and width dimensions equal to 19 m. The site is classified as rural, non-complex terrain. Hourly maximum concentration estimates are required. This example represents a continuous release of a gas with a specified emission rate through a stack with possible building downwash due to the influence of an adjacent building. The fenceline is 100 meters form the vent stack.

The following input information will be required:

| | |
|---|---|
| D | diameter at release point (0.1 m) |
| $H_b$ | building height (19 m) |
| $B_{min}$ | building minimum horizontal dimension (19 m) |
| $B_{max}$ | building maximum horizontal dimension (19 m) |
| $M_s$ | mean molecular weight (kg/kg-mole) |
| $Q_m$ | total material emission rate (2.13 g/s) |
| R | gas constant (8314 Pa•$m^3$/kg-mole•°K or 8314 J/kg-mole•°K) |
| $T_a$ | ambient temperature (298 °K) |
| $T_s$ | temperature of material released (298 °K) |
| V | volumetric flow rate of material released (0.14 $m^3$/s) |

<u>Procedure:</u>

1. **Density Check.** A density check will be performed for this example, therefore, proceed to step 2.

2. **Buoyancy Check.**

   A. **Mean Molecular Weight ($M_s$).** Stack tests show that HCN (molecular weight 27) is the primary constituent (13%) besides air in the gas stream. Mean density is calculated as follows using Equation (4.2.2-1):

$$M_s = \frac{1}{\frac{.87}{28.9} + \frac{.13}{27}} = 28.7 \text{ kg/kg-mole}$$

   B. **Discharge Density.** Calculate the discharge density $\rho_2$ (kg/$m^3$) using Equation (4.2.2-2):

$$\rho_2 = \frac{101325 \cdot 28.7}{8314 \cdot 298} = 1.17 \text{ kg/m}^3 \qquad (4.2.2\text{-}2)$$

   C. **Density of Air .** Calculate the density of air $\rho_{air}$ (kg/$m^3$) using Equation (4.2.2-3):

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 298} = 1.18 \text{ kg/m}^3 \qquad (4.2.2\text{-}3)$$

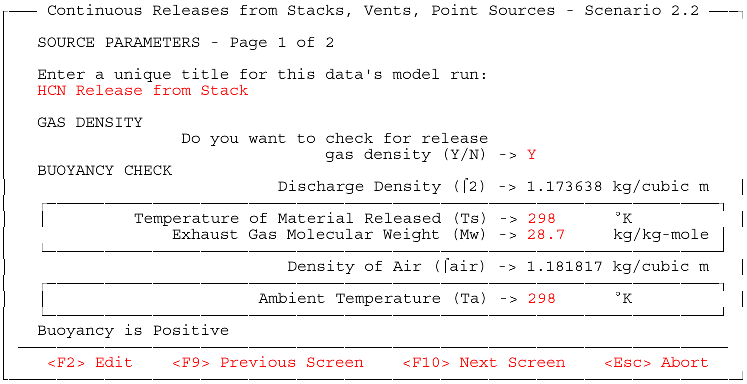
   D. **Perform Buoyancy Check.** Since discharge density is less than air density ($1.17(kg/m^3)/1.18(kg/m^3) < 1$), the release is positively buoyant. Proceed to step 4.

4. **Exit Velocity.** Calculate stack gas exit velocity ($V_s$) (m/s) using Equation (4.2.2-5):

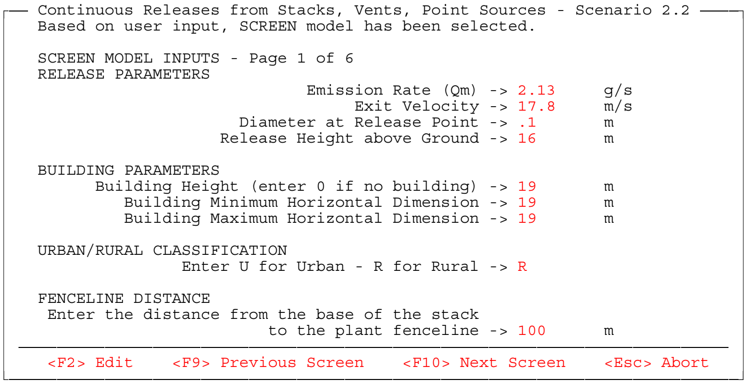
$$V_s = \frac{4 \cdot 0.14}{3.14\ (.1)^2} = 17.8\ m/s$$

5. Since the release is passive, dispersion calculations for this scenario are made using the SCREEN model for a point source.

Data entry in the TSCREEN model for this example is shown below:



```
Continuous Releases from Stacks, Vents, Point Sources - Scenario 2.2

SOURCE PARAMETERS - Page 1 of 2

Enter a unique title for this data's model run:
HCN Release from Stack

GAS DENSITY
               Do you want to check for release
                              gas density (Y/N) -> Y
BUOYANCY CHECK
                         Discharge Density (⌠2) -> 1.173638 kg/cubic m

          Temperature of Material Released (Ts) -> 298      °K
              Exhaust Gas Molecular Weight (Mw) -> 28.7     kg/kg-mole

                          Density of Air (⌠air) -> 1.181817 kg/cubic m

                          Ambient Temperature (Ta) -> 298   °K

Buoyancy is Positive

<F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



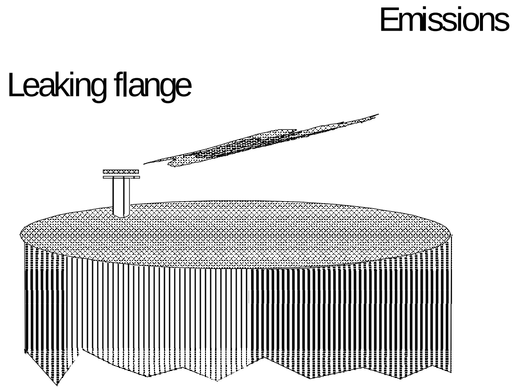
```
Continuous Releases from Stacks, Vents, Point Sources - Scenario 2.2
Based on user input, SCREEN model has been selected.

SCREEN MODEL INPUTS - Page 1 of 6
RELEASE PARAMETERS
                            Emission Rate (Qm) -> 2.13     g/s
                                 Exit Velocity -> 17.8     m/s
                      Diameter at Release Point -> .1      m
                    Release Height above Ground -> 16      m

BUILDING PARAMETERS
      Building Height (enter 0 if no building) -> 19       m
         Building Minimum Horizontal Dimension -> 19       m
         Building Maximum Horizontal Dimension -> 19       m

URBAN/RURAL CLASSIFICATION
               Enter U for Urban - R for Rural -> R

FENCELINE DISTANCE
 Enter the distance from the base of the stack
                       to the plant fenceline -> 100      m

<F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

A summary of the SCREEN model's output for this example is shown below.

```
     ***************************************
     *** SUMMARY OF SCREEN MODEL RESULTS ***
     ***************************************

 CALCULATION        MAX CONC     DIST TO   TERRAIN
  PROCEDURE        (UG/M**3)     MAX (M)    HT (M)
--------------    -----------    -------   -------
SIMPLE TERRAIN       .8543          100.        0.

BUILDING CAVITY-1    1.717           28.       --    (DIST = CAVITY LENGTH)
BUILDING CAVITY-2    1.717           28.       --    (DIST = CAVITY LENGTH)

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
```

### 4.2.3 Continuous Gas Leaks from a Reservoir

#### 4.2.3.1 Release Rate Estimates: Gas Leaks from a Reservoir



Similar Releases: A gas leak from a tank, a (small) gas leak from a pipe, or gas discharge from a pressure relief valve mounted on a tank.

Discussion:

This procedure applies to a continuous release of a gas (at constant pressure and temperature) from a containment (reservoir) through a hole or opening.

Limitations and Assumptions:

The hole or opening size must be sufficiently small, otherwise the reservoir temperature and pressure may no longer be constant. For the case of a leak from a tank, the assumption of constant reservoir temperature and pressure may be violated if a significant percentage of the tank contents is released. For the case of a leak from a pipe, the assumption of constant temperature and pressure may be violated if $\beta > 0.2$ (approximately) with $\beta$ as defined below; if $\beta > 0.2$, the scenario described in Section 4.2.5 may be appropriate. If the reservoir temperature and pressure are not constant, the release rate may vary with time, but the maximum release rate is generally obtained for the initial reservoir temperature and pressure (Spicer, 1992).

The released material must be an ideal gas at the reservoir conditions, during the depressurization process, and after depressurization to the atmosphere. For the case of a tank containing vapor and liquid, the hole must be in the vapor space of the tank.

Input Information:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($m^2$) |
| $A_1$ | flow area representing reservoir conditions ($m^2$) (In case of a leak from a tank, $A_1 \rightarrow \infty$ (and $\beta = 0$); in the case of a leak from a pipe, $A_1$ is the cross-sectional area of the pipe.) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (J/kg•°K) (For contaminant mixtures, see Appendix B) |
| $D_0$ | (equivalent) diameter of hole or opening ($D_0 = 2 \cdot \sqrt{A_0/\pi}$) (m) |
| $M_w$ | gas (contaminant) molecular weight (kg/kg-mole) (For contaminant mixtures, see Appendix B) |
| $P_v$ | vapor pressure as a function of temperature (Pa) |
| $P_a$ | ambient pressure (Pa) |
| $P_1$ | reservoir pressure (Pa) |
| R | gas constant (8314 J/kg-mole•°K or 8314 Pa•$m^3$/kg-mole•°K) |
| $T_b$ | contaminant normal boiling point (°K) |
| $T_c$ | critical temperature (for contaminant mixtures, see Appendix B) |
| $T_1$ | reservoir temperature (°K) |
| $\beta$ | $\sqrt{A_0/A_1}$ (dimensionless) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_pM))$ at $T_1$ (dimensionless) |
| $\lambda$ | heat of vaporization at the normal boiling point (J/kg) |
| $\rho_1$ | contaminant density at reservoir conditions ($T_1$ and $P_1$) ($kg/m^3$) |

Procedure:

1. **Choked Flow Pressure.** Estimate the choked flow pressure $P_*$ to determine if the flow is choked from Perry et al. (1984):

$$\frac{P_*}{P_1} = \left(\frac{2}{\gamma + 1}\right)^{\gamma/(\gamma-1)} \tag{4.2.3-1}$$

If $P_* \geq P_a$, then the flow is choked; go to step 2. If $P_* < P_a$, then the flow is subcritical (not choked); go to step 3.

2. **Choked Flow.** For choked flow, estimate the gas temperature $T_*$ when the pressure is $P_*$, the emission rate $Q_m$, and the discharge temperature $T_2$.

A. **Estimate $T_*$.** Estimate $T_*$ as follows:

$$\frac{T_*}{T_1} = \left(\frac{2}{\gamma + 1}\right) \qquad (4.2.3\text{-}2)$$

This estimate of $T_*$ must be checked to see if Equation (4.2.3-2) applies. If $T_*$ is greater than the (pseudo) critical temperature $T_c$, Equation (4.2.3-2) applies; if not, the following procedure is suggested. For single component contaminants, evaluate the contaminant vapor pressure at $T_*$ ($P_v(T_*)$) using the Clausius-Clapeyron equation:

$$P_v = 101325 \exp\left(\frac{\lambda Mw}{R}\left(\frac{1}{T_b} - \frac{1}{T_*}\right)\right)$$

If $P_v(T_*) \leq P_*$, then contaminant condensation occurs during the process of depressurization, and this approach is not valid; this release should be considered a two-phase release. If the release is two-phase go to step 5 (Section 4.2.3.2).

B. **Estimate Emission Rate.** Estimate the emission rate $Q_m$ (kg/s) as follows from Perry et al. (1984):

$$Q_m = C\, A_0 \left[P_1 \cdot \rho_1\, \gamma \left(\frac{2}{\gamma + 1}\right)^{(\gamma+1)/(\gamma-1)}\right]^{1/2} \qquad (4.2.3\text{-}3)$$

where $C \simeq 0.75$ (when $P_a = P_*$; when $P_* > P_a$, C can be higher).

C. **Estimate Discharge Temperature.** Estimate the discharge temperature $T_2$ (after depressurization). ($T_2$ is estimated assuming the expansion from reservoir conditions to choked conditions occurs adiabatically and reversibly; the expansion from choked conditions to atmospheric pressure is assumed to occur adiabatically but not reversibly. After Lewitt (1953), assume this adiabatical (irreversible) expansion is 85% efficient.) $T_2$ is estimated using:

$$T_2 = T_1 \left[1 - 0.85\left(\frac{\gamma - 1}{\gamma + 1}\right)\right] \qquad (4.2.3\text{-}4)$$

(Note that $T_2 > T_*$.) Proceed to Step 4.

3. **Subcritical Flow.** For subcritical (not choked) flow, estimate the emission rate $Q_m$ and the discharge temperature $T_2$.

A. **Estimate Emission Rate.** Estimate the emission rate $Q_m$ (kg/s) as follows from Perry et al. (1984):

$$Q_m = K\, Y\, A_0 \left[ 2\, \rho_1 \cdot \left( P_1 - P_a \right) \right]^{1/2} \qquad (4.2.3\text{-}5)$$

where

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

$$Y = 1 - \left( \frac{P_1 - P_a}{P_1\, \gamma} \right) (0.41 + 0.35\, \beta^4)$$

where $C \simeq 0.62$. (Although C can be larger for Reynolds numbers less than $10^4$, typical Reynolds numbers for these applications are larger than $10^4$.)

B. **Estimate Discharge Temperature.** Estimate the discharge temperature $T_2$ (after depressurization). $T_2$ is estimated from energy balance considerations (Lees, 1980):

$$T_2 = 2\, T_1 \,/\, \left\lfloor 1 + \left( 1 + 4\, a\, T_1 \right)^{1/2} \right\rfloor \qquad (4.2.3\text{-}6)$$

where

$$a = \frac{1}{2\gamma\, C_p} \left( \frac{Q_m\, R}{P_a \cdot M_w\, A_0} \right)^2 l$$

The estimate of $T_2$ must be checked. If $T_2$ is greater than the (pseudo) critical temperature $T_c$, the equation used to estimate $T_2$ applies; if not, the following procedure is suggested. For single component contaminants, evaluate the contaminant vapor pressure at $T_2$ ($P_v(T_2)$) using the Clausius-Clapeyron equation:

$$P_v = 101325 \exp\left( \frac{\lambda Mw}{R} \left( \frac{1}{T_b} - \frac{1}{T_2} \right) \right)$$

If $P_v(T_2) \le P_a$, then contaminant condensation occurs during the process of depressurization, and this approach is not valid; this release should be considered a two-phase release. If the release is two phase go to step 6 (Section 4.2.3.2).

4. **Discharge Density.** Estimate the discharge density $\rho_2$ from the discharge temperature $T_2$ using the ideal gas law: $\rho_2 = P_a M_w / R T_2$ where $R = 8314$ (Pa·m$^3$/kg-mole·°K). (Note that correct application of a dispersion model may require that the diameter of the hole or opening be modified to $D_0 (P_* T_2 / (P_a T_*))^{1/2}$ for choked flow and $D_0 (\rho_1/\rho_2)^{1/2}$ for subcritical flow if the model accounts for intial air dilution due to jetting or momentum effects using an initial velocity estimate; if this modification is not applied, the initial gas velocity is incorrectly over estimated. This correction is not needed in TSCREEN). Go to step 7 (Section 4.2.3.3) to select the appropriate dispersion model.

If the screening procedure above indicates that partial condensation of the released gas occurs, the following section should be used.

### 4.2.3.2 Continuous (Two-Phase) Release Rate Estimate: Gas Storage which Partially Condenses on Depressurization

Similar Releases: A gas leak from a tank, a gas leak from a pipe, or gas discharge from a pressure relief valve mounted on a tank.

Discussion:

Materials which are stored under pressure will depressurize when released to the atmosphere. This depressurization can result in the formation of two contaminant phases (saturated liquid and vapor) for: gases which cool so that condensation occurs during the depressurization process; and high volatility liquids (liquids whose normal boiling point is below the ambient temperature) which are stored at above ambient pressure (typically). (See Section 4.3.2 for more discussion on two-phase releases.) This scenario considers the release from a tank (or reservoir) and includes a provision for the effect of a pressure drop (piping) between the tank and the hole or opening.

This procedure applies to a continuous release of a gas which partially condenses during depressurization; the screening procedure for this scenario should only be applied if the screening procedure above indicated that partial condensation of the released gas occured. The release occurs (constant pressure and temperature) from a containment (reservoir) through a hole or opening; a provision is made for the effect of a pressure drop (piping) between the tank and the hole or opening.

Limitations and Assumptions:

The pressure and temperature of the tank (or reservoir) contents are essentially constant. The hole or opening size must be sufficiently small, otherwise the reservoir temperature and pressure may no longer be constant. For the case of a leak from a tank, the assumption of constant reservoir temperature and pressure may be violated if a significant percentage of the tank contents is released. If the reservoir temperature and pressure are not constant, the release rate may vary with time, but the maximum release rate is generally obtained for the initial reservoir temperature and pressure.

For the case of a leak from a pipe when $\beta > 0.2$ (as defined below), the assumption of constant temperature and pressure in the pipe may be violated; for such a case, the reservoir conditions should be taken from an upstream location (tank or reservoir) where the temperature and pressure will be (approximately) constant. For the case of a leak from a pipe when $\beta \leq 0.2$, the assumption of constant temperature and pressure in the pipe is reasonable, and the reservoir conditions should be taken to be the conditions within the pipe.

The vapor phase of the released material must be an ideal gas at the reservoir conditions, during the depressurization process, and after depressurization to the atmosphere; for the case of a tank containing vapor and liquid, the hole must be in the vapor space of the tank. For two phase flows, all released liquid is assumed to travel downwind as an aerosol with little rain out of liquid near the source (Spicer, 1992).

Input Information:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($m^2$) |
| $A_1$ | flow area representing reservoir conditions ($m^2$) (In case of a leak from a tank, $A_1 \rightarrow \infty$ (and $\beta = 0$); in the case of a leak from a pipe, $A_1$ is the cross-sectional area of the pipe.) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (J/kg-mole·°K) (For contaminant mixtures, see Appendix B) |
| $D_0$ | (equivalent) diameter of hole or opening ($D_0 = 2 \cdot \sqrt{A_0/\pi}$) (m) |
| $D_p$ | pipe diameter (as appropriate) (m) |
| $L_p$ | pipe length (as appropriate) (m) |
| $M_w$ | gas (contaminant) molecular weight (g/g-mole) (For contaminant mixtures, see Appendix B) |
| $P_a$ | ambient pressure (Pa) |
| $P_v$ | vapor pressure as a function of temperature (Pa) |
| $P_1$ | reservoir pressure (Pa) |
| R | gas constant (8314 J/kg-mole•°K or 8314 Pa•$m^3$/kg-mole•°K) |
| $T_b$ | contaminant normal boiling point (°K) |
| $T_c$ | critical temperature (°K) (For contaminant mixtures, see Appendix B) |
| $T_1$ | reservoir temperature (°K) |
| $\beta$ | $\sqrt{A_0/A_1}$ (dimensionless) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_pM))$ at $T_1$ (dimensionless) where R = 8314 (J/kg-mole·°K) |
| $\lambda$ | heat of vaporization at the normal boiling point (cal/g-mole) |
| $\rho_1$ | contaminant density at not normal boiling point ($kg/m^3$) |

Procedure:

5. **Two-Phase Choked Flow.** Estimate the choked flow pressure $P_*$ to determine if the flow is choked using the procedure described in Section 4.2.3.1. If the flow is not choked, proceed to Step 6. For choked flow, estimate the discharge temperature $T_2$, discharge density $\rho_2$, and the emission rate $Q_m$.

A. **Estimate $T_*$.** For pure components, estimate $T_*$ (the temperature which corresponds to $P_*$) from the vapor pressure (Clausius-Clapeyron) equation:

$$P_* = 101325 \cdot \exp\left( \frac{\lambda M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_*} \right) \right) \qquad (4.2.3\text{-}7)$$

which can be rewritten as:

$$T_* = \frac{1}{\dfrac{1}{T_b} - \dfrac{R}{\lambda\, M_w} \cdot \ln\left( \dfrac{P_*}{101325} \right)}$$

B. **Estimate Properties at Choked Flow Conditions.** Based on assumed isentropic behavior, estimate the vapor fraction at choked flow conditions $X_*$ as follows:

$$X_* = 1 + \frac{T_*}{\lambda\, M_w} \left[ M_w\, C_p \ln\left( \frac{T_1}{T_*} \right) - R \ln\left( \frac{P_1}{P_*} \right) \right] \qquad (4.2.3\text{-}8)$$

Using $X_*$ from Equation (4.2.3-8), estimate the enthalpy change ($H_1$-$H_*$) and the density $\rho_*$ as follows:

$$H_1 - H_* = C_p\, (T_1 - T_*) + \lambda\, (1 - X_*) \qquad (4.2.3\text{-}9)$$

$$\rho_* = \left[ X_* \left( \frac{R\, T_*}{P_*\, M_w} \right) + \left( \frac{1 - X_*}{\rho_1} \right) \right]^{-1} \qquad (4.2.3\text{-}10)$$

Note that values for individual enthalpies $H_1$ and $H_*$ are not required.

C. **Estimate Emission Rate.** Extending the ideas suggested by Lees (1950), estimate the emission rate $Q_m$ (kg/s) as follows:

$$Q_m = A_0\, \rho_* \left[ 2 \cdot 0.85 \left( \frac{H_1 - H_*}{1 + 4\, f\, L_p / D_p} \right) \right]^{1/2} \qquad (4.2.3\text{-}11)$$

where 0.85 is included to account for irreversibilities in the flow based on Lewitt (1953) and the term $4fL_p/D_p$ accounts for (piping) pressure drop between the reservoir and the hole or opening; as a preliminary estimate, use f=0.0045 (since typical Reynolds numbers for these applications are larger than $10^5$).

D. **Estimate Discharge Temperature and Density.** Estimate the discharge temperature $T_2$ (after depressurization). If a condensed phase is present, $T_2$ will be given by the Clausius Clapeyron equation:

$$P_a = 101325 \exp\left( \frac{\lambda\, M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_2} \right) \right) \qquad (4.2.3\text{-}12)$$

which can be rewritten as:

$$T_2 = \frac{1}{\dfrac{1}{T_b} - \dfrac{R}{\lambda\, M_w} \cdot \ln\left( \dfrac{P_a}{101324} \right)}$$

Using this estimate of $T_2$, estimate the vapor fraction $X_2$ as:

$$X_2 = X_* + C_p (T_* - T_2)/\lambda \qquad (4.2.3\text{-}13)$$

When $X_2$ (estimated from Equation (4.2.3-13)) satisfies $1 \geq X_2 \geq 0$, the estimate of $T_2$ is valid, and the density of the discharged material is given by:

$$\rho_2 = \left[ X_2 \left( \frac{R\, T_2}{P_a\, M_w} \right) + \left( \frac{1 - X_2}{\rho_L} \right) \right]^{-1} \qquad (4.2.3\text{-}14)$$

(Note that for choked flow conditions, correct application of a dispersion model may require that the diameter of the hole or opening be modified to $D_0(\rho_*/\rho_2)^{1/2}$ if the model accounts for initial air dilution due to jetting or momentum effects; if this modification is not applied, the initial aerosol velocity is incorrectly overestimated. This correction is not needed for TSCREEN.)

However, if $X_2 < 0$ or $X_2 > 1$, the contaminant condensed phase which was present at $P_*$ and $T_*$ is no longer present, and the released contaminant is a gas (without any condensed phase); the discharge temperature and density are estimated as follows:

$$T_2 = T_* + \lambda (1 - X_*)/C_p \qquad (4.2.3\text{-}15)$$

$$\rho_2 = \frac{P_a\, M_w}{R\, T_2} \qquad (4.2.3\text{-}16)$$

$X_2 = 0$.

E. Go to step 7 (Section 4.2.3.3) to select the dispersion model.

6. **Two-Phase Subcritical (Nonchoked) Flow.** For subcritical

flow, estimate the gas/liquid discharge temperature $T_2$, discharge density $\rho_2$, and the emission rate $Q_m$.

A. **Estimate $T_2$.** For pure components, estimate $T_2$ from the Clausius-Clapeyron equation:

$$P_a = 101325 \exp\left( \frac{\lambda M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_2} \right) \right) \qquad (4.2.3\text{-}17)$$

which can be rewritten as:

$$T_2 = \frac{1}{\dfrac{1}{T_b} - \dfrac{R}{\lambda M_w} \cdot \ln\left( \dfrac{P_a}{101325} \right)}$$

B. **Estimate Properties at Discharge Conditions.** Based on assumed isentropic behavior, estimate the vapor fraction at discharge flow conditions $X_2$ as:

$$X_2 = 1 + \frac{T_2}{\lambda M_w} \left[ M_w C_p \ln\left( \frac{T_1}{T_2} \right) - R \ln\left( \frac{P_1}{P_a} \right) \right] \qquad (4.2.3\text{-}18)$$

Using $X_2$ from Equation (4.2.3-18), estimate the enthalpy change $(H_1 - H_2)$ and the density $\rho_2$ as:

$$H_1 - H_2 = C_p (T_1 - T_2) + \lambda (1 - X_2) \qquad (2.3\text{-}19)$$

$$\rho_2 = \left[ X_2 \left( \frac{R T_2}{P_a M_w} \right) + \left( \frac{1 - X_2}{\rho_L} \right) \right]^{-1} \qquad (2.3\text{-}20)$$

Note that values for the individual enthalpies are not required.

C. **Estimate Emission Rate.** Extending the ideas suggested be Lees (1950), estimate the emission rate $Q_m$ as:

$$Q_m = A_0 \rho_2 \left[ 2 \cdot 0.85 \left( \frac{H_1 - H_2}{1 + 4 f L_p / D_p} \right) \right]^{1/2} \qquad (2.3\text{-}21)$$

where 0.85 is included to account for irrevesibilities in the flow based on Lewitt (1953) and the term $4fL_p/D_p$ accounts for the pressure drop (piping) between the reservoir and the hole or opening (as appropriate); as a preliminary estimate, use $f = 0.0045$ (since typical Reynolds numbers for these applications are larger than $10^5$).

D. Go to step 7 to select the dispersion model.

#### 4.2.3.3 Dispersion Model Selection

See Section 2.4 for a complete discussion of the model selection.

Input Information:

$T_a$ ambient temperature (°K)
$Q$ total amount of material released (kg)

Procedure:

7. **Buoyancy Check.** Evaluate release buoyancy as a first check.

   A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\ M_a}{R\ T_a} \qquad (4.2.3\text{-}22)$$

   where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmole).

   B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 8. If the buoyancy is neutral or positive, the SCREEN model for a point source should be used. (See Section 2.4 for more information on model selection.)

8. **Release Duration.** The release duration is used as an input into the RVD and Britter-McQuaid models. The release duration is used to determine if the release should be modeled as continuous or instantaneous (see Section 2.5). Calculate the release duration $T_d$ using the equation below:

$$T_d\ (\text{min}) = \frac{Q\ (\text{kg})}{Q_m\ (\text{kg/s}) \cdot 60\ (\text{s/min})} \qquad (4.2.3\text{-}23)$$

#### 4.2.3.4 Examples

##### 4.2.3.4.1 Example 1: Air Leak from Reservoir - Choked

Discussion:

In this example, 400 kg of a chemical with the same properties of (dry) air stored at $1.101\text{x}10^6$ Pa and 293.15 °K is released from a tank through a 5.25 cm hole on the side of the tank. The nearest distance to the fenceline is 100 meters.

Maximum 15-minute average concentration is needed. This example demonstrates the procedure when the flow is choked.

The following information will be required:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($\pi D_0^2/4 = 0.002165$ m$^2$) |
| $A_1$ | flow area representing reservoir conditions ($A_1 \rightarrow \infty$ m$^2$) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (1004 J/kg•°K) |
| $D_0$ | diameter of hole or opening ($D_0$ = 0.0525 m) |
| $M_w$ | gas (contaminant) molecular weight (29 kg/kmole) |
| $P_a$ | ambient pressure (101325 Pa) |
| $T_b$ | boiling point temperature (79 °K) |
| $P_1$ | reservoir pressure ($1.101\mathrm{x}10^6$ Pa) |
| R | gas constant (8314 J/kg-mole•°K or 8314 Pa•m$^3$/kg-mole•°K) |
| Q | total amount of material released (400 kg) |
| $T_a$ | ambient temperature (293.15 °K) |
| $T_c$ | critical temperature (132 °K) |
| $T_1$ | reservoir temperature (293.15 °K) |
| $\beta$ | $\sqrt{A_0/A_1}$ (0.0) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_pM_w))$ at $T_1$ (1.40) |
| $\rho_1$ | reservoir density (at $T_1$ and $P_1$) ($\rho_1 = P_1M_w/(RT_1) = (1.101\mathrm{x}10^6)(29)/((8314)(293.15)) = 13.10$ kg/m$^3$) |

With this information, the procedure discussed above is used to determine the release rate, the discharge temperature, and the discharge density. For dispersion calculations, 15-minute average concentrations at a fenceline of 100 m are desired.

Procedure:

1. **Choked Pressure.** Estimate the choked pressure $P_*$ to determine if the flow is choked. From Equation (4.2.3-1):

$$P_* = \left(\frac{2}{1.40 + 1}\right)^{1.40/(1.40-1)} \cdot 1.101\times10^6 = 5.82\times10^5 \; (P_a)$$

Since $P_* > P_a$, the flow is choked; go to step 2.

2. **Choked Flow.** For choked flow, estimate the gas temperature $T_*$ when the pressure is $P_*$, the emission rate is $Q_m$, and the discharge temperature is $T_2$.

A. **Estimate $T_*$.** Estimate $T_*$ using Equation (4.2.3-2) with $\gamma = 1.40$ and $T_1 = 293.15$ °K:

$$T_* = \left(\frac{2}{1.40 + 1}\right) \cdot 293.15 = 244 \; ^{\circ}\mathrm{K}$$

This estimate of $T_*$ must be checked to see if Equation (4.2.3-2) applies. If $T_*$ is greater than the (pseudo) critical temperature $T_c$ for air, Equation (4.2.3-2) applies. (The pseudo critical temperature of air is $T_c = 0.79(126.2) + 0.21(154.6) = 132^\circ K$ where the assumed composition (mole fraction) of air is 79% $N_2$ and 21% $O_2$, and the critical temperatures of $N_2$ and $O_2$ are 126.2 °K and 154.6 °K, respectively.)

B. **Estimate Emission Rate.** Estimate the emission rate $Q_m$ using Equation (4.2.3-3) with C = 0.75:

$$Q_m = C\cdot 0.002165\left[1.101\times10^6\cdot 13.10\cdot 1.40\left(\frac{2}{1.40+1}\right)^{(1.40+1)/(1.40-1)}\right]^{1/2}$$

$$Q_m = 4.22 \text{ kg/s}$$

C. **Estimate Discharge Temperature.** Estimate the discharge (after depressurization) temperature $T_2$ with Equation (4.2.3-4):

$$T_2 = 293.15\left[1 - 0.85\left(\frac{1.40-1}{1.40+1}\right)\right] = 252\ ^\circ K$$

Note that $T_2 > T_*$, so equations used were appropriate. Since flow is choked, proceed to Step 4.

4. **Discharge Density.** Estimate the discharge density $\rho_2$ from the discharge temperature $T_2$ using the ideal gas law:

$$(101325)(29)/(8314)(252) = 1.40 \text{ kg/m}^3$$

(For these choked flow conditions, correct application of a dispersion model may require that the diameter of the hole or opening be modified to $D_0(P_*T_2/P_aT_*)^{1/2} = 0.0525\ [(5.82x10^5)(252)/(101325)(244)]^{1/2} = 0.128$ m if the model accounts for initial air dilution due to jetting or momentum effects.) Since no partial condensation was indicated by screening calculations, proceed to Step 7.

7. **Perform Buoyancy Check.**

A. Calculate density of air using Equation (4.2.3-22):

$$\rho_{air} = \frac{101325\cdot 28.9}{8314\cdot 293.15} = 1.20 \text{ kg/m}^3$$

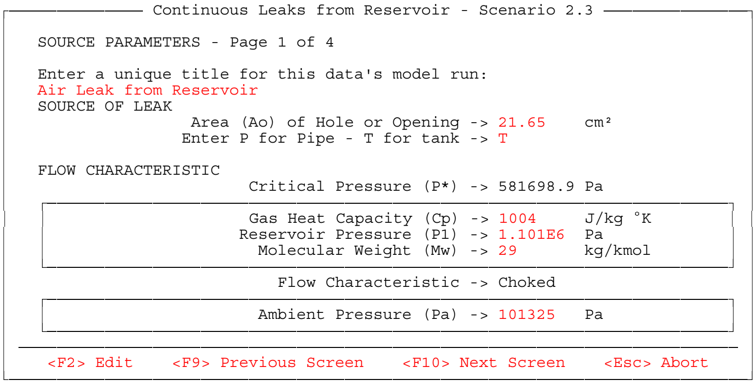
B. $\rho_2/\rho_{air} > 1$ therefore, buoyancy is negative.

8. **Release Duration.** Calculate the release duration $T_d$ using Equation (4.2.3-23) as follows:

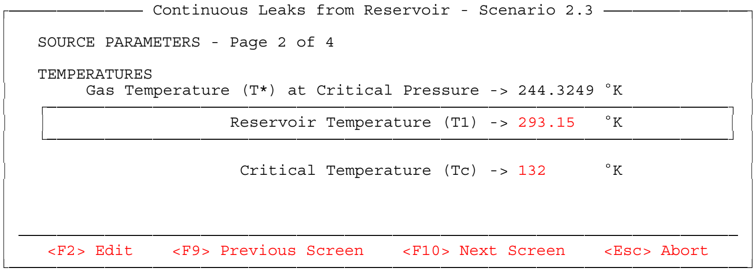
$$T_d\ (\text{min}) = \frac{400\ (\text{kg})}{4.22\ (\text{kg/s}) \cdot 60\ (\text{s/min})} = 1.58\ \text{min}$$

After this calculation run the Britter-McQuaid model since the release is not from a vertically directed jet. (See Section 5.4 for more information on the Britter-McQuaid model.)

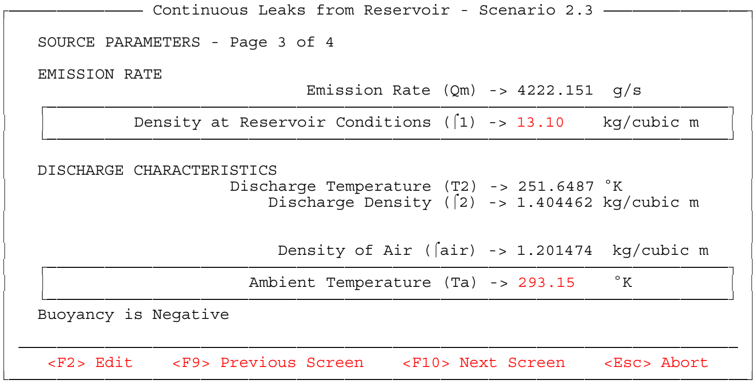
Data entry in the TSCREEN model for this example is shown below:



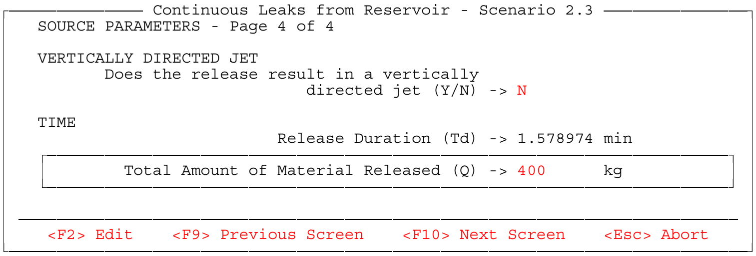
```
 Continuous Leaks from Reservoir - Scenario 2.3

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Air Leak from Reservoir
SOURCE OF LEAK
                Area (Ao) of Hole or Opening -> 21.65    cm²
               Enter P for Pipe - T for tank -> T

FLOW CHARACTERISTIC
                      Critical Pressure (P*) -> 581698.9 Pa

                      Gas Heat Capacity (Cp) -> 1004     J/kg °K
                     Reservoir Pressure (P1) -> 1.101E6  Pa
                       Molecular Weight (Mw) -> 29       kg/kmol

                         Flow Characteristic -> Choked

                       Ambient Pressure (Pa) -> 101325   Pa

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Continuous Leaks from Reservoir - Scenario 2.3

SOURCE PARAMETERS - Page 2 of 4

TEMPERATURES
     Gas Temperature (T*) at Critical Pressure -> 244.3249 °K

                    Reservoir Temperature (T1) -> 293.15   °K


                     Critical Temperature (Tc) -> 132      °K



 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

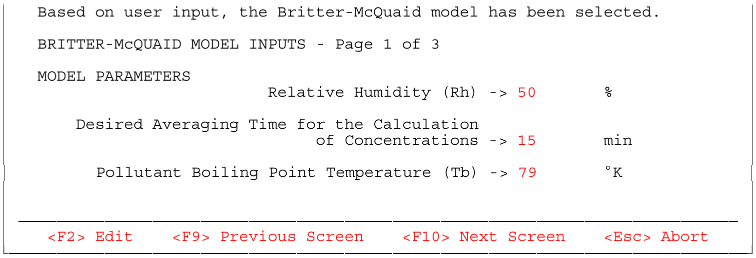


```
 Continuous Leaks from Reservoir - Scenario 2.3

SOURCE PARAMETERS - Page 3 of 4

EMISSION RATE
                          Emission Rate (Qm) -> 4222.151  g/s

          Density at Reservoir Conditions (⌈1) -> 13.10     kg/cubic m


DISCHARGE CHARACTERISTICS
                    Discharge Temperature (T2) -> 251.6487 °K
                        Discharge Density (⌈2) -> 1.404462 kg/cubic m


                         Density of Air (⌈air) -> 1.201474  kg/cubic m

                      Ambient Temperature (Ta) -> 293.15    °K

Buoyancy is Negative

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

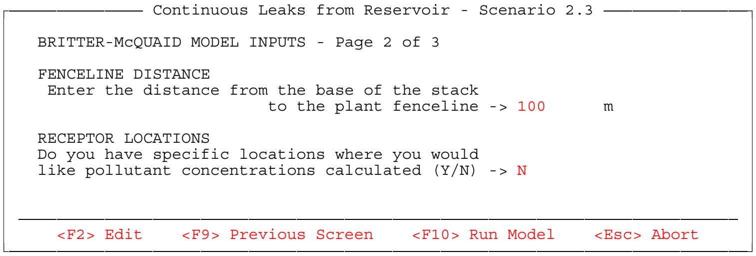


```
 Continuous Leaks from Reservoir - Scenario 2.3
SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET
       Does the release result in a vertically
                          directed jet (Y/N) -> N

TIME
                       Release Duration (Td) -> 1.578974 min

         Total Amount of Material Released (Q) -> 400      kg


 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

```
 Continuous Leaks from Reservoir - Scenario 2.3
```



```
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS
                        Relative Humidity (Rh) -> 50       %

    Desired Averaging Time for the Calculation
                             of Concentrations -> 15       min

      Pollutant Boiling Point Temperature (Tb) -> 79       °K

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
              Continuous Leaks from Reservoir - Scenario 2.3

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE
 Enter the distance from the base of the stack
                        to the plant fenceline -> 100      m

RECEPTOR LOCATIONS
Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

  <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

The Britter-McQuaid model's output is displayed below:

```
============================================================================
                                           11-19-92
                                                                13:34:04
 *** B&M MODEL RUN ***

Air Leak from Reservoir

INPUTS:
   AMBIENT PRESSURE (ATM)     =    1.000
   AMBIENT TEMP (K)           =    293.1
   AVERAGING TIME (MIN)       =    15.00
   BOILING PT TEMP (K)        =    79.00
   DURATION (S)               =    94.74
   EMISSION RATE (KG/S)       =    4.222
   EXIT TEMP (K)              =    251.6
   MASS (KG)                  =    400.0
   MOL. WEIGHT (G/G-MOLE)     =    29.00
   RELATIVE HUMIDITY (%)      =    50.00
   VAPOR FRACTION             =    1.000


     ***************************************
     ***   SUMMARY OF B&M MODEL RESULTS  ***
     ***************************************

   MAX CONC      MAX CONC     DIST TO    WIND SPEED
   (UG/M**3)      (PPM)       MAX (M)      (M/S)
   ---------    ---------     -------    ----------
   .7978E+08    .6617E+05      100.          3.

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************


**********************************
***        B&M DISTANCES      ***
**********************************


   DIST        CONC            CONC       WIND SPEED
    (M)      (UG/M**3)         (PPM)         (M/S)
  -------    ---------       ---------    ----------
   100.      .7978E+08       .6617E+05          3.
   200.      .1323E+08       .1098E+05          2.
   300.      .7453E+07       6182.              2.
   400.      .3704E+07       3072.              2.
   500.      .2371E+07       1966.              3.
   600.      .1821E+07       1510.              3.
   700.      .2115E+07       1754.              2.
   800.      .2861E+07       2373.              4.
   900.      .2132E+07       1768.              4.
  1000.      .1638E+07       1359.              4.
  1100.      .1291E+07       1071.              4.
  1200.      .1039E+07       861.4              4.
  1300.      .8502E+06       705.2              4.
  1400.      .7064E+06       585.9              4.
  1500.      .5945E+06       493.1              4.
  1600.      .5059E+06       419.6              4.
  1700.      .4348E+06       360.6              4.
  1900.      .3292E+06       273.1              4.
  2100.      .2564E+06       212.6              4.
  2300.      .2042E+06       169.4              4.
  2500.      .1658E+06       137.5              4.
  2700.      .1368E+06       113.4              4.
  2900.      .1144E+06       94.88              4.
  3100.      .9683E+05       80.31              4.
  3300.      .8282E+05       68.69              4.
  3600.      .6663E+05       55.26              4.
```

```
   3900.       .5455E+05       45.24            4.
   4200.       .4532E+05       37.59            4.
   4500.       .3814E+05       31.63            4.
   5000.       .2931E+05       24.31            4.


 CALCULATED VALUES:
    DENSITY OF DEPRESSURIZED CONTAMINANT (KG/M**3) =    1.405
    DENSITY OF AMBIENT AIR (KG/M**3)               =    1.199
    MOLE FRACTION                                  =    1.000
    MIN DIST INST (M)                              =    3158.
    MAX DIST CNST (M)                              =    757.9


 ***** NOTES & DEFINITIONS *****
(a) "inst" refers to an instantaneous release (Section 3.6 of B-M Workbook)
(b) "cnst" refers to a continuous release (Section 3.6 of B-M Workbook)
(c) "MIN DIST INST" is the minimum distance downwind at which the release
    may be treated as instantaneous
(d) "MAX DIST CNST" is the maximum distance downwind at which the release
    may be treated as continuous

 *********************************
 ***     END OF B&M OUTPUT      ***
 *********************************
```

### 4.2.3.4.2 Example 2: Air Leak from Reservoir - Subcritical (Not Choked)

Discussion:

In this example, (dry) air stored at $1.82 \times 10^5$ and 293.15 °K is released from a tank through a 5.25 cm hole in the tank; this example is the same as the previous example except for the reservoir pressure. This example demonstrates the procedure when the flow is not choked.

The following information will be required:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($\pi D_0^2/4 = 0.002165\ m^2$) |
| $A_1$ | flow area representing reservoir conditions ($A_1 \rightarrow \infty\ m^2$) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (6.959 cal/g-mole °K) |
| $D_0$ | diameter of hole or opening ($D_0 = 0.0525$ m) |
| $M_w$ | gas (contaminant) molecular weight (29 kg/kmole) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_1$ | reservoir pressure ($1.82 \times 10^5$ Pa) |
| R | gas constant (8314 J/kg-mole•°K or 8314 Pa•$m^3$/kg-mole•°K) |
| Q | total amount of material released (400 kg) |
| $T_a$ | ambient temperature (293.15 °K) |
| $T_c$ | critical temperature (132 °K) |
| $T_1$ | reservoir temperature (293.15 °K) |
| $\beta$ | $\sqrt{A_0/A_1}$ (0.0) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_p M_w))$ at $T_1$ (1.40) |
| $\rho_1$ | reservoir density (at $T_1$ and $P_1$) ($\rho_1 = P_1 M_w/(RT_1) = (1.82 \times 10^5)(29)/((8314)(293.15)) = 2.17\ kg/m^3$) |

With this information, the procedure discussed above is used to determine the release rate, the discharge temperature, and the discharge density.

Procedure:

1. **Choked Pressure.** Estimate the choked pressure $P_*$ to determine if the flow is choked. From Equation (4.2.3-1):

$$P_* = \left( \frac{2}{1.40 + 1} \right)^{1.40/(1.40-1)} \cdot 1.82\times10^5 = 9.61\times10^4 \; (P_a)$$

Since $P_* < P_a$, the flow is not choked; go to step 3.

3. **Subcritical Flow.** For subcritical (not choked) flow, estimate the emission rate $Q_m$ and the discharge temperature $T_2$.

   A. **Estimate Emission Rate.** Estimate the emission rate $Q_m$ using Equation (4.2.3-5):

$$Q_m = K \cdot Y \cdot .002165 \left[ 2 \cdot 2.17 (1.82\times10^5 - 101325) \right]^{1/2} = 0.691 \; kg/s$$

where

$$K = 0.62 \,/\, \sqrt{1 - 0.0^4} = 0.62$$

$$Y = 1 - \left( \frac{1.82\times10^5 - 101325}{1.82\times10^5 \cdot 1.40} \right) (0.41 + 0.35 \cdot 0^4) = 0.870$$

   B. **Estimate Discharge Temperature.** Estimate the discharge (after depressurization) temperature $T_2$. From Equation (4.2.3-6):

$$T_2 = 2 \cdot 293.15 \,/\, \left[ 1 + \left( 1 + 4 \cdot a \cdot 293.15 \right)^{1/2} \right] = 265 \; ^\circ K$$

where

$$a = \frac{1}{2 \cdot C_p} \left( \frac{0.691 \cdot 8314}{101325 \cdot 29 \cdot 0.002165} \right)^2 = 4.06\times10^{-4}$$

where

$$C_p^{/}(J/kg^\circ K) = 6.95889 (cal/g\text{-}mole \; ^\circ K) \cdot \frac{1000 (g/kg) \cdot 4.184 (J/cal)}{29 (g/g\text{-}mole)} = 1004 (J/kg^\circ K)$$

Since $T_2 > T_c$, proceed to Step 4.

4. **Discharge Density.** Estimate the discharge density $\rho_2$ from the discharge temperature $T_2$ using the ideal gas law:

$$(101325)(29)/(8314)(265) = 1.33 \; kg/m^3$$

(Correct application of a dispersion model may require that the diameter of the hole or opening be modified to

$D_0(\rho_1/\rho_2)^{1/2}$ = 0.0525 m $(2.17/1.33)^{1/2}$ = 0.0671 m if the model accounts for initial air dilution due to jetting or momentun effects; if this modification is not applied, the initial gas velocity is incorrectly overestimated.) Since no condensation is predicted from the above calculations, proceed to Step 7.

7. **Perform Buoyancy Check.**

A. Calculate density of air using Equation (4.2.3-22):

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 293.15} = 1.20 \text{ kg/m}^3$$

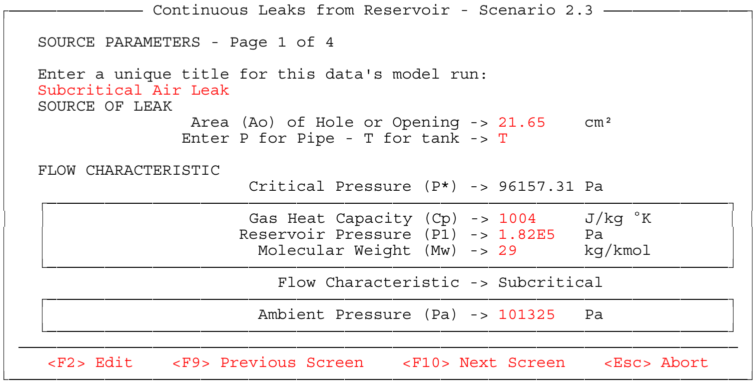
B. $\rho_2/\rho_{air} > 1$ therefore, buoyancy is negative.

8. **Release Duration.** Calculate the release duration $T_d$ using Equation (4.2.3-23) as follows:

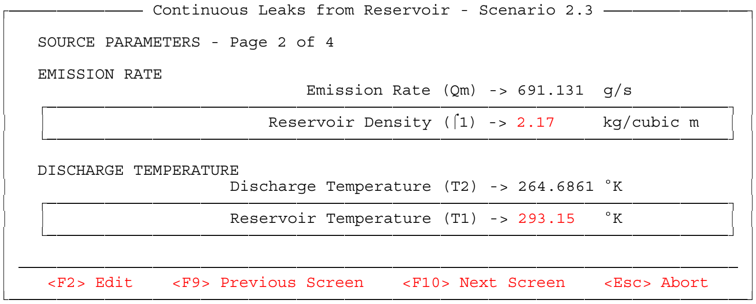
$$T_d \text{ (min)} = \frac{400 \text{ (kg)}}{0.691 \text{ (kg/s)} \cdot 60 \text{ (s/min)}} = 9.65 \text{ min}$$

After this calculation run the Britter-McQuaid model since the release is not from a vertically directed jet. (See Section 5.4 for more information on the Britter-McQuaid model.)

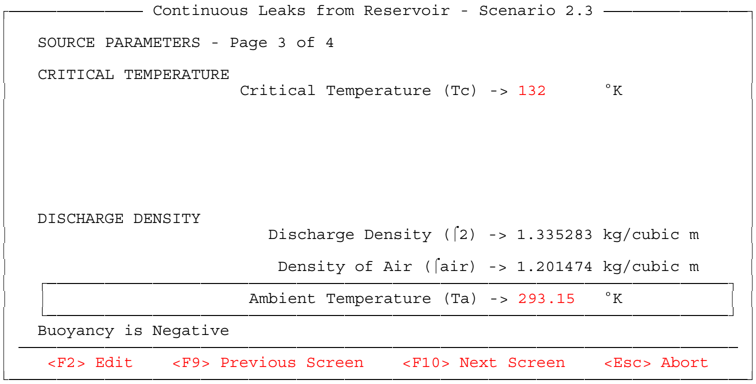
Data entry in the TSCREEN model for this example is shown below:



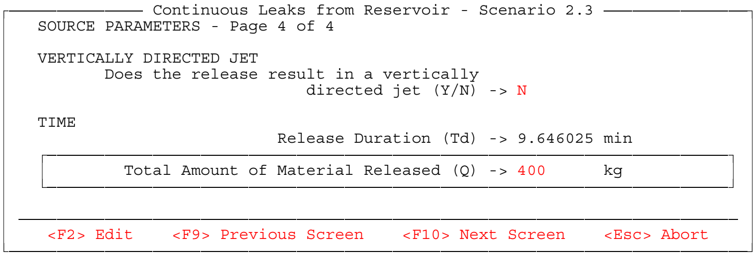
```
           Continuous Leaks from Reservoir - Scenario 2.3

  SOURCE PARAMETERS - Page 1 of 4

  Enter a unique title for this data's model run:
  Subcritical Air Leak
  SOURCE OF LEAK
                Area (Ao) of Hole or Opening -> 21.65    cm²
               Enter P for Pipe - T for tank -> T

  FLOW CHARACTERISTIC
                      Critical Pressure (P*) -> 96157.31 Pa

                      Gas Heat Capacity (Cp) -> 1004     J/kg °K
                     Reservoir Pressure (P1) -> 1.82E5   Pa
                       Molecular Weight (Mw) -> 29       kg/kmol

                         Flow Characteristic -> Subcritical

                       Ambient Pressure (Pa) -> 101325   Pa

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



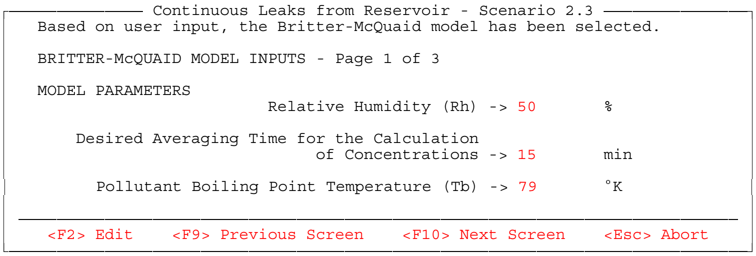
```
           Continuous Leaks from Reservoir - Scenario 2.3

  SOURCE PARAMETERS - Page 2 of 4

  EMISSION RATE
                         Emission Rate (Qm) -> 691.131  g/s

                     Reservoir Density (⌠1) -> 2.17     kg/cubic m

  DISCHARGE TEMPERATURE
                  Discharge Temperature (T2) -> 264.6861 °K

                  Reservoir Temperature (T1) -> 293.15   °K

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



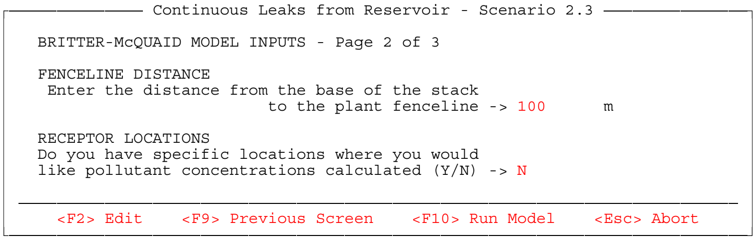
```
Continuous Leaks from Reservoir - Scenario 2.3

SOURCE PARAMETERS - Page 3 of 4

CRITICAL TEMPERATURE
                    Critical Temperature (Tc) -> 132      °K




DISCHARGE DENSITY
                       Discharge Density (⌠2) -> 1.335283 kg/cubic m

                        Density of Air (⌠air) -> 1.201474 kg/cubic m

                    Ambient Temperature (Ta) -> 293.15    °K

Buoyancy is Negative

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous Leaks from Reservoir - Scenario 2.3
SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET
       Does the release result in a vertically
                          directed jet (Y/N) -> N

TIME
                        Release Duration (Td) -> 9.646025 min

        Total Amount of Material Released (Q) -> 400      kg


 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous Leaks from Reservoir - Scenario 2.3
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS
                       Relative Humidity (Rh) -> 50       %

    Desired Averaging Time for the Calculation
                           of Concentrations -> 15       min

      Pollutant Boiling Point Temperature (Tb) -> 79       °K

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous Leaks from Reservoir - Scenario 2.3

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE
 Enter the distance from the base of the stack
                       to the plant fenceline -> 100      m

RECEPTOR LOCATIONS
Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

  <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

A summary of the Britter-McQuaid model's output is displayed below:

```
                    ***************************************
                    ***   SUMMARY OF B&M MODEL RESULTS  ***
                    ***************************************

                  MAX CONC      MAX CONC     DIST TO    WIND SPEED
                  (UG/M**3)       (PPM)      MAX (M)      (M/S)
                  ---------     ---------    -------    ----------
                   .3102E+08     .2573E+5      100.          1.

               ***************************************************
               ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
               ***************************************************
```

### 4.2.3.4.3 Example 3: Chlorine Gas Leak - Choked

Discussion:

In the example, chlorine gas stored at 6.7999 atm and 320 °K is released through a 2.8 cm hole. This example demonstrates the procedure when the flow is choked.

The following information will be required:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($\pi D_0^2/4$ = 0.0006158 m$^2$) |
| $A_1$ | flow area representing reservoir conditions ($A_1 \rightarrow \infty$ m$^2$) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (489 J/kg•°K) |
| $D_0$ | diameter of hole or opening ($D_0$ = 0.028 m) |
| $M_w$ | gas (contaminant) molecular weight (70.9 kg/kmole) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_1$ | reservoir pressure (6.89x10$^5$ Pa) |
| R | gas constant (8314 J/kg-mole•°K or 8314 Pa•m$^3$/kg-mole•°K) |
| Q | total amount of material released (400 kg) |
| $T_a$ | ambient temperature (293 °K) |
| $T_c$ | critical temperature (417.15 °K) |
| $T_1$ | reservoir temperature (320 °K) |
| $\beta$ | $\sqrt{A_0/A_1}$ (0.0) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_pM_w))$ at $T_1$ (1.32) |
| | heat of vaporization at normal boiling point (2.879x10$^5$ J/kg) |
| $\rho_1$ | contaminant liquid density at the normal boiling point (18.36 kg/m$^3$) |

With this information, the procedure discussed above determines the release rate, the discharge temperature, and the discharge density.

Procedure:

1. **Choked Pressure.** Estimate the choked pressure $P_*$ to determine if the flow is choked. From Equation (4.2.3-1):

$$P_* = \left(\frac{2}{1.32 + 1}\right)^{1.32/(1.32-1)} \cdot 6.89\times10^5 = 3.74\times10^5 \ P_a$$

Since $P_* > P_a$, the flow is choked; go to step 2.

2. **Choked Flow.** For choked flow, estimate the gas temperature $T_*$ when the pressure is $P_*$, the emission rate $Q_m$, and the discharge temperature $T_2$.

   A. **Estimate $T_*$.** Estimate $T_*$ using Equation (4.2.3-2) with $\gamma$ = 1.32 and $T_1$ = 320 °K:

$$T_* = \left( \frac{2}{1.32 + 1} \right) \cdot 320 = 276\ ^\circ\mathrm{K}$$

The Clausius-Clapeyron equation can be conveniently used to estimate the vapor pressure at $T_*$ as follows:

$$P_v = 101325 \exp\left( \frac{2.879\times10^5 \cdot 70.9}{8314} \left( \frac{1}{239.05} - \frac{1}{276} \right) \right) = 4.01\times10^5\ \mathrm{Pa}$$

Since $P_v(T_*) > P_*$, no condensation occurs.

B. **Estimate Emission Rate.** Estimate the emission rate $Q_m$ using Equation (4.2.3-3) with C = 0.75:

$$Q_m = C \cdot 0.0006158 \left[ 6.89\times10^5 \cdot 18.36 \cdot 1.32 \left( \frac{2}{1.32 + 1} \right)^{(1.32+1)/(1.32-1)} \right]^{1/2}$$

$$Q_m = 1.10\ \mathrm{kg/s}$$

C. **Estimate Discharge Temperature.** Estimate the emission discharge (after depressurization) temperature $T_2$ with Equation (4.2.3-4):

$$T_2 = 320 \left[ 1 - 0.85 \left( \frac{1.32 - 1}{1.32 + 1} \right) \right] = 283\ ^\circ\mathrm{K}$$

Since flow is choked, proceed to Step 4.

4\. **Discharge Density.** Estimate the discharge density $\rho_2$ from the discharge temperature $T_2$ using the ideal gas law:

$$(101325)(70.9)/(8314)(283) = 3.05\ \mathrm{kg/m^3}$$

(For these choked flow conditions, correct application of a dispersion model may require that the diameter of the hole or opening be modified to $D_0(P_*/P_a)^{1/2} = 0.028\ \mathrm{m}\ (3.69/1)^{1/2} = 0.0538\ \mathrm{m}$ if the model accounts for the initial air dilution due to jetting or momentum effects. Since flow is one-phase, proceed to Step 7.

7\. **Perform Buoyancy Check.**

A. Calculate density of air use Equation (4.2.3-22) as follows:

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 293} = 1.20\ \mathrm{kg/m^3}$$

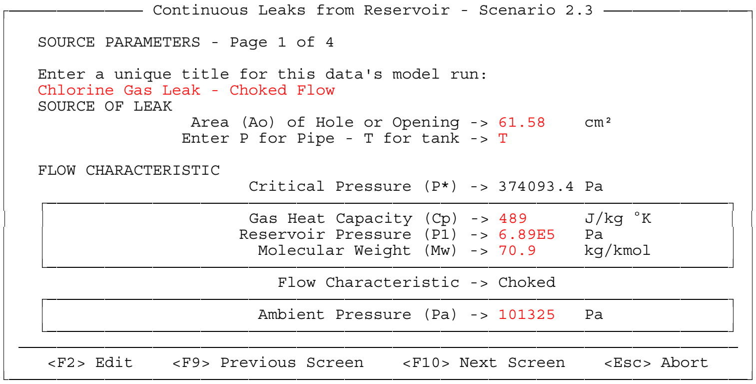
B. $\rho_2/\rho_{air} > 1$ therefore, buoyancy is negative.

8. **Release Duration.** Calculate the release duration $T_d$ using Equation (4.2.3-23) as follows:

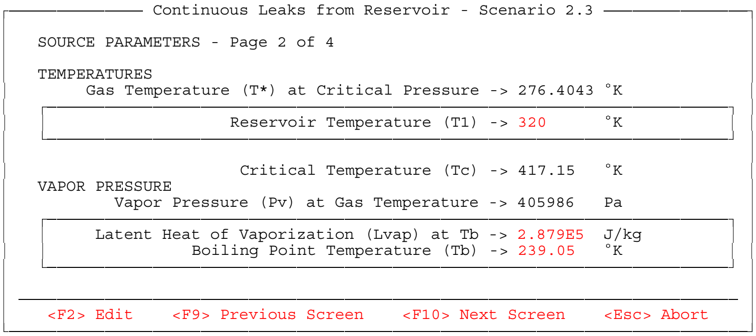
$$T_d \text{ (min)} = \frac{400 \text{ (kg)}}{1.10 \text{ (kg/s)} \cdot 60 \text{ (s/min)}} = 6.06 \text{ min}$$

After this calculation run the Britter-McQuaid model since the release is not from a vertically directed jet. (See Section 5.4 for more information on the Britter-McQuaid model.)

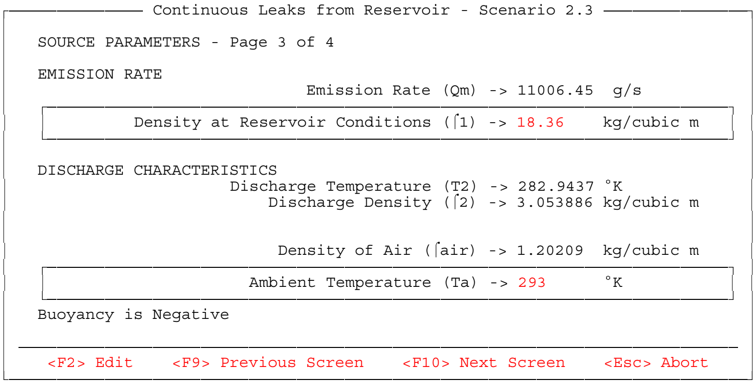
Data entry in the TSCREEN model for this example is shown below:



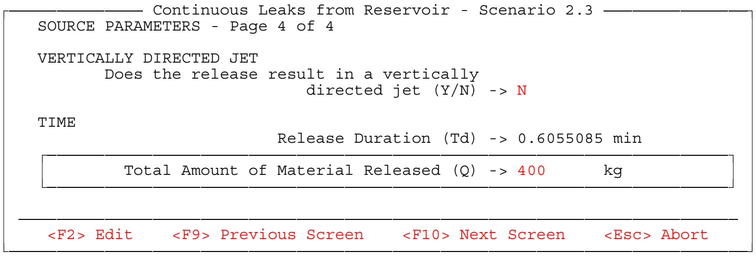
```
              Continuous Leaks from Reservoir - Scenario 2.3

   SOURCE PARAMETERS - Page 1 of 4

   Enter a unique title for this data's model run:
   Chlorine Gas Leak - Choked Flow
   SOURCE OF LEAK
                   Area (Ao) of Hole or Opening -> 61.58    cm²
                  Enter P for Pipe - T for tank -> T

   FLOW CHARACTERISTIC
                         Critical Pressure (P*) -> 374093.4 Pa

                         Gas Heat Capacity (Cp) -> 489      J/kg °K
                        Reservoir Pressure (P1) -> 6.89E5   Pa
                          Molecular Weight (Mw) -> 70.9     kg/kmol

                            Flow Characteristic -> Choked

                          Ambient Pressure (Pa) -> 101325   Pa

    <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



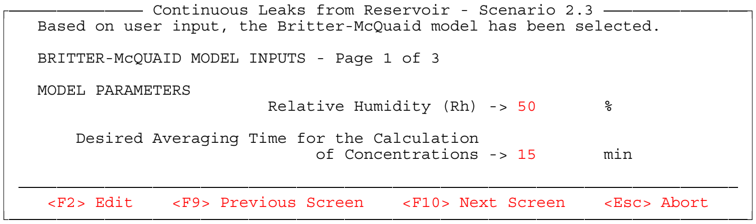
```
              Continuous Leaks from Reservoir - Scenario 2.3

   SOURCE PARAMETERS - Page 2 of 4

   TEMPERATURES
        Gas Temperature (T*) at Critical Pressure -> 276.4043 °K

                       Reservoir Temperature (T1) -> 320      °K


                        Critical Temperature (Tc) -> 417.15   °K
   VAPOR PRESSURE
           Vapor Pressure (Pv) at Gas Temperature -> 405986   Pa

         Latent Heat of Vaporization (Lvap) at Tb -> 2.879E5  J/kg
                   Boiling Point Temperature (Tb) -> 239.05   °K


    <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



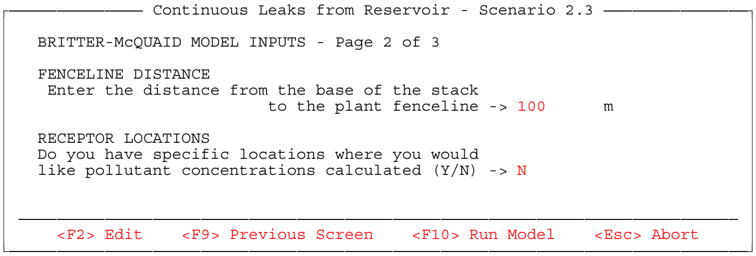
```
              Continuous Leaks from Reservoir - Scenario 2.3

   SOURCE PARAMETERS - Page 3 of 4

   EMISSION RATE
                             Emission Rate (Qm) -> 11006.45  g/s

          Density at Reservoir Conditions (⌠1) -> 18.36     kg/cubic m


   DISCHARGE CHARACTERISTICS
                     Discharge Temperature (T2) -> 282.9437 °K
                         Discharge Density (⌠2) -> 3.053886 kg/cubic m


                          Density of Air (⌠air) -> 1.20209  kg/cubic m

                       Ambient Temperature (Ta) -> 293      °K

   Buoyancy is Negative

    <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Continuous Leaks from Reservoir - Scenario 2.3
SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET
       Does the release result in a vertically
                    directed jet (Y/N) -> N

TIME
                 Release Duration (Td) -> 0.6055085 min

        Total Amount of Material Released (Q) -> 400       kg

 <F2> Edit   <F9> Previous Screen   <F10> Next Screen   <Esc> Abort
```



```
 Continuous Leaks from Reservoir - Scenario 2.3
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS
                  Relative Humidity (Rh) -> 50       %

    Desired Averaging Time for the Calculation
                     of Concentrations -> 15       min

 <F2> Edit   <F9> Previous Screen   <F10> Next Screen   <Esc> Abort
```



```
 Continuous Leaks from Reservoir - Scenario 2.3

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE
 Enter the distance from the base of the stack
                  to the plant fenceline -> 100      m

RECEPTOR LOCATIONS
Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

  <F2> Edit   <F9> Previous Screen   <F10> Run Model   <Esc> Abort
```

A summary of the Britter-McQuaid model's output is displayed below:

```
      ***************************************
      ***   SUMMARY OF B&M MODEL RESULTS  ***
      ***************************************

    MAX CONC      MAX CONC     DIST TO    WIND SPEED
    (UG/M**3)      (PPM)       MAX (M)      (M/S)
    ---------    ---------     -------    ----------
    .2442E+08    8280.           100.          3.

 *****************************************************
 ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
 *****************************************************
```

### 4.2.3.4.4 Example 4: Saturated Vapor Chlorine Leak

Discussion:

In this example, saturated chlorine vapor is discharged through a pressure relief valve (10.16 cm diameter) designed to open at $2.586\text{x}10^6 P_a$ (375 psia); the chlorine vapor temperature is estimated to be 349.2 °K using the Clausius-Clapeyron equation and the normal boiling point of chlorine (239.05 °K). Condensation will be present in this release (at the choked flow conditions). This example demonstrates the procedure when the flow is choked.

The following information will be required:

- $A_0$ area of reservoir hole or opening ($\pi D_0^2/4 = 0.008107\ m^2$)
- $A_1$ flow area representing reservoir conditions ($A_1 \rightarrow \infty\ m^2$)
- $C_p$ gas (contaminant) heat capacity at $T_1$ (489 J/kg·°K)

| | |
|---|---|
| $D_0$ | diameter of hole or opening ($D_0$ = 0.1016 m) |
| $M_w$ | gas (contaminant) molecular weight (70.9 kg/kmol) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_1$ | reservoir pressure ($2.586 \times 10^6$ Pa) |
| R | gas constant (8314 J/kg-mole·°K or 8314 Pa•$m^3$/kg-mole•°K) |
| Q | total amount of material released (400 kg) |
| $T_a$ | ambient temperature (293 °K) |
| $T_b$ | contaminant normal boiling temperature (239.05 °K) |
| $T_c$ | critical temperature (417.15 °K) |
| $T_1$ | reservoir temperature (349.2 °K) |
| $\beta$ | $\sqrt{A_0/A_1}$ (0.0) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_p M_w))$ at $T_1$ (1.32) |
| $\lambda$ | heat of vaporization at the normal boiling point ($2.879 \times 10^5$ J/kg) |
| $\rho_1$ | contaminant liquid density at the normal boiling point (1574 kg/$m^3$) |

With this information, the procedure discussed above determines the release rate, the discharge temperature, and the discharge density.

Procedure:

1. **Choked Flow Pressure.** Estimate the choked flow pressure $P_*$ to determine if the flow is choked. From Equation (4.2.3-1):

$$P_* = \left( \frac{2}{1.32 + 1} \right)^{1.32/(1.32-1)} \cdot 2.586 \times 10^6 = 1.40 \times 10^6 \text{ (Pa)}$$

   Since $P_* > P_a$, the flow is choked; go to step 2.

2. **Choked Flow.** For choked flow, estimate the gas temperature $T_*$ when the pressure is $P_*$, the emission rate $Q_m$, and the discharge temperature $T_2$.

   A. **Estimate $T_*$.** Estimate $T_*$ using Equation (4.2.3-2) with $\gamma = 1.32$ and $T_1 = 349.2$ °K:

$$T_* = \left( \frac{2}{1.32 + 1} \right) \cdot 349.2 = 301 \text{ °K}$$

   This estimate of $T_*$ must be checked to see if Equation (4.2.3-2) applies. $T_*$ is not greater than the (pseudo) critical temperature $T_c$ (417.15 °K); therefore, the contaminant vapor pressure at $T_*$ ($P_v(T_*)$) must be calculated using the Clausius-Clapeyron equation:

$$P_v = 101325 \exp\left( \frac{2.879 \times 10^5 \cdot 70.9}{8314} \left( \frac{1}{239.05} - \frac{1}{301} \right) \right) = 8.39 \times 10^5 \text{ Pa}$$

The chlorine vapor pressure at 301 °K is less than $P_*$; so, condensation was predicted; proceed to step 5.

5. **Two-Phase Choked Flow.** For choked flow, estimate the discharge temperature $T_2$, discharge density $\rho_2$, and the emission rate $Q_m$.

   A. **Estimate $T_*$.** Estimate $T_*$ (the temperature which corresponds to $P_*$) from Equation (4.2.3-7):

$$T_* = \frac{1}{\dfrac{1}{239.05} - \dfrac{8314}{2.879\times10^5\cdot70.9}\cdot\ln\left(\dfrac{2.586\times10^6}{101325}\right)} = 321\ ^\circ K$$

   B. **Estimate Properties at Choked Flow Conditions.** Based on assumed isentropic behavior, the vapor fraction at choked flow conditions is estimated from Equation (4.2.3-8):

$$X_* = 1 + \frac{321.2}{2.879\times10^5\cdot70.9}\left[70.9\cdot489\ \ln\left(\frac{349.2}{321}\right) - 8314\ \ln\left(\frac{2.586\times10^6}{1.40\times10^6}\right)\right]$$

$$= .966$$

Using Equation (4.2.3-9), the enthalpy change is estimated as:

$$H_1 - H_* = 489\ (349.2 - 321) + 2.879\times10^5\ (1 - .966) = 2.36\times10^4\ (\mathrm{J/kg})$$

The density is estimated using Equation (4.2.3-10):

$$\rho_* = \left[0.966\left(\frac{8314\cdot321}{1.40\times10^6\cdot70.9}\right) + \left(\frac{1 - 0.966}{1574}\right)\right]^{-1} = 38.5\ \mathrm{kg/m^3}$$

   C. **Estimate Emission Rate.** Using Equation (4.2.3-11), the emission rate is estimated as:

$$Q_m = 0.008107\cdot38.5\left[2\cdot0.85\left(\frac{2.36\times10^4}{1}\right)\right]^{1/2} = 62.5\ \mathrm{kg/s}$$

   D. **Estimate Discharge Temperature and Density.** Application of Equation (4.2.3-12) gives the discharge temperature ($T_2$) as:

$$T_2 = \frac{1}{\dfrac{1}{239.05} - \dfrac{8314}{2.879\times10^5\cdot70.9}\cdot\ln\left(\dfrac{101325}{101325}\right)} = 239.05\ ^\circ K$$

and Equation (4.2.3-13) gives the vapor fraction ($X_2$) as:

$$X_2 = .966 + 489(321 - 239.05)/2.879\times10^5 = 1.11$$

since $X_2 > 1$, these estimates are not valid. Using Equation (4.2.3-15) gives $T_2$ as:

$$T_2 = 321 + 2.879\times10^5(1 - .966)/489 = 341\ ^\circ K$$

and Equation (4.2.3-16) gives the discharge density ($\rho_2$) as:

$$\rho_2 = \frac{101325 \cdot 70.9}{8314 \cdot 341} = 2.53\ kg/m^3$$

(For these choked flow conditions, correct application of a dispersion model may require that the diameter of the hole or opening be modified to $D_0(\rho_*/\rho_2)^{1/2}$ = $0.1016(38.5/2.53)^{1/2}$ = 0.396 m if the model accounts for initial air dilution due to jetting or momentum effects; if this modification is not applied, the initial gas velocity is incorrectly overestimated.) Proceed to Step 7.

7. **Perform Buoyancy Check.**

   A. Calculate density of air using Equation (4.2.3-22) as follows:

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 293} = 1.20\ kg/m^3$$

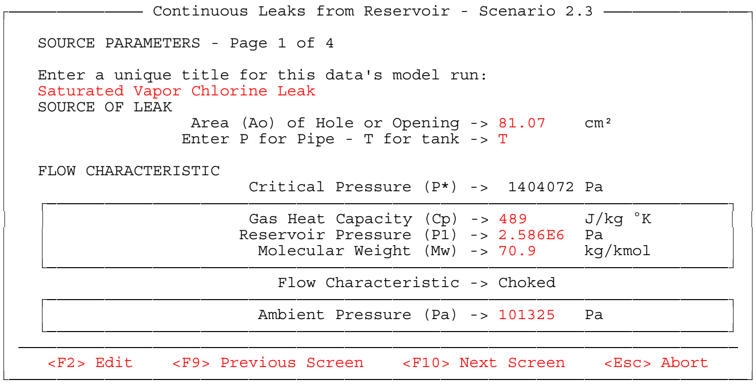
   B. $\rho_2/\rho_{air} > 1$ therefore, buoyancy is negative.

8. **Release Duration.** Calculate the release duration $T_d$ using Equation (4.2.3-23) as follows:

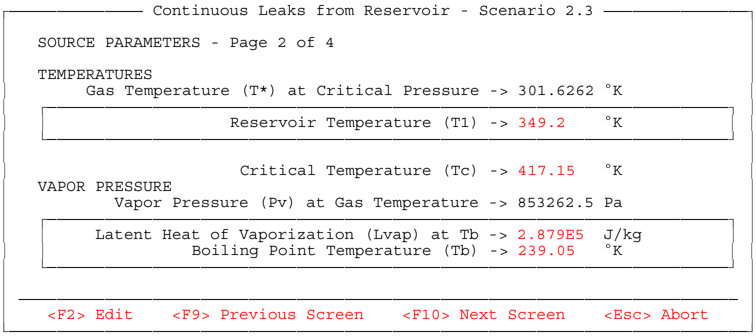
$$T_d\ (min) = \frac{400\ (kg)}{62.5\ (kg/s) \cdot 60\ (s/min)} = 0.107\ min$$

Since the release is from a relief valve, run the RVD model. (See Section 5.2 for more information on the RVD model.)

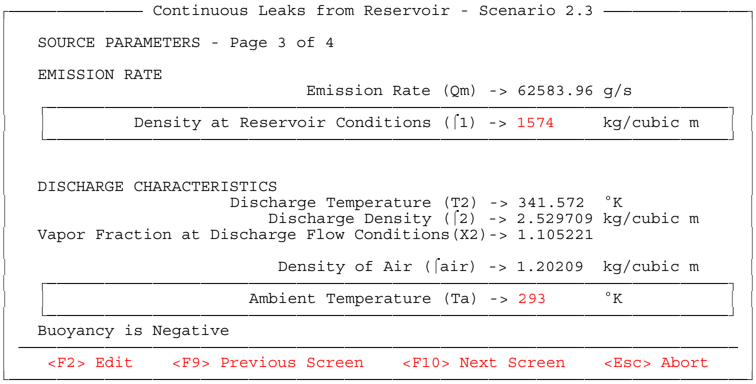
Data entry in the TSCREEN model for this example is shown below:



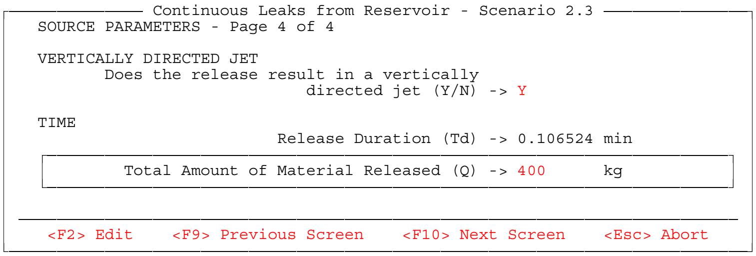
```
              Continuous Leaks from Reservoir - Scenario 2.3

  SOURCE PARAMETERS - Page 1 of 4

  Enter a unique title for this data's model run:
  Saturated Vapor Chlorine Leak
  SOURCE OF LEAK
                Area (Ao) of Hole or Opening -> 81.07    cm²
               Enter P for Pipe - T for tank -> T

  FLOW CHARACTERISTIC
                      Critical Pressure (P*) ->  1404072 Pa

                      Gas Heat Capacity (Cp) -> 489      J/kg °K
                     Reservoir Pressure (P1) -> 2.586E6  Pa
                       Molecular Weight (Mw) -> 70.9     kg/kmol

                         Flow Characteristic -> Choked

                       Ambient Pressure (Pa) -> 101325   Pa

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



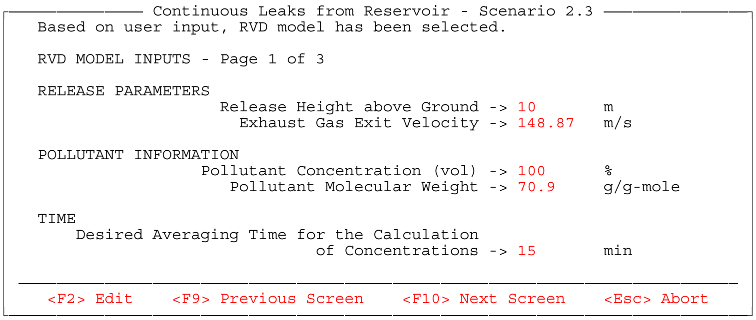
```
              Continuous Leaks from Reservoir - Scenario 2.3

  SOURCE PARAMETERS - Page 2 of 4

  TEMPERATURES
       Gas Temperature (T*) at Critical Pressure -> 301.6262 °K

                    Reservoir Temperature (T1) -> 349.2     °K


                     Critical Temperature (Tc) -> 417.15    °K
  VAPOR PRESSURE
          Vapor Pressure (Pv) at Gas Temperature -> 853262.5 Pa

         Latent Heat of Vaporization (Lvap) at Tb -> 2.879E5  J/kg
                   Boiling Point Temperature (Tb) -> 239.05   °K


   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



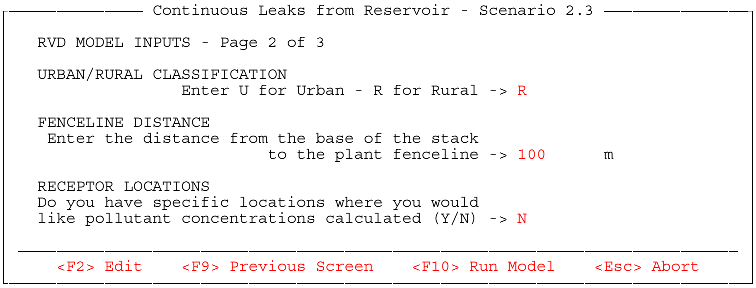
```
              Continuous Leaks from Reservoir - Scenario 2.3

  SOURCE PARAMETERS - Page 3 of 4

  EMISSION RATE
                             Emission Rate (Qm) -> 62583.96 g/s

          Density at Reservoir Conditions (⌠1) -> 1574      kg/cubic m


  DISCHARGE CHARACTERISTICS
                     Discharge Temperature (T2) -> 341.572  °K
                         Discharge Density (⌠2) -> 2.529709 kg/cubic m
  Vapor Fraction at Discharge Flow Conditions(X2)-> 1.105221

                           Density of Air (⌠air) -> 1.20209  kg/cubic m

                       Ambient Temperature (Ta) -> 293      °K

  Buoyancy is Negative

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
              Continuous Leaks from Reservoir - Scenario 2.3
  SOURCE PARAMETERS - Page 4 of 4

  VERTICALLY DIRECTED JET
         Does the release result in a vertically
                             directed jet (Y/N) -> Y

  TIME
                          Release Duration (Td) -> 0.106524 min

         Total Amount of Material Released (Q) -> 400      kg


   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
─────────────── Continuous Leaks from Reservoir - Scenario 2.3 ───────────────
   Based on user input, RVD model has been selected.

   RVD MODEL INPUTS - Page 1 of 3

   RELEASE PARAMETERS
                      Release Height above Ground -> 10       m
                        Exhaust Gas Exit Velocity -> 148.87   m/s

   POLLUTANT INFORMATION
                    Pollutant Concentration (vol) -> 100      %
                       Pollutant Molecular Weight -> 70.9     g/g-mole

   TIME
       Desired Averaging Time for the Calculation
                               of Concentrations -> 15       min

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
─────────────── Continuous Leaks from Reservoir - Scenario 2.3 ───────────────

   RVD MODEL INPUTS - Page 2 of 3

   URBAN/RURAL CLASSIFICATION
                 Enter U for Urban - R for Rural -> R

   FENCELINE DISTANCE
    Enter the distance from the base of the stack
                          to the plant fenceline -> 100      m

   RECEPTOR LOCATIONS
   Do you have specific locations where you would
   like pollutant concentrations calculated (Y/N) -> N

    <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

## The RVD model's output is displayed below:

```
═══════════════════════════════════════════════════════════════════════════════ Saturated Vapor
Chlorine Leak    07-30-1992

                                Input Data

Pollutant emission rate (kg/sec) =  62.58396
Exit gas velocity (m/sec)=  148.87
Exit Temperature (K)=  341.572
Stack Height (m) =  10     Diameter (m) =  .101598
Pollutant Concentration (volume %) =  100
Exhaust Gas Density (kg/m3) =  2.523289
Exhaust Gas Molecular Weight =  70.9
Exhaust Gas Mass Flow Rate (kg/sec) =  62.58396
Pollutant Molecular Weight =  70.9
Release duration (min) =  .106524  Av. Time (min) =  15
Wind Speeds (m/sec) =  1.0    2.0    3.0    4.0    5.0
                       8.0   10.0   15.0   20.0
Distances (m) =  100    200    300    400    500    600    700
                 800    900    1000    1100    1200    1300    1400
                 1500    1600    1700    1900    2100    2300    2500
                 2700    2900    3100    3300    3600    3900    4200
                 4500    5000
Ambient Temperature (K) =  293  293  293  293  293  293
Rural Wind Speed Profile Exponents


*************************************************************
***              SUMMARY OF RVD MODEL RESULTS             ***
*************************************************************

Maximum offsite concentration is  582952.8  ug/m3
                or equivalently   201.4435  ppm
                 occurring at     112.2981  m downwind
              when wind speed is  1  m/sec
                and stability is  A

*************************************************************
***      REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS    ***
*************************************************************
```

```
***********************
***  RVD DISTANCES  ***
***********************

Distance Concentration  Stability  Wind
                          Class    Speed
  (m)      (ug/m3)                (m/sec)      (ppm)
------------------------------------------------------
  100.0  0.00000E+00        F      20.0     0.0000E+00
  200.0  0.40060E+06        F       1.0     0.1384E+03
  300.0  0.36385E+06        F       2.0     0.1257E+03
  400.0  0.33158E+06        F       3.0     0.1146E+03
  500.0  0.30604E+06        E       4.0     0.1058E+03
  600.0  0.27184E+06        E       4.0     0.9394E+02
  700.0  0.25833E+06        E       5.0     0.8927E+02
  800.0  0.23685E+06        E       5.0     0.8185E+02
  900.0  0.21940E+06        E       5.0     0.7581E+02
 1000.0  0.20488E+06        E       5.0     0.7080E+02
 1100.0  0.21288E+06        D       8.0     0.7356E+02
 1200.0  0.20117E+06        D       8.0     0.6952E+02
 1300.0  0.19097E+06        D       8.0     0.6599E+02
 1400.0  0.19054E+06        D      10.0     0.6584E+02
 1500.0  0.18218E+06        D      10.0     0.6296E+02
 1600.0  0.17470E+06        D      10.0     0.6037E+02
 1700.0  0.16795E+06        D      10.0     0.5804E+02
 1900.0  0.15624E+06        D      10.0     0.5399E+02
 2100.0  0.14640E+06        D      10.0     0.5059E+02
 2300.0  0.14955E+06        D      15.0     0.5168E+02
 2500.0  0.14166E+06        D      15.0     0.4895E+02
 2700.0  0.13475E+06        D      15.0     0.4656E+02
 2900.0  0.12863E+06        D      15.0     0.4445E+02
 3100.0  0.13010E+06        D      20.0     0.4496E+02
 3300.0  0.12492E+06        D      20.0     0.4317E+02
 3600.0  0.11805E+06        D      20.0     0.4079E+02
 3900.0  0.11207E+06        D      20.0     0.3873E+02
 4200.0  0.10680E+06        D      20.0     0.3690E+02
 4500.0  0.10116E+06        D      20.0     0.3496E+02
 5000.0  0.84574E+05        D      20.0     0.2923E+02


          Dense Gas Behavior

           Stability  Class

 Wind    A   B   C   D   E   F
Speed
  1.0    1   1   1   1   2   1
  2.0    1   1   1   1   1   1
  3.0    1   1   1   1   1   1
  4.0    2   1   1   1   1   2
  5.0    2   1   1   1   1   2
  8.0    2   2   1   1   2   2
 10.0    2   2   1   1   2   2
 15.0    2   2   1   1   2   2
 20.0    2   2   1   1   2   2

(0=Non-Dense Behavior   1=Dense Gas Behavior
     2=Combinations that cannot occur)
```

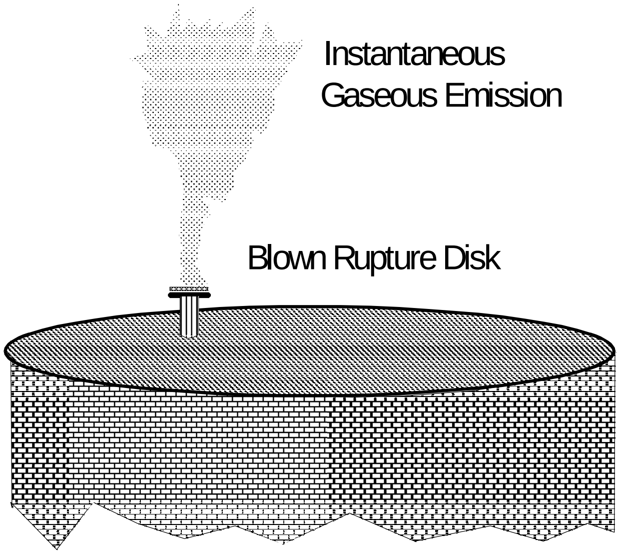
```
            Release Richardson Numbers

                  Stability Class

   Wind       A         B         C         D         E         F
   Speed
   1.0    729135.7  729135.7  729135.7  729135.7  729135.7  729135.7
   2.0     91142.0   91142.0   91142.0   91142.0   91142.0   91142.0
   3.0     27005.0   27005.0   27005.0   27005.0   27005.0   27005.0
   4.0     11392.7   11392.7   11392.7   11392.7   11392.7   11392.7
   5.0      5833.1    5833.1    5833.1    5833.1    5833.1    5833.1
   8.0      1424.1    1424.1    1424.1    1424.1    1424.1    1424.1
  10.0       729.1     729.1     729.1     729.1     729.1     729.1
  15.0       216.0     216.0     216.0     216.0     216.0     216.0
  20.0        91.1      91.1      91.1      91.1      91.1      91.1


            Dense Plume Trajectory

Stability  Wind Plume Touchdown       Touchdown
  Class   Speed  Rise  Distance      Concentration
         (m/sec)  (m)     (m)      (ug/m3)      (ppm)
----------------------------------------------------------
    A       1.0   31.8  112.30   0.58295E+06   0.20144E+03
    A       2.0   25.2  234.32   0.42725E+06   0.14764E+03
    A       3.0   22.0  361.81   0.35393E+06   0.12230E+03
----------------------------------------------------------
    B       1.0   31.8  112.30   0.58295E+06   0.20144E+03
    B       2.0   25.2  234.32   0.42725E+06   0.14764E+03
    B       3.0   22.0  361.81   0.35393E+06   0.12230E+03
    B       4.0   20.0  493.46   0.30867E+06   0.10666E+03
    B       5.0   18.6  628.57   0.27705E+06   0.95737E+02
----------------------------------------------------------
    C       1.0   31.8  112.30   0.58295E+06   0.20144E+03
    C       2.0   25.2  234.32   0.42725E+06   0.14764E+03
    C       3.0   22.0  361.81   0.35393E+06   0.12230E+03
    C       4.0   20.0  493.46   0.30867E+06   0.10666E+03
    C       5.0   18.6  628.57   0.27705E+06   0.95737E+02
    C       8.0   15.9 1050.62   0.21933E+06   0.75791E+02
    C      10.0   14.8 1343.49   0.19571E+06   0.67630E+02
    C      15.0   12.9 2107.74   0.15828E+06   0.54696E+02
    C      20.0   11.7 2909.84   0.13557E+06   0.46846E+02
----------------------------------------------------------
    D       1.0   31.8  112.30   0.58295E+06   0.20144E+03
    D       2.0   25.2  234.32   0.42725E+06   0.14764E+03
    D       3.0   22.0  361.81   0.35393E+06   0.12230E+03
    D       4.0   20.0  493.46   0.30867E+06   0.10666E+03
    D       5.0   18.6  628.57   0.27705E+06   0.95737E+02
    D       8.0   15.9 1050.62   0.21933E+06   0.75791E+02
    D      10.0   14.8 1343.49   0.19571E+06   0.67630E+02
    D      15.0   12.9 2107.74   0.15828E+06   0.54696E+02
    D      20.0   11.7 2909.84   0.13557E+06   0.46846E+02
----------------------------------------------------------
    E       2.0   25.2  234.32   0.42725E+06   0.14764E+03
    E       3.0   22.0  361.81   0.35393E+06   0.12230E+03
    E       4.0   20.0  493.46   0.30867E+06   0.10666E+03
    E       5.0   18.6  628.57   0.27705E+06   0.95737E+02
----------------------------------------------------------
    F       1.0   31.8  112.30   0.58295E+06   0.20144E+03
    F       2.0   25.2  234.32   0.42725E+06   0.14764E+03
    F       3.0   22.0  361.81   0.35393E+06   0.12230E+03
```

```
 Concentrations at Specific Receptor Distances

Stability  Wind Distance Concentration
  Class   Speed
         (m/sec)   (m)      (ug/m3)      (ppm)
--------------------------------------------------

    A       1.0    200.0  0.40060E+06   0.1384E+03

    A       1.0    300.0  0.30778E+06   0.1064E+03
    A       2.0    300.0  0.36385E+06   0.1257E+03

    A       1.0    400.0  0.25529E+06   0.8822E+02
    A       2.0    400.0  0.30180E+06   0.1043E+03
    A       3.0    400.0  0.33158E+06   0.1146E+03
.
.
.

    F       1.0   4500.0  0.18137E+05   0.6267E+01
    F       2.0   4500.0  0.28100E+05   0.9710E+01
    F       3.0   4500.0  0.35945E+05   0.1242E+02

    F       1.0   5000.0  0.15163E+05   0.5240E+01
    F       2.0   5000.0  0.23492E+05   0.8118E+01
    F       3.0   5000.0  0.30050E+05   0.1038E+02


*******************************
*** END OF RVD MODEL OUTPUT ***
*******************************
```

#### 4.2.3.5 Considerations for Time-Varying and Time-Limited Releases

See Section 2.5 for a discussion of considerations for time-varying and time-limited releases.

## 4.2.4 Instantaneous Gas Leaks from a Reservoir



Similar Releases: A gas leak from a tank or a (small) gas leak from a pipe.

Discussion:

This procedure applies to an instantaneous release of a gas (at constant pressure and temperature) from a containment (reservoir) through a hole or opening.

Limitations and Assumptions:

Same as Scenario 4.2.3.

Input Information:

Same as Scenario 4.2.3.

Procedure:

1-6. Same as Scenario 4.2.3

7. **Buoyancy Check.** Perform buoyancy check as a first check.

A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a \, M_a}{R \, T_a} \qquad (4.2.4\text{-}1)$$

where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

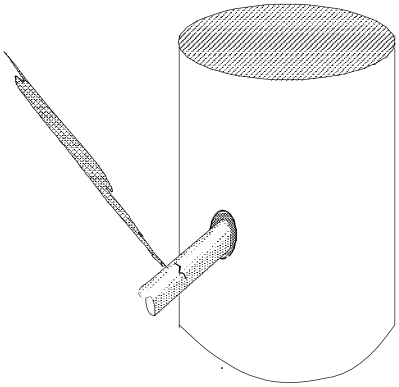
B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 8. If the buoyancy is positive, the PUFF model for a point source should be used. (See Section 2.4 for more information on model selection.)

8. Same as Section 4.2.3

### 4.2.4.1 Examples

See the examples in Section 4.2.3.

### 4.2.5 Continuous Gas Leaks from a Pipe Attached to a Reservoir



#### 4.2.5.1 Release Rate Estimates: Gas Leaks from a Pipe Attached to a Reservoir

Similar Releases: Continuous release of a gas (at constant pressure and temperature) from a containment through a long pipe.

Limitations and Assumptions:

The hole or opening size must be sufficiently small, otherwise the reservoir temperature and pressure may no longer be constant. For the case of a leak from a tank, the assumption of constant reservoir temperature and pressure may be violated if a significant percentage of the tank contents is released. If the reservoir temperature and pressure are not constant, the release rate may vary with time, but the maximum release rate is generally obtained for the initial reservoir temperature and pressure.

The flow through the pipe is assumed to be adiabatic (i.e., the heat transfer to the gas being released is unimportant); this assumption is not very restrictive (Levenspiel (1977)).

The released material must be a (ideal) gas at the reservoir conditions, during the depressurization process, and after depressurization to the atmosphere, and for the case of a tank containing vapor and liquid, the pipe must be attached to the vapor space of the tank (Spicer, 1992).

Input Information:

$A_0$ area of reservoir hole or opening ($m^2$)

$D_0$ (equivalent) diameter of hole or opening ($D_0 = 2\cdot\sqrt{A_0/\pi}$)

| | |
|---|---|
| | (m) |
| $D_p$ | pipe diameter (m) |
| $L_p$ | pipe length (m) |
| $M_w$ | gas (contaminant) molecular weight (g/g-mole) (For contaminant mixtures, see Appendix B) |
| $N_e$ | number of pipe elbows (dimensionless) |
| $P_v$ | vapor pressure as a function of temperature (Pa) |
| $P_a$ | ambient pressure (Pa) |
| $P_1$ | reservoir pressure (Pa) |
| R | gas constant (8314 J/kg-mole•°K or 8314 $P_a$•$m^3$/kg-mole•°K) |
| $T_c$ | critical temperature (°K) |
| $T_1$ | reservoir temperature (°K) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_pM_w))$ at $T_1$ (dimensionless) |

<u>Procedure:</u>

1. **Pipe Friction Loss.** Estimate the friction loss in the piping system. After Perry et al. (1984), estimate the frictional loss N as:

$$N = \frac{4\ f\ L_p}{D_p} + 0.5 + 0.75\ N_e + [0.5] \qquad (4.2.5\text{-}1)$$

In Equation (4.2.5-1), the first term represents the skin friction losses in the pipe; $f \simeq 0.0045$ (the coefficient of skin friction) can be used as a preliminary estimate (i.e., a tighter estimate of f would probably be less than 0.0045, and although f can be larger for Reynolds numbers less than $10^5$, typical Reynolds numbers for these applications are larger than $10^5$). The second term provides for the effect of friction losses in the reservoir-to-pipe connection. The third term accounts for frictional losses in any pipe elbows. The fourth term (written in brackets) should only be included if $D_0/D_p \leq 0.2$, otherwise it should be left off.

2. **Discharge for Choked Flow.** Estimate the discharge rate as if the flow is choked (the validity of this assumption will be checked); in this case, the gas approaches the speed of sound at the exit. For choked flow, the following equations must be solved simultaneously for the Mach number at the pipe entrance $M_2$ and a dimensionless parameter (at the pipe entrance) $Y_2$:

$$Y_2 = 1 + \left(\frac{\gamma - 1}{2}\right) M_2^2 \qquad (4.2.5\text{-}2)$$

$$\left(\frac{\gamma + 1}{2}\right) \ln\left(\frac{2\ Y_2}{M_2^2\ (\gamma + 1)}\right) - \left(\frac{1}{M_2^2} - 1\right) + \gamma\ N = 0 \qquad (4.2.5\text{-}3)$$

After $M_2$ and $Y_2$ are known, the mass flux G is fixed by:

$$G = P_1\, M_2 \left( \frac{M_w\, \gamma}{R\, T_1}\, Y_2^{(\gamma+1)/(1-\gamma)} \right)^{1/2} \qquad (4.2.5\text{-}4)$$

The discharge pressure must be checked to determine if the flow is indeed choked:

$$P_3\ (\mathrm{Pa}) = G \left( \frac{R\, T_1}{M_w\, \gamma} \left( \frac{2}{\gamma + 1} \right) \right)^{1/2} \qquad (4.2.5\text{-}5)$$

If $P_3 < P_a$ or $P_3 > P_1$, then the flow is not choked, and these estimates for G, $M_2$, $Y_2$, and $P_3$ are not valid; proceed to step 3. If $P_1 > P_3 \geq P_a$, then the flow is choked, and the release rate is given by $Q_m$ (kg/s) = G $A_0$. The discharge temperature $T_3$ is given by $2T_1/(\gamma+1)$. Proceed to step 4.

3. **Discharge for Subcritical Flow.** Estimate the discharge rate for subcritical flow; in this case, the gas pressure at the pipe exit approaches ambient pressure ($P_3=P_a$). For subcritical flow, the following eight equations must be solved simultaneously for the mass flux G; the Mach number at the pipe entrance and exit $M_2$ and $M_3$; the pressure at the pipe entrance $P_2$ (Pa); the temperature at the pipe entrance and exit $T_2$ and $T_3$; and the dimensionless flow parameters (at the pipe entrance and exit) $Y_2$ and $Y_3$:

$$Y_2 = 1 + \left( \frac{\gamma - 1}{2} \right) M_2^2 \qquad (4.2.5\text{-}6)$$

$$Y_3 = 1 + \left( \frac{\gamma - 1}{2} \right) M_3^2 \qquad (4.2.5\text{-}7)$$

$$\left( \frac{\gamma + 1}{2} \right) \ln \left( \frac{M_3^2\, Y_2}{M_2^2\, Y_3} \right) - \left( \frac{1}{M_2^2} - \frac{1}{M_3^2} \right) + \gamma\, N = 0 \qquad (4.2.5\text{-}8)$$

$$G = P_1\, M_2 \left( \frac{M_w\, \gamma}{R\, T_1}\, Y_2^{(\gamma+1)/(1-\gamma)} \right)^{1/2} \qquad (4.2.5\text{-}9)$$

$$M_2 = \frac{G}{P_2} \left( \frac{R\, T_2}{\gamma\, M_w} \right)^{1/2} \qquad (4.2.5\text{-}10)$$

$$M_3 = \frac{G}{P_2} \left( \frac{R\, T_3}{\gamma\, M_w} \right)^{1/2} \qquad (4.2.5\text{-}11)$$

$$\frac{P_2}{P_1} = \left( \frac{T_2}{T_1} \right)^{\gamma/(\gamma-1)} \qquad (4.2.6\text{-}12)$$

$$\frac{T_3}{T_2} = \frac{Y_2}{Y_3} \qquad (4.2.5\text{-}13)$$

The solution to these equations must be checked particularly to ensure that $M_3<1$, $P_1>P_2$, and $T_1>T_2$. If these conditions are not met, the value of f is probably too low and should be increased. The release rate is given by $Q_m$ (kg/s) = G $A_0$. Proceed to step 4.

4. **Check Discharge Temperature $T_3$.** The estimate of $T_3$ must be checked. If $T_3$ is greater than the (pseudo) critical temperature $T_c$, the equation used to estimate $T_3$ applies; if not, the following procedure is suggested. For single component contaminants, evaluate the contaminant vapor pressure at $T_3$ ($P_v(T_3)$). If $P_v(T_3) \leq P_a$, then contaminant condensation occurs during the process of depressurization, and this approach is not valid; this release should be considered a two-phase release. If this is a two-phase release proceed to step 6, otherwise proceed to step 5.

5. **Discharge Density.** Estimate the discharge density from the discharge temperature $T_3$ using the ideal gas law: $\rho_3 = P_aM_w/(RT_3)$. (Note that for choked flow conditions, correct application of a dispersion model may require that the diameter of the hole or opening be modified $D_0(P_3/P_a)^{1/2}$ if the model accounts for initial air dilution due to jetting or momentum effects; if this modification is not applied, the initial gas velocity is incorrectly overestimated.) Proceed to step 9.

### 4.2.5.2 Continuous (Two-Phase) Release Rate Estimate: Gas Storage which Partially Condenses on Depressurization

Similar Releases: A gas leak from a tank, a gas leak from a pipe.

Discussion:

Materials which are stored under pressure will depressurize when released to the atmosphere. This depressurization results in the formation of two contaminant phases (saturated liquid and vapor) for: gases which cool so that condensation occurs during the depressurization process; and high volatility liquids (liquids whose normal boiling point is below the ambient temperature) which are stored at (typically) above ambient pressure. (See Section 4.3.2 for more discussion on two-phase releases.) In this scenario, the terms gas, saturated liquid, and subcooled liquid all refer to the state of the tank contents.) This scenario considers the release from a tank (or reservoir) and includes provision for the effect of a pressure drop (piping) between the tank and the hole or opening.

This procedure applies to a continuous release of a gas which partially condenses during depressurization; the screening procedure for this scenario should only be applied if the screening procedure above indicated that partial condensation of the released gas occurs. The release occurs (at constant pressure and temperature) from a containment (reservoir) through a hole or opening; a provision is made for the effect of a pressure drop (piping) between the tank and the hole or opening.

## Limitations and Assumptions:

The pressure and temperature of the tank (or reservoir) contents are essentially constant. The hole or opening size must be sufficiently small, otherwise the reservoir temperature and pressure may no longer be constant. For the case of a leak from a tank, the assumption of constant reservoir temperature and pressure may be violated if a significant percentage of the tank contents is released. If the reservoir temperature and pressure are not constant, the release rate may vary with time, but the maximum release rate is generally obtained for the initial reservoir temperature and pressure.

For the case of a leak from a pipe when $\beta > 0.2$ (as defined below), the assumption of constant temperature and pressure in the pipe may be violated; for such a case, the reservoir conditions should be taken from an upstream location (tank or reservoir) where the temperature and pressure will be (approximately) constant. For the case of a leak from a pipe when $\beta \leq 0.2$, the assumption of constant temperature and pressure in the pipe is reasonable, and the reservoir conditions should be taken to be the conditions within the pipe.

The vapor phase of the release material must be an ideal gas at the reservoir conditions, during the depressurization process, and after depressurization to the atmosphere; for the case of a tank containing vapor and liquid, the hole must be in the vapor space of the tank. For two phase flows, all released liquid is assumed to travel downwind as an aerosol with little rain out of liquid near the source (Spicer, 1992).

## Input Information:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($m^2$) |
| $A_1$ | flow area representing reservoir conditions ($m^2$) (In case of a leak from a tank, $A_1 \rightarrow \infty$ (and $\beta = 0$); in the case of a leak from a pipe, $A_1$ is the cross-sectional area of the pipe.) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (J/kg·°K) (For contaminant mixtures, see Appendix B) |
| $D_0$ | (equivalent) diameter of hole or opening ($D_0 = 2\cdot\sqrt{A_0/\pi}$) (m) |
| $D_p$ | pipe diameter (as appropriate) (m) |
| $L_p$ | pipe length (appropriate) (m) |
| $M_w$ | gas (contaminant) molecular weight (kg/kmol) (For contaminant mixtures, see Appendix B) |
| $P_a$ | ambient pressure (Pa) |

| | |
|---|---|
| $P_v$ | vapor pressure as a function of temperature (Pa) |
| $P_1$ | reservoir pressure (Pa) |
| R | gas constant (8314 J/kg-mole·°K or 8314 $P_a$•$m^3$/kg-mole•°K) |
| $T_b$ | contaminant normal boiling point (°K) |
| $T_c$ | critical temperature (for contaminant mixtures, see Appendix B) |
| $T_1$ | reservoir temperature (°K) |
| β | $\sqrt{A_0/A_1}$ (dimensionless) |
| γ | $(C_p/C_v) \simeq 1/(1 - R/(C_p M_w))$ at $T_1$ (dimensionless) |
| λ | heat of vaporization at the normal boiling point (J/kg) |
| $\rho_1$ | contaminant density at reservoir conditions ($T_1$ and $P_1$) (kg/$m^3$) |

Procedure:

6. **Choked Pressure.** Estimate the choked pressure $P_*$ to determine if the flow is choked from Perry et al. (1984).

$$\frac{P_*}{P_1} = \left( \frac{2}{\gamma + 1} \right)^{\gamma/(\gamma-1)} \qquad (4.2.5\text{-}14)$$

If $P_* \geq P_a$, then the flow is choked; go to step 7. If $P_* < P_a$, then the flow is subcritical (not choked); go to step 8.

7. **Two-Phase Choked Flow.** For choked flow, estimate the discharge temperature $T_2$, discharge density $\rho_2$, and the emission rate $Q_m$.

   A. **Estimate $T_*$.** For pure components, estimate $T_*$ (the temperature which corresponds to $P_*$) from the Clausius-Clapeyron equation:

$$P_* = 101325 \exp\left( \frac{\lambda\, M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_*} \right) \right) \qquad (4.2.5\text{-}15)$$

   which can be rewritten as:

$$T_* = \frac{1}{\dfrac{1}{T_b} - \dfrac{R}{\lambda\, M_w} \cdot \ln\left( \dfrac{P_*}{101325} \right)}$$

   B. **Estimate Properties at Choked Flow Conditions.** Based on assumed isentropic behavior, estimate the vapor fraction at choked flow conditions $X_*$ as follows:

$$X_* = 1 + \frac{T_*}{\lambda\ M_w} \left[ M_w\ C_p\ \ln\left(\frac{T_1}{T_*}\right) - R\ \ln\left(\frac{P_1}{P_*}\right) \right] \qquad (4.2.5\text{-}16)$$

Using $X_*$ from Equation (4.2.5-16), estimate the enthalpy change $(H_1 - H_*)$ and the density $\rho_*$ as follows:

$$H_1 - H_* = C_p\ (T_1 - T_*) + \lambda\ (1 - X_*) \qquad (4.2.5\text{-}17)$$

$$\rho_* = \left[ X_* \left( \frac{R\ T_*}{P_*\ M_w} \right) + \left( \frac{1 - X_*}{\rho_1} \right) \right]^{-1} \qquad (2.5\text{-}17)$$

Note that values for the individual enthalpies $H_1$ and $H_*$ are not required.

C. **Estimate Emission Rate.** Extending the ideas suggested by Lees (1950), estimate the emission rate $Q_m$ (kg/s) as follows:

$$Q_m = A_0\ \rho_* \left[ 2 \cdot 0.85 \left( \frac{H_1 - H_*}{1 + 4\ f\ L_p\ /\ D_p} \right) \right]^{1/2} \qquad (4.2.5\text{-}19)$$

where 0.85 is included to account for irrevesibilities in the flow based on Lewitt (1953) and the term $4fL_p/D_p$ accounts for the pressure drop (piping) between the reservoir and the hole or opening; as a preliminary estimate, use f=0.0045 (since typical Reynolds numbers for these applications are larger than $10^5$).

D. **Estimate Discharge Temperature and Density.** Estimate the discharge temperature $T_2$ (after depressurization). If a condensed phase is present, $T_2$ will be given by the Clausius-Clapeyron equation:

$$P_a = 101325\ \exp\left( \frac{\lambda\ M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_2} \right) \right) \qquad (4.2.5\text{-}20)$$

which can be rewritten as:

$$T_2 = \frac{1}{\dfrac{1}{T_b} - \dfrac{R}{\lambda\ M_w} \cdot \ln\left( \dfrac{P_a}{101325} \right)}$$

Using this estimate of $T_2$, estimate the vapor fraction $X_2$ as:

$$X_2 = X_* + C_p(T_* - T_2)/\lambda \qquad (4.2.5\text{-}21)$$

When $X_2$ estimated from Equation (4.2.5-21) satisfies $1 \geq X_2 \geq 0$, the estimate of $T_2$ is valid, and the density of the discharged material is given by:

$$\rho_2 = \left[ X_2 \left( \frac{R\ T_2}{P_a\ M_w} \right) + \left( \frac{1 - X_2}{\rho_L} \right) \right]^{-1} \qquad (4.2.5\text{-}22)$$

However, if $X_2 < 0$ or $X_2 > 1$, the contaminant condensed phase which was present at $P_*$ and $T_*$ is no longer present, and the released contaminant is a gas (without any condensed phase); the discharge temperature and density are estimated as follows:

$$T_2 = T_* + \lambda (1 - X_*)/C_p \qquad (4.2.5\text{-}23)$$

$$\rho_2 = \frac{P_a\ M_w}{R\ T_2} \qquad (4.2.5\text{-}24)$$

where $X_2 = 0$.

E. Go to step 9 to select the dispersion model.

8. **Two-Phase Subcritical (Nonchoked) Flow.** For subcritical flow, estimate the gas/liquid discharge temperature $T_2$, discharge density $\rho_2$, and the emission rate $Q_m$.

A. **Estimate $T_2$.** For pure components, estimate $T_2$ from the Clausius-Clapeyron equation:

$$P_a = 101325 \exp \left( \frac{\lambda\ M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_2} \right) \right) \qquad (4.2.5\text{-}25)$$

which can be rewritten as:

$$T_2 = \frac{1}{\dfrac{1}{T_b} - \dfrac{R}{\lambda\ M_w} \cdot \ln \left( \dfrac{P_a}{101325} \right)}$$

B. **Estimate Properties at Discharge Conditions.** Based on assumed isentropic behavior, estimate the vapor fraction $X_2$ at discharge flow conditions as:

$$X_2 = 1 + \frac{T_2}{\lambda\ M_w} \left[ M_w\ C_p \ln \left( \frac{T_1}{T_2} \right) - R \ln \left( \frac{P_1}{P_a} \right) \right] \qquad (4.2.5\text{-}26)$$

Using $X_2$ from Equation (4.2.5-26), estimate the enthalpy change $(H_1 - H_2)$ and the density $\rho_2$ as:

$$H_1 - H_2 = C_p (T_1 - T_2) + \lambda (1 - X_2) \qquad (4.2.5\text{-}27)$$

$$\rho_2 = \left[ X_2 \left( \frac{R\,T_2}{P_a\,M_w} \right) + \left( \frac{1 - X_2}{\rho_L} \right) \right]^{-1} \qquad (4.2.5\text{-}28)$$

C. **Estimate Emission Rate.** Extending the ideas suggested be Lees (1950), estimate the emission rate $Q_m$ (kg/s) as:

$$Q_m = A_0\,\rho_2 \left[ 2 \cdot 0.85 \left( \frac{H_1 - H_2}{1 + 4\,f\,L_p / D_p} \right) \right]^{1/2} \qquad (4.2.5\text{-}29)$$

where 0.85 is included to account for irrevesibilities in the flow based on Lewitt (1953) and the term $4fL_p/D_p$ accounts for the pressure drop (piping) between the reservoir and the hole or opening (as appropriate); as a preliminary estimate, use f = 0.0045 (since typical Reynolds numbers for these applications are larger than $10^5$).

D. Go to step 9 to determine the dispersion model.

4.2.5.3 Dispersion Model Determination

See Section 2.4 for a complete discussion of the model determination.

Input Information:

$T_a$ ambient temperature (°K)
Q total amount of material released (kg)

Procedure:

9. **Buoyancy Check.** Evaluate release buoyancy as a first check.

A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\,M_a}{R\,T_a} \qquad (4.2.5\text{-}30)$$

where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 10. If the buoyancy is positive, the SCREEN model for a point source should be used. (See Section 2.4 for more information on model selection.)

10. **Release Duration.** The release duration is used as an input into the RVD and Britter-McQuaid models. The release duration can be used to determine if the release is continuous or instantaneous (see Section 2.5). Calculate the release duration $T_d$ using the equation below:

$$T_d\ (\text{min}) = \frac{Q\ (\text{kg})}{Q_m\ (\text{kg/s}) \cdot 60\ (\text{s/min})} \qquad (4.2.5\text{-}31)$$

### 4.2.5.4 Examples

### 4.2.5.4.1 Example 1: Air Leak - Choked

Discussion:

In this example (from Perry et al. (1984)), (dry) air stored at $1.101 \times 10^6$ Pa and 293.15 °K is released from a tank through 10 m of a 5.25 cm (inside diameter) Schedule 40 steel pipe; there are three elbows in the line. The diameter of the opening is the diameter of the pipe. The fenceline is 100 m from the tank. This example demonstrates the procedure when the flow is choked.

The following information will be required:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($\pi D_0/4 = 0.002165\ m^2$) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (1004 J/kg °K) |
| $D_0$ | diameter of hole or opening ($D_0 = 0.0525$ m) |
| $L_p$ | pipe length (10 m) |
| $M_w$ | gas (contaminant) molecular weight (29 kg/kmol) |
| $N_e$ | number of pipe elbows (3) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_1$ | reservoir pressure ($1.101 \times 10^6$ Pa) |
| R | gas constant (8314 J/kg-mole·°K) |
| $T_b$ | normal boiling point (79 °K) |
| Q | total amount of material released (400 kg) |
| $T_a$ | ambient temperature (293 °K) |
| $T_c$ | critical temperature (154.6 °K) |
| $T_1$ | reservoir temperature (293.15 °K) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_p M_w))$ at $T_1$ (1.40) |

With this information, the procedure discussed above determines the release rate, the discharge temperature, and the discharge density.

1. **Pipe Friction Loss.** Estimate the friction loss in the piping system. In Equation (4.2.5-1), the first term is 4(0.0045)(10)/(0.0525) = 3.43; the second term is 0.5; the third term is 0.76(3)=2.25; and the fourth term is not

included:

$$N = 3.43 + 0.5 + 2.25 = 6.18$$

2. **Discharge for Choked Flow.** Estimate the discharge rate as if the flow is choked (the validity of this assumption will be checked). For choked flow, Equations (4.2.5-2) and (4.2.5-3) are solved simultaneously for $M_2$ and $Y_2$; computer solution gives $M_2 = 0.283$ and $Y_2 = 1.016$. With $M_2$ and $Y_2$ known, the mass flux G is given by Equation (4.2.5-4) as:

$$G = 1.101\times10^6 \cdot 0.283 \left( \frac{29 \cdot 1.40}{R\ 293.15} 1.016^{(1.40+1)/(1-1.40)} \right)^{1/2} = 1210\ \mathrm{kg/m^2s}$$

The discharge pressure $P_3$ is given by Equation (4.2.5-5) as:

$$P_3\ (\mathrm{Pa}) = 1210 \left( \frac{8314 \cdot 293.15}{29 \cdot 1.40} \left( \frac{2}{1.40 + 1} \right) \right)^{1/2} = 2.71\times10^5\ \mathrm{Pa}$$

Since $P_3 \geq P_a$, the flow is choked, and release rate is given by $Q_m$=(1210) (0.002165) = 2.62 kg/s. (Note that the estimated release rate for the same reservoir conditions is reduced from 4220 g/s to 2620 g/s if the piping pressure drop is included.) The discharge temperature $T_3$ is given by $2T_1/(\gamma+1)$; $T_3$ = 244 °K. Go to step 4.

4. **Check Discharge Temperature $T_3$.** The estimate of $T_3$ must be checked. For this example, $T_3$ = 244 °K, and the pseudo critical temperature of air is 154.6 °K, so no condensation occurs for these conditions.

5. **Discharge Density.** Estimate the discharge density $\rho_3$ from the discharge temperature $T_3$ using the ideal gas law:

$$\rho_3 = (101325)(29)/((8314)(244)) = 1.45\ \mathrm{kg/m^3}$$

(For these choked flow conditions, correct application of a dispersion model may require that the diameter of the hole or opening be modified to $D_0(P_3/P_a)^{1/2}$ = 0.0525 m $(2.71\times10^5/101325)^{1/2}$ = 0.0859 m if the model accounts for initial air dilution due to jetting or momentum effects; if this modification is not applied, the initial gas velocity is incorrectly overestimated.) Go to step 9.

9. **Perform Buoyancy Check.**

A. Calculate density of air.

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 293} = 1.20\ \mathrm{kg/m^3}$$

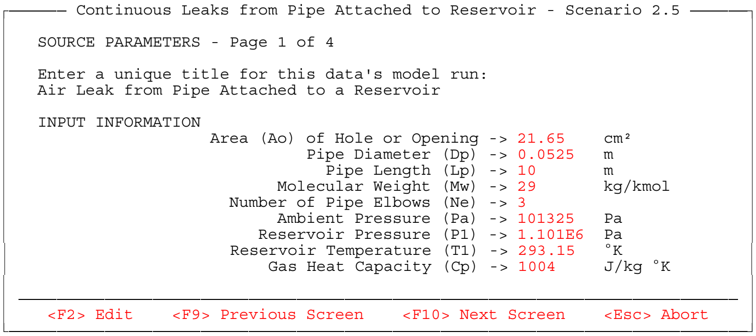
B. $\rho_3/\rho_{air} > 1$ therefore, buoyancy is negative.

10. **Release Duration.** Calculate the release duration $T_d$ using the equation below:

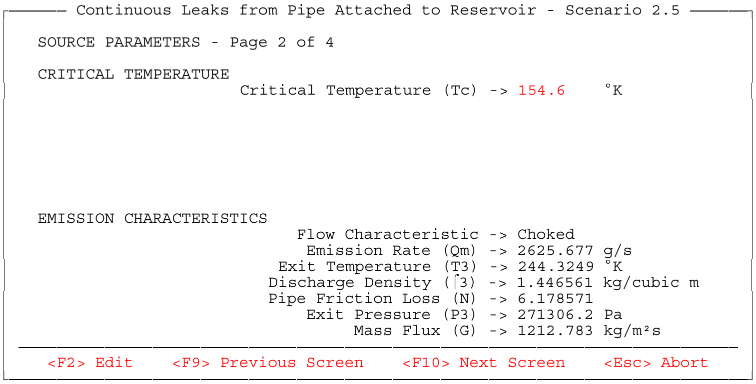
$$T_d\ (\text{min}) = \frac{400\ (\text{kg})}{2.62\ (\text{kg/s}) \cdot 60\ (\text{s/min})} = 2.54\ \text{min}$$

Since the release is not from a vertically directed jet, the Britter-McQuaid model is used. (See Section 5.4 for more information on the Britter-McQuaid model.)

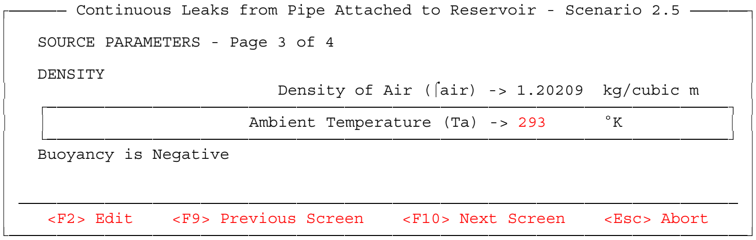
Data entry in the TSCREEN model for this example is shown below:



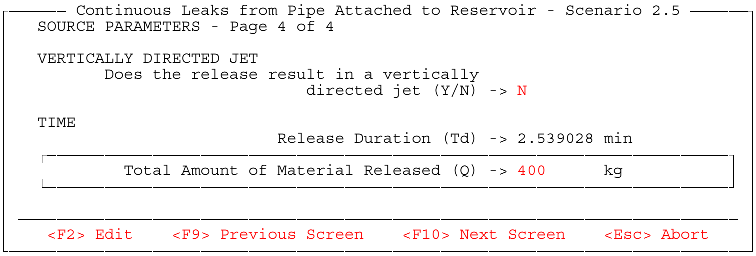
```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Air Leak from Pipe Attached to a Reservoir

INPUT INFORMATION
                  Area (Ao) of Hole or Opening -> 21.65     cm²
                            Pipe Diameter (Dp) -> 0.0525    m
                              Pipe Length (Lp) -> 10        m
                         Molecular Weight (Mw) -> 29        kg/kmol
                    Number of Pipe Elbows (Ne) -> 3
                         Ambient Pressure (Pa) -> 101325    Pa
                       Reservoir Pressure (P1) -> 1.101E6   Pa
                    Reservoir Temperature (T1) -> 293.15    °K
                        Gas Heat Capacity (Cp) -> 1004      J/kg °K

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



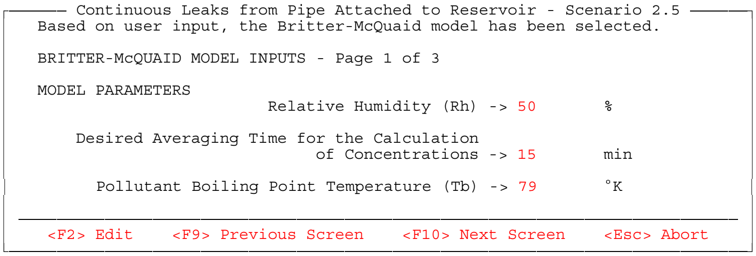
```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5

SOURCE PARAMETERS - Page 2 of 4

CRITICAL TEMPERATURE
                     Critical Temperature (Tc) -> 154.6     °K




EMISSION CHARACTERISTICS
                           Flow Characteristic -> Choked
                            Emission Rate (Qm) -> 2625.677 g/s
                          Exit Temperature (T3) -> 244.3249 °K
                         Discharge Density (⌠3) -> 1.446561 kg/cubic m
                         Pipe Friction Loss (N) -> 6.178571
                             Exit Pressure (P3) -> 271306.2 Pa
                                  Mass Flux (G) -> 1212.783 kg/m²s

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



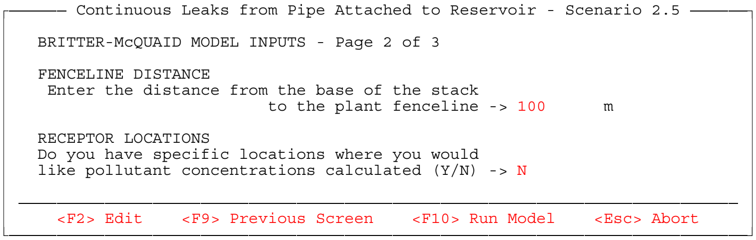
```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5

SOURCE PARAMETERS - Page 3 of 4

DENSITY
                         Density of Air (⌠air) -> 1.20209  kg/cubic m

                      Ambient Temperature (Ta) -> 293       °K

Buoyancy is Negative


   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
────── Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5 ──────
   SOURCE PARAMETERS - Page 4 of 4

   VERTICALLY DIRECTED JET
          Does the release result in a vertically
                                directed jet (Y/N) -> N

   TIME
                             Release Duration (Td) -> 2.539028 min

            Total Amount of Material Released (Q) -> 400      kg

    <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
────── Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5 ──────
   Based on user input, the Britter-McQuaid model has been selected.

   BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

   MODEL PARAMETERS
                            Relative Humidity (Rh) -> 50       %

       Desired Averaging Time for the Calculation
                                 of Concentrations -> 15       min

         Pollutant Boiling Point Temperature (Tb) -> 79       °K

    <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
────── Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5 ──────

   BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

   FENCELINE DISTANCE
    Enter the distance from the base of the stack
                            to the plant fenceline -> 100      m

   RECEPTOR LOCATIONS
   Do you have specific locations where you would
   like pollutant concentrations calculated (Y/N) -> N

     <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

A summary of the Britter-McQuaid model's output is displayed below:

```
     ***************************************
     ***   SUMMARY OF B&M MODEL RESULTS  ***
     ***************************************

   MAX CONC      MAX CONC     DIST TO   WIND SPEED
   (UG/M**3)      (PPM)       MAX (M)     (M/S)
   ---------    ---------     -------   ----------
   .7283E+08    .6037E+05      100.         2.

****************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
****************************************************
```

### 4.2.5.4.2 Example 2: Air Leak - Subcritical (Not Choked)

**Discussion:**

In this example, (dry) air stored at $1.82 \times 10^5$ atm and 293.15 °K is released from a tank through 10 m of a 5.25 cm (inside diameter) Schedule 40 steel pipe; there are three elbows in the line. The diameter of the opening is the diameter of the pipe. The fenceline is located 100 m from the tank. This example demonstrates the procedure when the flow is not choked and is similar to the last example except for the reservoir pressure.

The following information will be required:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($\pi D_0/4 = 0.002165$ m$^2$) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (1004 J/kg °K) |
| $D_0$ | diameter of hole or opening ($D_0 = 0.0525$ m) |

| | |
|---|---|
| $L_p$ | pipe length (10 m) |
| $M_w$ | gas (contaminant) molecular weight (29 kg/kmol) |
| $N_e$ | number of pipe elbows (3) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_1$ | reservoir pressure ($1.82 \times 10^5$ Pa) |
| R | gas constant (8314 J/kg-mole·°K) |
| $T_b$ | normal boiling point (79 °K) |
| Q | total amount of material released (400 kg) |
| $T_a$ | ambient temperature (293 °K) |
| $T_c$ | critical temperature (154.6 °K) |
| $T_1$ | reservoir temperature (293.15 °K) |
| $\gamma$ | $(C_p/C_v) \simeq 1/(1 - R/(C_p M_w))$ at $T_1$ (1.40) |

With this information, the procedure discussed above determines the release rate, the discharge temperature, and the discharge density.

Procedure:

1. **Pipe Friction Loss.** Estimate the friction loss in the piping system. In Equation (2.5-1), the first term is 4(0.0045)(10)/(0.0525) = 3.43; the second term is 0.5; the third term is 0.76(3)=2.25; and the fourth term is not included:

$$N = 3.43 + 0.5 + 2.25 = 6.18$$

2. **Discharge for Choked Flow.** Estimate the discharge rate as if the flow is choked (the validity of this assumption will be checked). For choked flow, Equations (4.2.5-2) and (4.2.5-3) are solved simultaneously for $M_2$ and $Y_2$; computer solution gives $M_2 = 0.283$ and $Y_2 = 1.016$. With $M_2$ and $Y_2$ known, the mass flux G is given by Equation (4.2.5-4) as:

$$G = 1.82\times10^5 \cdot 0.283 \left( \frac{29 \cdot 1.40}{R\ 293.15}\ 1.016^{(1.40+1)/(1-1.40)} \right)^{1/2} = 201\ \mathrm{kg/m^2 s}$$

The discharge pressure $P_3$ is given by Equation (4.2.5-5) as:

$$P_3 = 201 \left( \frac{R\ 293.15}{29 \cdot 1.40} \left( \frac{2}{1.40 + 1} \right) \right)^{1/2} = 4.50\times10^4\ \mathrm{Pa}$$

Since $P_a < P_3$, the flow is not choked; go to step 3.

3. **Discharge for Subcritical Flow.** Estimate the discharge rate for subcritical flow. Equations (4.2.5-6) thru (4.2.5-13) are solved simultaneously for: the mass flux G = 184 kg/m²s; the Mach number at the pipe entrance and exit $M_2 = 0.257$ and $M_3 = 0.436$; the pressure at the pipe entrance $P_2 = 1.74\times10^5$ (Pa); the temperature at the pipe entrance and exit $T_2$=289

°K and $T_3$=282 °K; and the dimensionless flow parameters (at the pipe entrance and exit) $Y_2$=1.013 and $Y_3$=1.038. The solution to these equations meets the conditions that $M_3<1$, $P_1>P_2$, and $T_1>T_2$. The release rate is given be $Q_m$ = (184) (0.002165) = 0.398 kg/s. (Note that the estimated release rate for the same reservoir conditions is reduced from 693 g/s to 398 g/s if the piping pressure drop is included.) Go to step 4.

4. **Check Discharge Temperature $T_3$.** The estimate of $T_3$ must be checked. For this example, $T_3$ = 282 °K, and the pseudo critical temperature of air is 154.6 °K, so no condensation occurs for these conditions.

5. **Discharge Density.** Estimate the discharge density $\rho_3$ from the discharge temperature $T_3$ using the ideal gas law:

$$\rho_3 = (101325)(29)/((8314)(282)) = 1.25\ \mathrm{kg/m^3}$$

Go to step 9.

9. **Perform Buoyancy Check.**

A. Calculate density of air.

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 293} = 1.20\ \mathrm{kg/m^3}$$

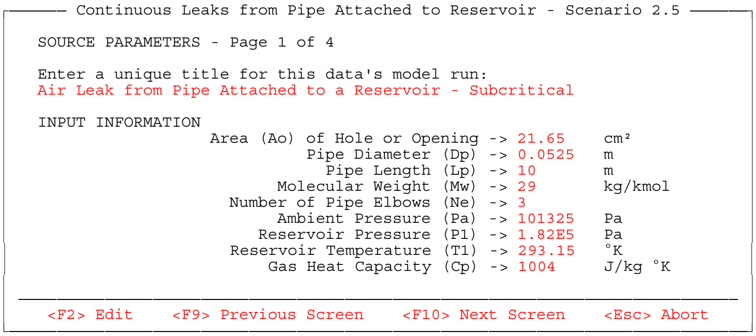
B. $\rho_3/\rho_{air} > 1$ therefore, buoyancy is negative.

10. **Release Duration.** Calculate the release duration $T_d$ using the equation below:

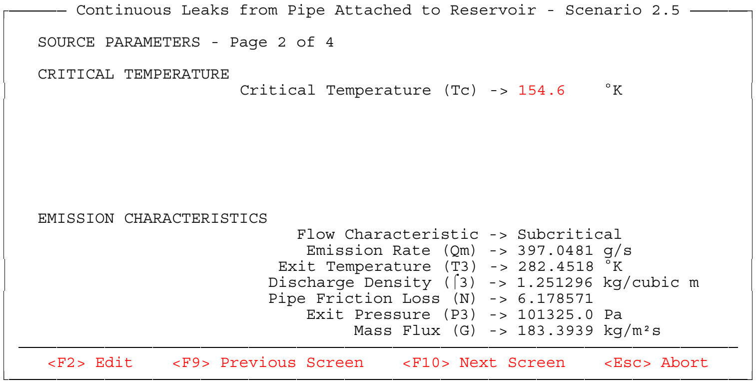
$$T_d\ (\mathrm{min}) = \frac{400\ (\mathrm{kg})}{0.398\ (\mathrm{kg/s}) \cdot 60\ (\mathrm{s/min})} = 16.8\ \mathrm{min}$$

After this calculation run the Britter-McQuaid model since the release is not from a vertically directed jet. (See Section 5.4 for more information on the Britter-McQuaid model.)

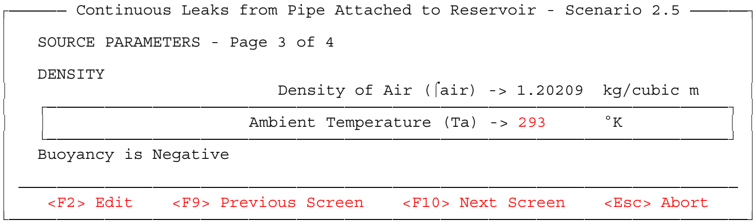
Data entry in the TSCREEN model for this example is shown below:



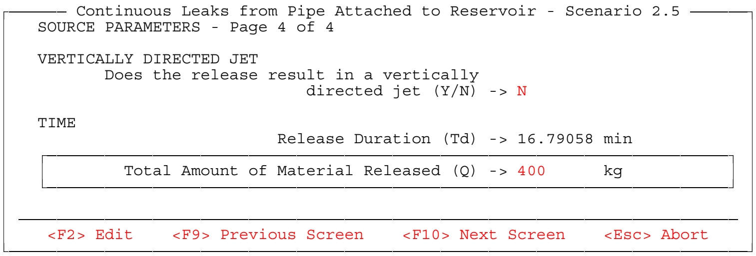
```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Air Leak from Pipe Attached to a Reservoir - Subcritical

INPUT INFORMATION
                  Area (Ao) of Hole or Opening -> 21.65     cm²
                            Pipe Diameter (Dp) -> 0.0525    m
                              Pipe Length (Lp) -> 10        m
                         Molecular Weight (Mw) -> 29        kg/kmol
                    Number of Pipe Elbows (Ne) -> 3
                         Ambient Pressure (Pa) -> 101325    Pa
                       Reservoir Pressure (P1) -> 1.82E5    Pa
                    Reservoir Temperature (T1) -> 293.15    °K
                        Gas Heat Capacity (Cp) -> 1004      J/kg °K

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



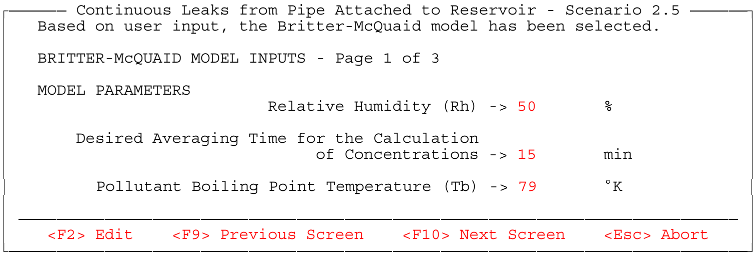
```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5

SOURCE PARAMETERS - Page 2 of 4

CRITICAL TEMPERATURE
                     Critical Temperature (Tc) -> 154.6     °K




EMISSION CHARACTERISTICS
                           Flow Characteristic -> Subcritical
                            Emission Rate (Qm) -> 397.0481 g/s
                         Exit Temperature (T3) -> 282.4518 °K
                        Discharge Density (⌠3) -> 1.251296 kg/cubic m
                        Pipe Friction Loss (N) -> 6.178571
                            Exit Pressure (P3) -> 101325.0 Pa
                                 Mass Flux (G) -> 183.3939 kg/m²s

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



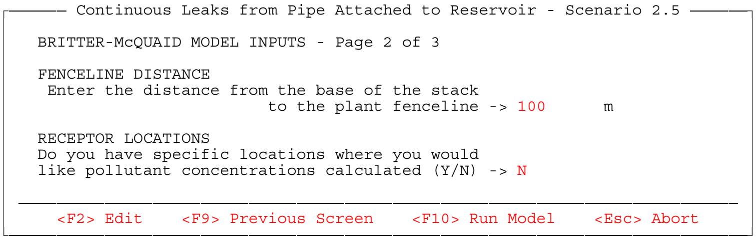
```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5

SOURCE PARAMETERS - Page 3 of 4

DENSITY
                         Density of Air (⌠air) -> 1.20209  kg/cubic m

                      Ambient Temperature (Ta) -> 293       °K

Buoyancy is Negative

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5
SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET
       Does the release result in a vertically
                           directed jet (Y/N) -> N

TIME
                        Release Duration (Td) -> 16.79058 min

         Total Amount of Material Released (Q) -> 400       kg

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS
                        Relative Humidity (Rh) -> 50        %

    Desired Averaging Time for the Calculation
                           of Concentrations -> 15        min

      Pollutant Boiling Point Temperature (Tb) -> 79        °K

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous Leaks from Pipe Attached to Reservoir - Scenario 2.5

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE
 Enter the distance from the base of the stack
                       to the plant fenceline -> 100      m

RECEPTOR LOCATIONS
Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

    <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

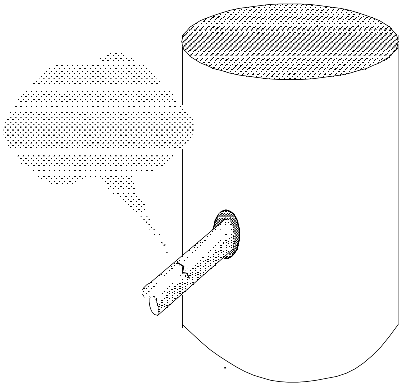
A summary of the Britter-McQuaid model's output is displayed below:

```
     ***************************************
     ***   SUMMARY OF B&M MODEL RESULTS  ***
     ***************************************

   MAX CONC      MAX CONC     DIST TO    WIND SPEED
   (UG/M**3)      (PPM)       MAX (M)      (M/S)
   ---------    ---------     -------    ----------
   .2459E+08    .2038E+05      100.          1.

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
```

### 4.2.5.5 Considerations for Time-Varying and Time-Limited Releases

See Section 2.5 for a discussion of considerations for time-varying and time-limited releases.

## 4.2.6 Instantaneous Gas Leaks from a Pipe Attached to a Reservoir



Similar Releases: Instantaneous release of a gas from a containment (at constant pressure and temperature) through a long pipe.

Limitations and Assumptions:

Same as for Scenario 4.2.5.

Input Information:

Same as for Scenario 4.2.5.

Procedure:

1-8. Same as for Scenario 4.2.5

9. **Buoyancy Check.** Evaluate release buoyancy as a first check.

A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a \, M_a}{R \, T_a} \qquad (4.2.6\text{-}1)$$

where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

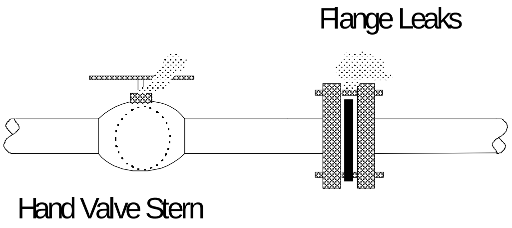
B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 10. If the buoyancy is positive, the PUFF model for a point source should be used. (See Section 2.4 for more information on model selection.)

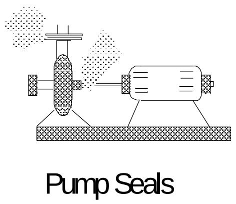
10. Same as Section 4.2.5

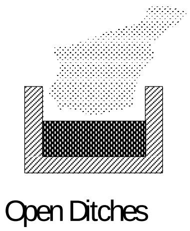
### 4.2.6.1 Examples

See the examples in Section 4.2.5.

### 4.2.7 Continuous Multiple Fugitive Emissions







Similar Releases: Releases from any continuous area or volume source where the emissions that are uniformly released over the area or the area represents a collection of small sources poorly defined in terms of location (e.g., multiple vents on large manufacturing buildings, fugitive VOC sources in refineries or chemical process manufacturing plants).

Discussion:

Fugitive gaseous emissions resulting from a collection of small sources and gaseous area source emissions of different types (e.g., process equipment, valves, etc.) are modeled in this section. Often, areas of fugitive emissions can be specified for elevated releases such as manufacturing facilities where substantial numbers of hood and vent sources are found on the roof and fugitive emissions identified in mass balances are suspected from ventilation sources. In these cases, the area of release can be considered as a volume source using a characteristic height such as a building height. Dispersion calculations can assume area and volume source releases. However, currently, the TSCREEN model does not include volume source releases.

The use of EPA fugitive emission factors for selected equipment are found in the EPA report Protocol for Generating Unit-Specific Emission Estimates for Equipment Leaks of VOC and VHAP, EPA-450/3-88-010 (Appendix A). For selected air toxic, fugitive factors are also found in Appendix A (items 1 and 3).

Limitations and Assumptions:

- Dispersion calculations assume area source releases only.

Input Information:

EF emission factor from various fugitive emissions (Mg/yr)
Pd production rate (kg/Mg)
$Q_m$ emission rate (g/s)

4.2.7.1 Procedure

1. **Emission Rate.** Fugitive gaseous emissions resulting from a collection of small sources and gaseous area source emissions of different types (e.g., process equipment, valves, etc.) are modeled using a source specific emission rate or fugitive emission factors. The document Protocols for Generating Unit-Specific Emissions Estimates for Equipment Leaks or VOC, and VHAP, EPA-450/3-88-010 describes methodologies the EPA considers appropriate for development of unit specific emission estimates for equipment leaks of organic compounds: volatile organic compounds (VOC) and volatile hazardous air pollutants (VHAP). Estimates generated using this document would be specific to process units (or groups of sources) for which an estimate was made. EPA has made provisions for extending such estimates beyond the limits of that group of sources. Five methods for estimating emissions from equipment leaks from a specific chemical processing unit are included in the protocol: average emission factor method; leak/no-leak emission factor method; three-strata emission factor method; application of EPA correlations; and development of new correlations. For selected air toxics, factors are also found in Appendix A items 1 and 3.

   If the emission rate is not known it can be calculated as follows:

   A. **Emission Rate in kg/yr.** Calculate emission rate in kg/yr.

   $$Q_m\,(\text{kg/yr}) = \text{Pd}\,(\text{Mg/yr})\ \text{EF}\,(\text{kg/Mg}) \qquad (4.2.7\text{-}1)$$

   B. **Emission Rate in g/s.** Convert emission rate from kg/yr to g/s.

   $$Q_m\,(\text{g/s}) = \frac{Q_m\,(\text{kg/yr})\ 1000\,(\text{g/kg})}{365\,(\text{dy/yr})\ 86400\,(\text{s/dy})}$$

2. TSCREEN will run the SCREEN model for an area source. See Section 5.1.2 for a complete list of inputs.

#### 4.2.7.2 Example: Ethylene Dichloride Release

Discussion:

The maximum hourly average concentration estimate is required for ambient ethylene dichloride at a fenceline receptor 100 meters downwind from a production facility. The area of emissions at the plant is 100 m x 100 m, and production rate is 204,000 Mg/yr in continuous operation over the year.

Normal production of ethylene dichloride in vinyl chloride plants results in fugitive emissions from storage vents. Specific sources of emissions cannot be specified. As a result, simulations make use of emission factors to provide average emissions plantwide. These emissions are then used in a continuous ground level area source dispersion model.

Procedure:

1. **Emission Rate.** Emissions are obtained from emission factors published by EPA (1987b). Plant-wide emissions are calculated from the production rate and an emission factor from various fugitive sources. The emission factor per production unit is given by:

| | |
|---|---|
| chlorination vent | 0.0216 kg/Mg |
| column vents | 0.06 kg/Mg |
| process storage vents | 0.0003 kg/Mg |
| process fugitive | 0.265 kg/Mg |
| Total | 0.3469 kg/Mg |

A. **Emission Rate in kg/yr.** Total emissions (in kg/yr) for the plant are given by Equation (4.2.7-1):

$$Q_m \text{ (kg/yr)} = 204{,}000 \text{ (Mg/yr) X } 0.3469 \text{ (kg/Mg)} = 70{,}768 \text{ (kg/yr)}$$

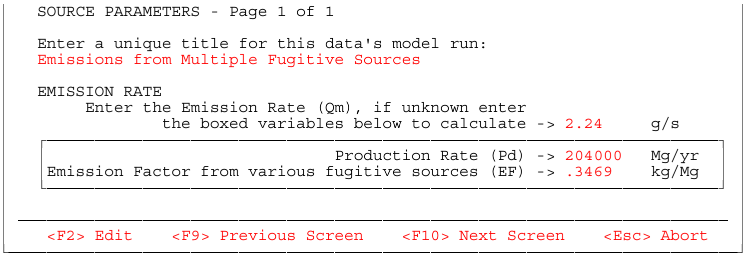
B. **Emission Rate in g/s.** Convert emission rate to g/s:

$$Q_m \text{ (g/s)} = \frac{70{,}768 \text{ (kg/yr) } 1000 \text{ (g/kg)}}{365 \text{ (dy/yr) } 86400 \text{ (s/dy)}} = 2.24 \text{ (g/s)}$$

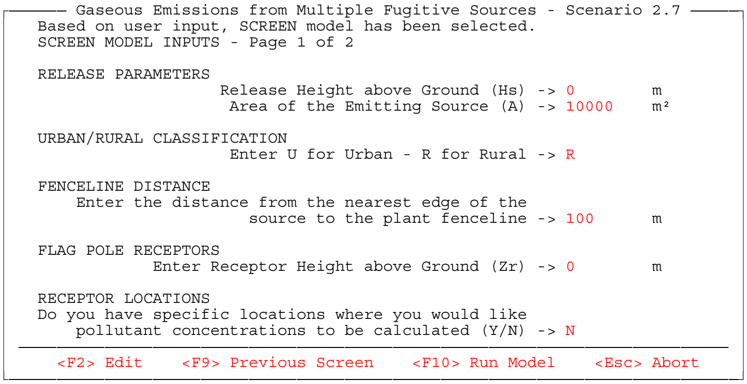
2. Run the SCREEN model for an area source. For a complete explanation of the inputs for the SCREEN model for an area source, see Section 5.1.2. The default release height ($H_s$) for this scenario is 0.

Data entry in the TSCREEN model for this is shown below:

```
┌──── Gaseous Emissions from Multiple Fugitive Sources - Scenario 2.7 ─────┐
```



```
SOURCE PARAMETERS - Page 1 of 1

Enter a unique title for this data's model run:
Emissions from Multiple Fugitive Sources

EMISSION RATE
     Enter the Emission Rate (Qm), if unknown enter
             the boxed variables below to calculate -> 2.24     g/s

                               Production Rate (Pd) -> 204000   Mg/yr
Emission Factor from various fugitive sources (EF) -> .3469    kg/Mg
```

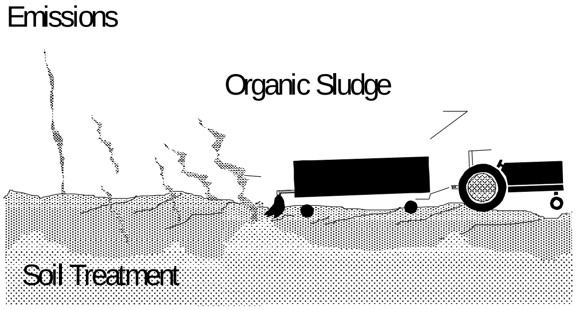


```
Gaseous Emissions from Multiple Fugitive Sources - Scenario 2.7
Based on user input, SCREEN model has been selected.
SCREEN MODEL INPUTS - Page 1 of 2

RELEASE PARAMETERS
                   Release Height above Ground (Hs) -> 0        m
                    Area of the Emitting Source (A) -> 10000    m²

URBAN/RURAL CLASSIFICATION
                    Enter U for Urban - R for Rural -> R

FENCELINE DISTANCE
    Enter the distance from the nearest edge of the
                      source to the plant fenceline -> 100      m

FLAG POLE RECEPTORS
            Enter Receptor Height above Ground (Zr) -> 0        m

RECEPTOR LOCATIONS
Do you have specific locations where you would like
    pollutant concentrations to be calculated (Y/N) -> N
```

A summary of the SCREEN model's output for this example is shown below:

```
     ***************************************
     *** SUMMARY OF SCREEN MODEL RESULTS ***
     ***************************************

 CALCULATION         MAX CONC     DIST TO    TERRAIN
  PROCEDURE          (UG/M**3)    MAX (M)     HT (M)
--------------     -----------    -------    -------
SIMPLE TERRAIN       1190.           100.         0.

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
```

## 4.2.8 Continuous Emissions from Land Treatment Facilities



Similar Releases: Landfarms; ground level application of sludge (volatile organic material in oil) to soil surface.

Discussion:

The emissions equation is a simplification of the Thibodeaux-Hwang model, assuming ground-level application of the waste, more rapid diffusion through the oil layer, and vapor-liquid equilibrium between the oil layer and pore spaces.

Limitations and Assumptions:

- Waste is a sludge consisting of organics in oil.
- Methods are a simplification of the Thibodeax-Hwang emission model (Thibodeax and Hwang, 1982).
- Assumes no subsurface injection, slower diffusion of organic component through air-filled pore spaces than through the oil layer, and vapor-liquid equilibrium between the air in the pore spaces and the oil layer.
- Assumes that Raoult's Law applies.
- Effective diffusivity is assumed to be 40 % of pure component diffusivity.

Input Information:

$A$ release area ($m^2$)
$L_{vap}$ latent heat of vaporization (J/kmol)
$T_b$ boiling point temperature (°K)
$M_w$ molecular weight (kg/kmol)

ppm grams of organic component per million grams of waste oil (g/Mg)
$P_v$ vapor pressure as a function of temperature (Pa)
R gas constant (8314 J/kg-mole·°K)

### 4.2.8.1 Procedure

1. **Vapor Pressure.** Calculate the vapor pressure ($P_v$) in Pa. The vapor pressure of a pure substance is temperature dependent. The Antoine equation could be used to estimate vapor pressure; however, the Clausius-Clapeyron equation is used in TSCREEN because the required input is readily available for most chemicals in TSCREEN's chemical database. The Clausius-Clapeyron equation is:

$$P_v = 101325 \exp\left( \frac{L_{vap}\, M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T} \right) \right) \qquad (4.2.8\text{-}1)$$

   where T = liquid temperature (°K), assumed = 298 °K. The vapor pressure must be greater than 0.

2. **Emission Rate.** Calculate Emission Rate ($Q_m$) (g/s). Since typical applications involve applications of volatile liquids such as benzene, the Thibodeux-Hwang emission model has been simplified for screening purposes using default values:

$$Q_m = K \cdot \text{ppm (g/Mg)} \cdot A\ (m^2) \cdot (P_v)^{1/2}\ \text{(Pa)} \qquad (4.2.8\text{-}2)$$

   where: $K = 9.101 \times 10^{-10} (g/Pa^{1/2}\text{-}m^2\text{-}s)$

3. Run the SCREEN model for an area source. For an explanation of inputs to the SCREEN model to an area source, see Section 5.1.2.

### 4.2.8.2 Example: Emission from sludge containing benzene

Discussion:

Sludge containing 1000 ppm benzene is applied to a one acre land treatment site at a rate of 1 lb/ft$^2$ and filled to a depth of 8 inches. Hourly average concentrations at the fenceline of 200 m are needed.

The following input information will be required:

A release area (one acre or 4046.8 m$^2$)
$L_{vap}$ latent heat of vaporization ($3.9393 \times 10^5$ J/kg)
$T_b$ boiling point temperature of benzene (351 °K)
$M_w$ molecular weight (78.12 kg/kmol)

| | |
|---|---|
| ppm | grams of benzene per million grams of waste oil (1000 g benzene/Mg oil) |
| R | gas constant (8314 J/kg-mole·°K) |

Procedure:

1. **Vapor Pressure.** The vapor pressure is calculated using Equation (4.2.8-1) as follows:

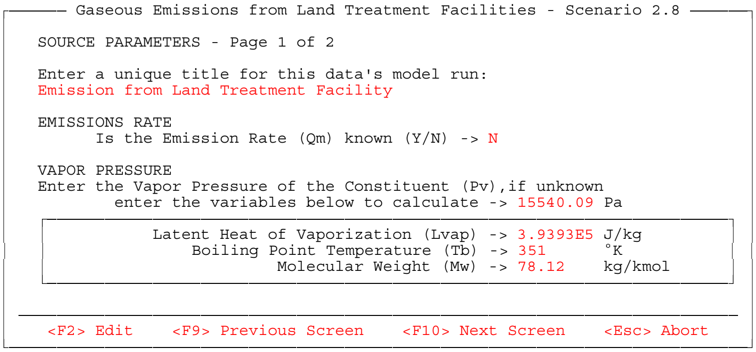
$$P_v = 101325 \exp\left( \frac{3.9393\times10^5 \cdot 78.12}{8314} \left( \frac{1}{351} - \frac{1}{298} \right) \right) = 1.55\text{x}10^4 \text{ Pa}$$

2. **Emission Rate.** Calculate the emission rate ($Q_m$) in g/s using Equation (4.2.8-2):

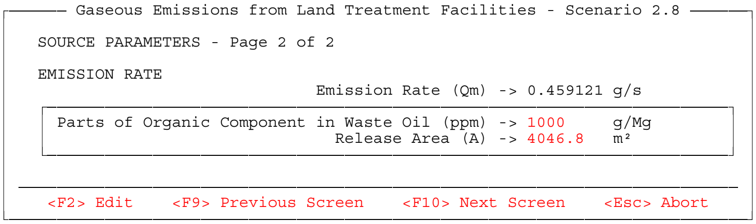
$$Q_m = 9.101\times10^{-10} \cdot (1000) \cdot 4046.8 \cdot (1.55\times10^4)^{1/2} = 0.46 \text{ g/s}$$

3. Run the SCREEN model for an area source.

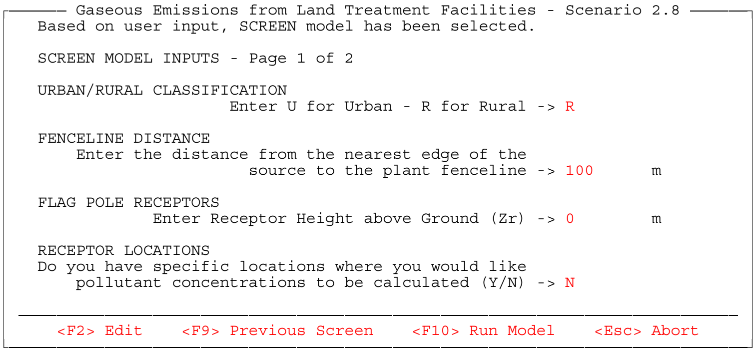
Data entry in the TSCREEN model for this example is shown below:



```
 Gaseous Emissions from Land Treatment Facilities - Scenario 2.8

SOURCE PARAMETERS - Page 1 of 2

Enter a unique title for this data's model run:
Emission from Land Treatment Facility

EMISSIONS RATE
      Is the Emission Rate (Qm) known (Y/N) -> N

VAPOR PRESSURE
Enter the Vapor Pressure of the Constituent (Pv),if unknown
        enter the variables below to calculate -> 15540.09 Pa

           Latent Heat of Vaporization (Lvap) -> 3.9393E5 J/kg
               Boiling Point Temperature (Tb) -> 351      °K
                        Molecular Weight (Mw) -> 78.12    kg/kmol
```



```
 Gaseous Emissions from Land Treatment Facilities - Scenario 2.8

SOURCE PARAMETERS - Page 2 of 2

EMISSION RATE
                             Emission Rate (Qm) -> 0.459121 g/s

  Parts of Organic Component in Waste Oil (ppm) -> 1000     g/Mg
                               Release Area (A) -> 4046.8   m²
```

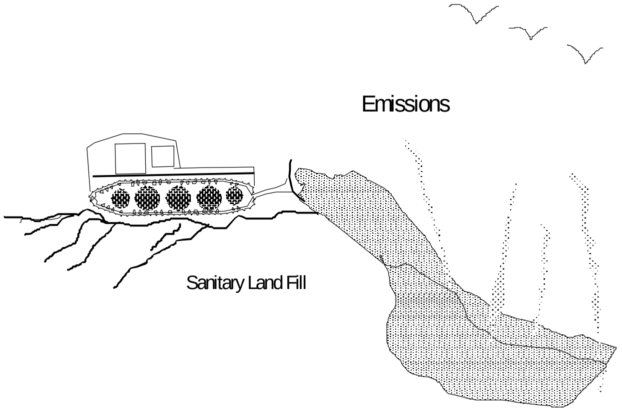


```
 Gaseous Emissions from Land Treatment Facilities - Scenario 2.8
Based on user input, SCREEN model has been selected.

SCREEN MODEL INPUTS - Page 1 of 2

URBAN/RURAL CLASSIFICATION
                    Enter U for Urban - R for Rural -> R

FENCELINE DISTANCE
    Enter the distance from the nearest edge of the
                      source to the plant fenceline -> 100      m

FLAG POLE RECEPTORS
            Enter Receptor Height above Ground (Zr) -> 0        m

RECEPTOR LOCATIONS
Do you have specific locations where you would like
    pollutant concentrations to be calculated (Y/N) -> N
```

A summary of the SCREEN model's output for this example is shown below:

```
     ***************************************
     *** SUMMARY OF SCREEN MODEL RESULTS ***
     ***************************************

 CALCULATION        MAX CONC    DIST TO   TERRAIN
  PROCEDURE        (UG/M**3)    MAX (M)    HT (M)
--------------    -----------   -------   -------
SIMPLE TERRAIN      3464.          100.        0.

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
```

## 4.2.9 Continuous Emissions from Municipal Solid Waste Landfills



Similar Releases: None. Emission rates applicable to municipal solid waste landfills only.

Discussion:

A New Source Performance Standard was proposed on May 30, 1991 for Municipal Solid Waste Landfills (MSWLFs). Air emissions from MSWLFs contribute to the formation of ambient ozone and potentially to global warming. The U.S. EPA estimates that MSWLFs emit about 1% of the national stationary source volatile organic compound (VOC) emissions. Also, the methane produced from landfills is between one third and one half of the national total. Toxics, explosion potential, and odor nuisance are additional problems related to air emissions from MSWLFs.

Landfill air emissions are controlled through application of a gas collection system and control device. Three engineering components comprise the collection and control system. Extraction wells pull the gas up from the depth of the fill. A header system links all the wells and collects the gas by vacuum. A control device either burns the gas or uses it for fuel.

In the proposed regulation, the U.S. EPA has developed a system to determine which landfills should be controlled. A non-methane organic compound (NMOC) emission rate was selected for determining applicability under this regulation. Each landfill calculates its annual emissions. If a landfill emits over a certain amount of NMOC per year, a gas collection and control system must be installed.

The information in this section is taken from the background document for proposal of air regulations for municipal solid waste landfills (EPA, 1991b). This document explains how emissions can be estimated using either (1) an equation based on default values or (2) sampling data (e.g., field measurements of the gas flow rate and composition). The equation is based on the Scholl Canyon model (EMCON Associates, 1982) and uses default or measured values of methane generation potential and nonmethane organic compounds (NMOCs). The total VOC emissions determined by this procedure can be speciated using a profile as shown in Table 4.2.9-1. There are a number of factors contributing to the variability in gaseous emissions from municipal solid waste landfills (e.g., waste composition, landfill moisture content, age of refuse, pH and alkalinity of landfill, amount of buried waste, climate, and physical and operating characteristics of the landfill). The greatest sources of uncertainty are the type and amount of waste buried in a landfill. Use of sampling data is strongly recommended (as described in the EPA background document for proposed regulations for municipal solid waste landfills). However, the use of an equation is considered appropriate as a simple screening tool, and this approach is described below.

Ambient concentrations resulting from municipal solid waste landfill emissions are determined using area source techniques in the SCREEN model.

Limitations and Assumptions:

- Emission rates are applicable to municipal solid waste landfills only.

- An average NMOC emission rate is provided. (To obtain the individual toxic constituent emission rate, the individual toxic constituent percent of total emissions is needed. The background document for the proposed regulations provides the range in the vapor phase concentration of toxic constituents that has been measured from landfills nationwide.)

- Emission rates are assumed to be steady-state, with no seasonal or diurnal variation.

Output:

$M_{NMOC}$ = Average annual NMOC emission rate, Mg/yr
$M_{NMOC}$ (g/s) = $M_{NMOC}$ (Mg/yr) X 0.0317

Input Information:

| | |
|---|---|
| $L_o$ | refuse methane generation potential ($m^3$/Mg refuse) |
| R | average annual waste acceptance rate (Mg/yr) |
| k | methane generation rate constant (1/yr) |
| c | year since closure (c=0 for new/active landfills) |
| t | age of landfill (yrs) |
| $C_{NMOC}$ | concentration of NMOC (ppmv as hexane) |
| ConstPer | constituent percent of total VOC emissions (%) |

$3.595 \times 10^{-9}$ conversion factor

The variables R, c, and t should be known for each landfill. The average annual acceptance rate, R, can be determined by dividing the refuse in place by the age of the landfill. If site-specific values of k, $L_o$, or $C_{NMOC}$ are unknown, default values of 0.02/yr, 230 $m^3$/Mg, and 8000 ppmv as hexane may be used, respectively.

### 4.2.9.1 Procedure:

1. **Mass Emission Rate of NMOC, Mg/yr.** Calculate the average annual NMOC emission rate. The following equation is best suited for the purposes of the U.S. EPA to determine the NMOC emission rate:

$$M_{NMOC} = 2L_oR(e^{-kc} - e^{-kt})(C_{NMOC})(3.595 \times 10^{-9}) \qquad (4.2.9\text{-}1)$$

2. **Mass Emission Rate of NMOC, g/s.** Convert Mass Emission Rate of NMOC from Mg/yr to g/s.

$$M_{NMOC}\ (g/s) = M_{NMOC}\ (Mg/yr) \times 0.0317 \qquad (4.2.9\text{-}2)$$

3. **Fraction of total NMOC emissions, $Q_m$ (g/s).**

$$Q_m\ (g/s) = M_{NMOC}\ (g/s) \times ConstPer\ (\%)/100 \qquad (4.2.9\text{-}3)$$

4. Dispersion of emissions from a landfill is simulated as an area source, involving determination of dispersion parameters based on virtual distances before concentrations can be calculated at each receptor location. The SCREEN model for an area source is used for this scenario. For an explanation of inputs for the SCREEN model for an area source, see Section 5.1.2.

### 4.2.9.2 Example: Municipal Solid Waste Landfill

Discussion:

Hourly concentration estimates are required for emissions of perchloroethene from a municipal landfill in Ohio. The landfill area is 3 hectares and the distance to the nearest offsite receptor is 100 m.

Concentration estimates from landfills are determined using an emissions model or site-specific measurements. In this example, measurements are not available and the NMOC emission model in Section 4.2.9.1 is used. Once NMOC emissions are calculated, NMOC emission profiles (Table 4.2.9-1) are used to determine what fraction of the total is perchloroethene. The example concentrations listed are averages; site-specific concentrations are dependent on the type of waste in the landfill.

The following input information will be required:

$L_o$ refuse methane generation potential (230 $m^3$/Mg refuse)
R average annual waste acceptance rate (13,000 Mg/yr)
k methane generation rate constant (0.02 (1/yr))
c year since closure (0)
t age of landfill (10 yrs)
$C_{NMOC}$ concentration of NMOC (8000 ppmv as hexane)
$MW_{NMOC}$ molecular weight of NMOC (87.00 lb/mole NMOC)

**TABLE 4.2.9-1**
**SPECIATED VOC EMISSION PROFILE**

| Air Toxic Chemical | Molecular Wt. | Concentration(ppmv) |
|---|---|---|
| Benzene | 78.12 | 3.52 |
| Carbon Tetrachloride | 153.81 | 1.49 |
| Chloroform | 119.38 | 0.06 |
| Ethylene Dichloride | 98.96 | 1.85 |
| Methylene Chloride | 84.93 | 19.70 |
| Perchloroethene | 165.83 | 6.82 |
| Trichloroethene | 131.29 | 3.80 |
| Vinyl Chloride | 62.50 | 7.04 |
| 1,1-Dichloroethylene | 96.94 | 0.16 |

Procedure:

1. **Mass Emission Rate of NMOC, Mg/yr.** From Equation (4.2.9-1), emissions are calculated as:

$$M_{NMOC} = 2(230)(13{,}000)(1 - e^{-(0.02)(10)})(8{,}000)(3.595X10^{-9})$$
$$M_{NMOC} = 31.2 \text{ Mg/yr}$$

2. **Mass Emission Rate of NMOC, g/s.** From Equation (4.2.9-2) the emissions in g/s are calculated as:

$$M_{NMOC} = 31.2 \text{ Mg/yr X } 0.0317 = .989 \text{ g/sec}$$

3. **Fraction of total NMOC emissions, $Q_m$ (g/s).** The fraction of perchloroethylene to the total NMOC emissions can be calculated as follows:

$$\frac{6.82\,(\text{ppmv})}{8000\,(\text{ppmv})} \text{ X } \frac{165.83\,(\text{lb/mole})}{87.00\,(\text{lb/mole NMOC})} = 0.0016$$

(ConstPer = 0.0016 x 100% = 0.16%)

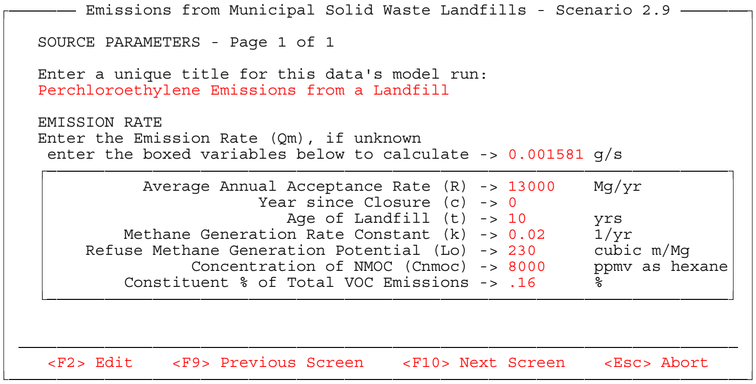
Perchloroethylene emissions $Q_m$ can then be calculated as follows:

$$Q_m = .989 \text{ (g/s) X } .0016 = .0016 \text{ g/s}$$

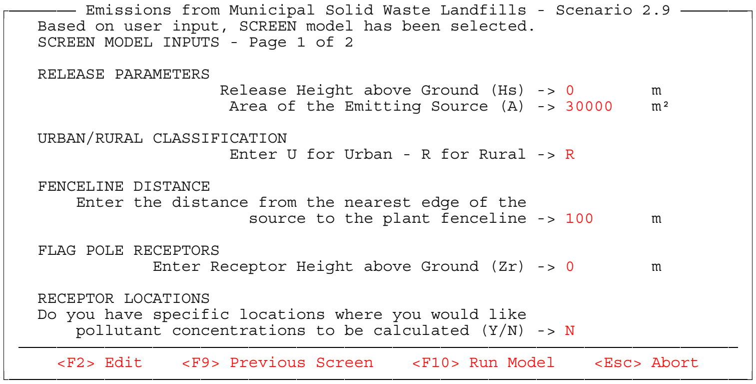
4. TSCREEN will run the SCREEN model for an area source.

Landfill area = 3 hectares (30,000 $m^2$)
Distance to nearest offsite receptor = 100 m

Data entry in the TSCREEN model for this example is shown below:



```
────── Emissions from Municipal Solid Waste Landfills - Scenario 2.9 ──────

 SOURCE PARAMETERS - Page 1 of 1

 Enter a unique title for this data's model run:
 Perchloroethylene Emissions from a Landfill

 EMISSION RATE
 Enter the Emission Rate (Qm), if unknown
  enter the boxed variables below to calculate -> 0.001581 g/s

            Average Annual Acceptance Rate (R) -> 13000    Mg/yr
                        Year since Closure (c) -> 0
                           Age of Landfill (t) -> 10       yrs
          Methane Generation Rate Constant (k) -> 0.02     1/yr
     Refuse Methane Generation Potential (Lo) -> 230      cubic m/Mg
               Concentration of NMOC (Cnmoc) -> 8000     ppmv as hexane
        Constituent % of Total VOC Emissions -> .16      %


   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

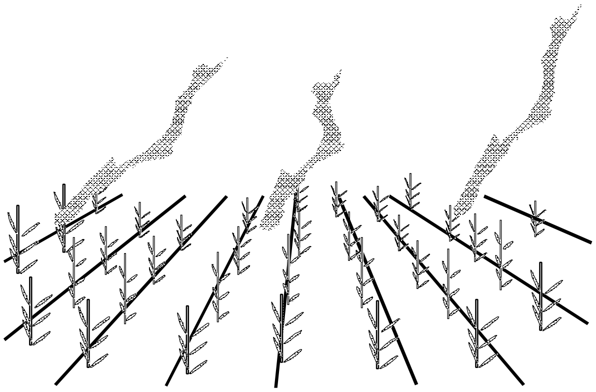


```
────── Emissions from Municipal Solid Waste Landfills - Scenario 2.9 ──────
 Based on user input, SCREEN model has been selected.
 SCREEN MODEL INPUTS - Page 1 of 2

 RELEASE PARAMETERS
                    Release Height above Ground (Hs) -> 0        m
                     Area of the Emitting Source (A) -> 30000    m²

 URBAN/RURAL CLASSIFICATION
                     Enter U for Urban - R for Rural -> R

 FENCELINE DISTANCE
     Enter the distance from the nearest edge of the
                       source to the plant fenceline -> 100      m

 FLAG POLE RECEPTORS
             Enter Receptor Height above Ground (Zr) -> 0        m

 RECEPTOR LOCATIONS
 Do you have specific locations where you would like
     pollutant concentrations to be calculated (Y/N) -> N

    <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

A summary of SCREEN model's output for this example is displayed below:

```
     ***************************************
     *** SUMMARY OF SCREEN MODEL RESULTS ***
     ***************************************

 CALCULATION         MAX CONC    DIST TO   TERRAIN
  PROCEDURE         (UG/M**3)    MAX (M)    HT (M)
--------------     -----------   -------   -------
 SIMPLE TERRAIN      5.008          100.        0.

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
```

### 4.2.10 Continuous Emissions of Pesticides



Emissions

Similar Releases: Emissions resulting from the volatilization of pesticides or herbicides applied to open fields.

Discussion:

Pesticides are classified according to the targeted pest. The most widely used pesticides, particularly in agriculture, are herbicides, insecticides, fungicides, and nematicides. A pesticide, otherwise known as the active ingredient, is combined with inert ingredients in formulations such as sprays, dusts, granules, aerosols, fumigants, and microencapsulation.

There are several factors that influence the extent and rate of pesticide volatilization, including physical and chemical properties of the pesticide, method of application, the type of surface to which the pesticide is applied, and degree of incorporation into the soil.

Evaporative losses during application and post-application are proportional to vapor pressure. The vapor pressure of active ingredients generally range from $10^{-3}$ to $10^{-8}$ millimeters of mercury (mm Hg). Fumigants usually have higher vapor pressures. Ethylene bromide, a common fumigant, has a vapor pressure of 0.8 mm Hg at 20°C. Often the inert ingredient is an organic solvent such as xylene, which has a vapor pressure of 8 mm Hg.

For pesticides applied to soils, the soil moisture content and the depth of the tilling are important factors affecting volatilization. Pesticides applied to dry soils do not volatilize as rapidly as pesticides applied to moist soils because of greater adsorption of pesticides on dry soil. The evaporation rate of pesticides incorporated into the soil is limited primarily by pesticide movement through the soil to the surface. The resistance increases with mixing depth.

Ambient concentrations resulting from the volatilization of applied pesticides are determined by using area source techniques in the SCREEN model.

Limitations and Assumptions:

- Maximum evaporation rates of pesticides are estimated based on the rate of evaporation of a compound such as water.
- The method is based on the principle that loss of a pure substance into the atmosphere from an inert surface is proportional to the vapor pressure and the square root of the molecular weight of the substance.
- The water evaporation rate is adjusted for the type of surface and relative humidity.

References:

The best sources of information are technical literature searches and contacts with agricultural research stations. Information on pesticide formulations, air emissions potential, and control strategies can be found in the Alternative Control Technology (ACT) for Application of Agricultural Pesticides report. The draft report was released April 1992 for peer review by the Emissions Standards Division of the Environmental Protection Agency located in Research Triangle Park, North Carolina. The reader may also find the following reference to be helpful:

Spencer, W.F. and Cliath M.M., 1973: "Pesticide Volatilization as Related to Water Loss from Soil," Journal of Environmental Quality.

Input Information:

| | |
|---|---|
| E | evaporation rate of water per acre (inches of water evaporated X 226,600 pounds per inch on one acre) (in/day) |
| aE | adjusted water evaporation rate in lb/acre; aE=0.73E, 0.40E, and 0.70E for application to vegetated land, soil surfaces, and water surfaces, respectively |
| RH | relative humidity (%) |
| $P_W$ | vapor pressure of water at same temperature as $P_P$ (atm) |

| | |
|---|---|
| $P_P$ | vapor pressure of pesticide ingredient (atm) |
| $M_W$ | molecular weight of water (18 g/g-mole) |
| $M_P$ | molecular weight of pesticide ingredient (g/g-mole) |
| A | area of application ($m^2$) |

### 4.2.10.1 Procedure

1. **Evaporation Rate of Water.** Convert the evaporation rate of water (E) from in/day to g/s.

$$E(\text{lb/s/acre}) = E(\text{in/day})\,226600(\text{lb/in/acre})(\text{day}/86400\text{s}) \qquad (4.2.10\text{-}1)$$

$$E\ (\text{lb/s}) = E\ (\text{lb/s/acre}) \cdot \frac{A\ (m^2)}{3910.3445\ (m^2/\text{acre})} \qquad (4.2.10\text{-}2)$$

$$E\ (\text{g/s}) = E\ (\text{lb/s}) \cdot 493.593\ (\text{g/lb}) \qquad (4.2.10\text{-}3)$$

2. **Emission Rate $Q_m$.** The following equation developed by Spencer is used to determine the evaporation rate of a pesticide ingredient per acre:

$$Q_m = \frac{[aE/(1 - RH/100)]\ [P_p \cdot 760 \cdot M_p^{1/2}]}{P_w \cdot 760 \cdot M_w^{1/2}} \qquad (4.2.10\text{-}4)$$

3. Area source dispersion techniques are used for the emissions from pesticide application. The SCREEN model for an area source is used for this scenario. For an explanation of inputs to the SCREEN model for an area source, see Section 5.1.2

### 4.2.10.2 Example: Continuous Emissions from an Herbicide

Discussion:

Bentazon is applied to 14.5 acres (56,700 $m^2$) for postemergence control of broadleaf weeds. The active ingredient is sodium bentazon at 40 percent by weight. The molecular weight of sodium bentazon is 262 grams per mole. The vapor pressure at 25°C is approximately $1x10^{-7}$ mm Hg ($1.32x10^{-10}$ atm). Rate of application is one pound of active ingredient per acre. The evaporation rate of water is 0.20 inches per day. The property boundary is located 100 meters from the edge of the study field. Maximum post-application one-hour average concentrations are to be estimated. The relative humidity is 60 percent.

The following input information will be required:

| | |
|---|---|
| E | evaporation rate of water per acre (lb/day/acre) (inches of water evaporated per day X 226,600 pounds per inch on one acre); 0.20 in/day of water evaporated |

| | |
|---|---|
| aE | adjusted water evaporation rate in lb/acre; aE=0.73E for application to vegetated land |
| RH | relative humidity (60 %) |
| $P_W$ | vapor pressure of water at same temperature as $P_P$ (.03158 atm) |
| $P_P$ | vapor pressure of pesticide ingredient ($1.32 \times 10^{-10}$ atm) |
| $M_W$ | molecular weight of water (18 g/g-mole) |
| $M_P$ | molecular weight of pesticide ingredient (262 g/g-mole) |
| A | area of application (56,700 $m^2$) |

Procedure:

1. **Evaporation Rate of Water.** Calculate the evaporation rate of water using Equations (4.2.10-1), (4.2-10.2), and (4.2-10.3):

$$E(lb/s/acre)=0.20(in/day)226600(lb/in/acre)(day/86400s)=0.52(lb/s/acre)$$

$$E\ (lb/s) = E\ (lb/s/acre) \cdot \frac{A\ (m^2)}{3910.3445\ (m^2/acre)} = 7.6\ (lb/s)$$

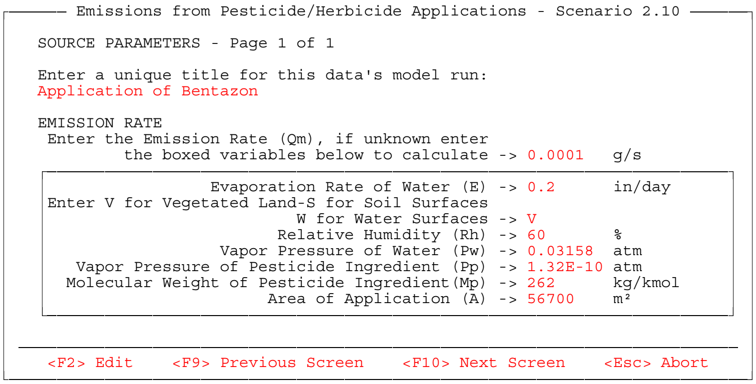
$$E\ (g/s) = E\ (lb/s) \cdot 493.593\ (g/lb) = 3440\ (g/s)$$

2. **Emission Rate $Q_m$.** Use the evaporation rate of water to estimate emissions of sodium bentazon from the field with Equation (4.2.10-4):

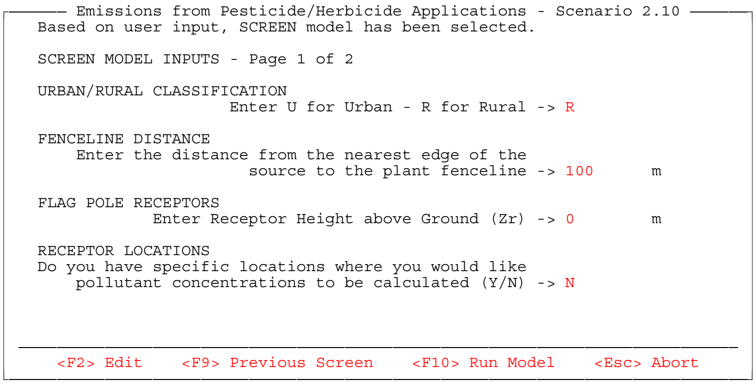
$$Q_m = \frac{[0.73 \cdot 3440/(1 - 60/100)]\ [1.32 \times 10^{-10} \cdot 760 \cdot 262^{1/2}]}{.03158 \cdot 760 \cdot 18^{1/2}} = .0001(g/s)$$

3. TSCREEN will run the SCREEN model for an area source:

Data entry in the TSCREEN model for this example is shown below:



```
Emissions from Pesticide/Herbicide Applications - Scenario 2.10

SOURCE PARAMETERS - Page 1 of 1

Enter a unique title for this data's model run:
Application of Bentazon

EMISSION RATE
 Enter the Emission Rate (Qm), if unknown enter
        the boxed variables below to calculate -> 0.0001   g/s

                 Evaporation Rate of Water (E) -> 0.2      in/day
 Enter V for Vegetated Land-S for Soil Surfaces
                          W for Water Surfaces -> V
                        Relative Humidity (Rh) -> 60       %
                  Vapor Pressure of Water (Pw) -> 0.03158  atm
   Vapor Pressure of Pesticide Ingredient (Pp) -> 1.32E-10 atm
  Molecular Weight of Pesticide Ingredient(Mp) -> 262      kg/kmol
                       Area of Application (A) -> 56700    m²

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

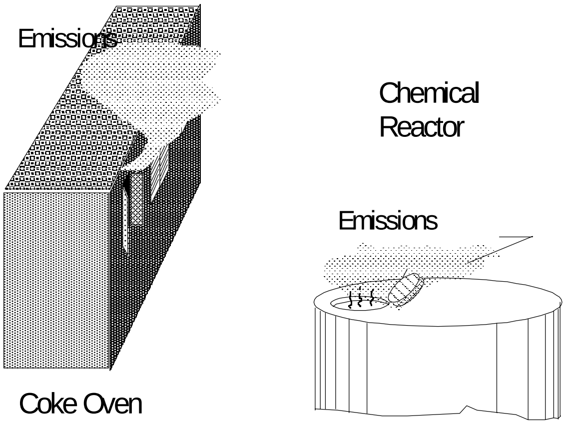


```
Emissions from Pesticide/Herbicide Applications - Scenario 2.10
Based on user input, SCREEN model has been selected.

SCREEN MODEL INPUTS - Page 1 of 2

URBAN/RURAL CLASSIFICATION
                    Enter U for Urban - R for Rural -> R

FENCELINE DISTANCE
    Enter the distance from the nearest edge of the
                      source to the plant fenceline -> 100      m

FLAG POLE RECEPTORS
            Enter Receptor Height above Ground (Zr) -> 0        m

RECEPTOR LOCATIONS
Do you have specific locations where you would like
    pollutant concentrations to be calculated (Y/N) -> N
```

A summary of the SCREEN model's output for this example is displayed below:

```
          ***************************************
          *** SUMMARY OF SCREEN MODEL RESULTS ***
          ***************************************

 CALCULATION        MAX CONC    DIST TO   TERRAIN
  PROCEDURE        (UG/M**3)    MAX (M)    HT (M)
--------------    -----------   -------   -------
SIMPLE TERRAIN      .2360         100.        0.

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
```

### 4.2.11 Instantaneous Discharges from Equipment Openings



Similar Releases: Any puff or burst type release with short duration emissions resulting from the opening of equipment after processing (e.g., coke ovens or chemical reactors), from routine sampling of product processing or gaseous emissions from disconnected lines.

Discussion:

Sources of this type are modeled as instantaneous point sources of gaseous emissions due to the momentum of their release. Emissions can either be estimated on a source-specific basis by the user or calculated from representative emission factors. Emissions estimates are available in AP-42 for some batch operations. VOC profiles are also available to identify toxic components (Appendix A, item 4). Simple estimates of emissions from failed or disconnected transfer lines or similar sources can be calculated from the gas volume between the break point and nearest shutoff valve. Ambient concentrations resulting from instantaneous discharges are determined by using the PUFF model (see Section 5.3).

Limitations and Assumptions:

- Release is presumed to be neutrally buoyant.
- There is no plume rise algorithm in the current version of the PUFF model. The height of release should be set to stack height.

Input Information:

EF total emission times fraction associated with particular pollutant (g/kg)
Pd total production of the facility of all emissions (kg)

### 4.2.11.1 Procedure

1. **Total Amount of Material Released.** Calculate the total amount of material released (Q) (g).

$$Q\ (g) = Pd\ (kg) \cdot EF\ (g/kg) \qquad (4.2.11\text{-}1)$$

2. Since the release is neutrally buoyant, dispersion estimates are determined using the PUFF model. For an explanation of inputs to the PUFF model, see Section 5.3.

### 4.2.11.2 Example: Release from equipment opening

Discussion:

A common source of emissions due to equipment openings is found in the production of coke where the opening of the ovens at the completion of processing results in a near instantaneous release. One toxic component of the emission is toluene. A coke oven battery produces 20,000 kg total emissions. The oven door is 5 m above ground. An estimate of 15-minute average concentration at distances beyond 50 m downwind of this source is needed.

Emissions from coke ovens result primarily from charging and discharging operations and fugitive losses which occur on a continuous basis. The example presented is for the near instantaneous emissions which result from discharge in the completed coke through the oven doors. Sample simulations are based on the impact of a single furnace although in real applications total emissions from a battery of ovens over time would be more typical. Simulations require determinations of an emission factor for the oven and total emissions based on oven capacity. Dispersion estimates are made assuming that the release is instantaneous with no initial dispersion.

The following input information will be required:

EF total emission times fraction associated with particular pollutant
Pd total production at the facility of all emissions
Hs release height above ground (5m)

Procedure:

1. **Total Amount of Material Released.** To begin, the emissions are estimated using emission factors (EPA, 1987b). Assume

that VOC emissions are approximately 3% of total coke pushing emissions. (Note, AP-42 suggests 0.2 lb/ton). The total VOC production is:

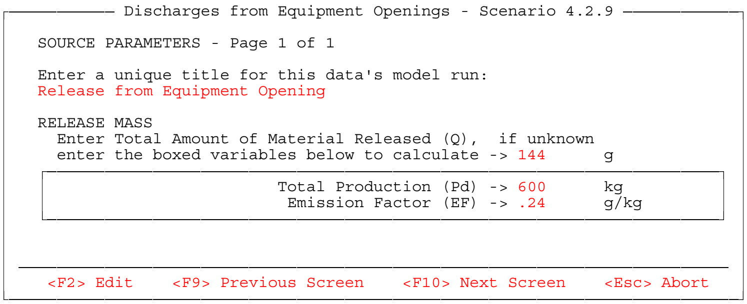
$$0.03 \times 20,000 \text{ kg} = 600 \text{ kg}.$$

Assume that total toluene emissions from coke production are 0.48 lb/ton of VOC (0.24 g/kg). Coke pushing emissions are then given by multiplying the emission factor times the total production using Equation (4.2.11-1):

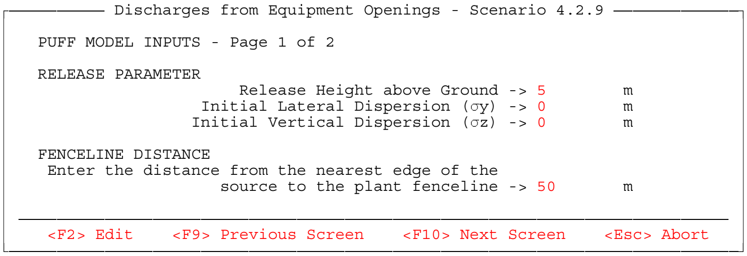
$$Q(g) = 0.24 \ (g/kg) \bullet 600 \ (kg) = 144 \ (g) \text{ toluene}$$

2. Because the release is neutrally buoyant, the cloud is treated as passive for this example. TSCREEN will run the PUFF model.

Data entry in the TSCREEN model for this example is shown below:



```
 Discharges from Equipment Openings - Scenario 4.2.9

SOURCE PARAMETERS - Page 1 of 1

Enter a unique title for this data's model run:
Release from Equipment Opening

RELEASE MASS
  Enter Total Amount of Material Released (Q),  if unknown
  enter the boxed variables below to calculate -> 144      g

                          Total Production (Pd) -> 600      kg
                           Emission Factor (EF) -> .24      g/kg

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Discharges from Equipment Openings - Scenario 4.2.9

PUFF MODEL INPUTS - Page 1 of 2

RELEASE PARAMETER
                     Release Height above Ground -> 5        m
                 Initial Lateral Dispersion (σy) -> 0        m
                Initial Vertical Dispersion (σz) -> 0        m

FENCELINE DISTANCE
 Enter the distance from the nearest edge of the
                   source to the plant fenceline -> 50       m

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

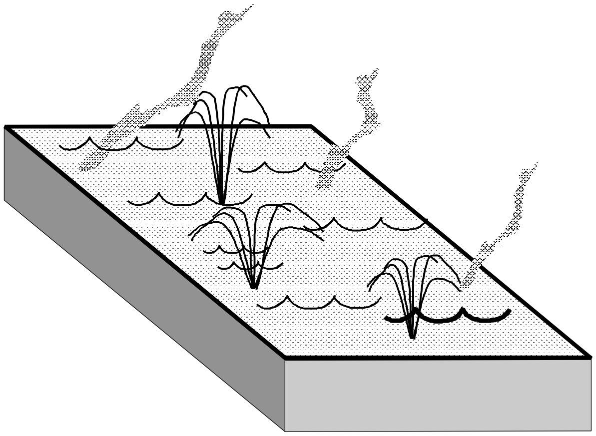
A summary of the PUFF model's output for this example is shown below:

```
 ******************************************************
 ***         SUMMARY OF PUFF MODEL RESULTS          ***
 ******************************************************

THE MAXIMUM CONCENTRATION AND THE DISTANCE TO MAXIMUM
CONCENTRATION FOR DISTANCES BEYOND FENCELINE    .050 (KM).
FOR NEAR SURFACE RELEASE MAXIMUM CONCENTRATION WILL OCCUR AT
THE FENCELINE.

    AVERAGING          MAXIMUM             DISTANCE TO         STABILITY
    TIME (MIN)     CONCENTRATION (G/M**3)   MAX. CONC. (KM)     CLASS

 INSTANTANEOUS            1.693E-01           .060              N
       1                  2.107E-02           .082              N
       5                  4.213E-03           .082              N
*      15                 1.404E-03           .082              N
       60                 3.511E-04           .082              N

 ******************************************************
 **   REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS  **
 ******************************************************
```

## 4.3 Liquid Release

A liquid release is a release of material that may immediately evaporate (no pooling results) ort may pool first and then evaporate.

### 4.3.1 Continuous Evaporation from Surface Impoundments (Lagoons)



Similar Releases: Waste lagoons and other impoundments with emissions resulting from the evaporation of volatile chemicals from liquid mixtures with biological activity.

Discussion:

Emission rates from well-mixed aqueous waste in surface impoundments are modeled in this scenario. Techniques are provided for both quiescent and aerated impoundments. Emission estimates account for volatilization solely, with other removal mechanisms assumed to be negligible. Ambient concentrations resulting from continuous evaporation from surface impoundments are determined by using area source techniques in the SCREEN model.

Limitations and Assumptions:

- Equations are simplifications of EPA methods (EPA, 1987a) for quiescent surface impoundments with and without flow and for aeration basins.

- Equations are simplified by assuming a wind speed of 5 m/s, a constituent diffusivity in water of $10^{-5}$ $cm^2/s$, and a constituent diffusivity in air of 0.10 $cm^2/s$.

- Assumes waste is well mixed in impoundment.
- Assumes removal entirely by volatilization, with no loss due to biodegradation, seepage, or absorption.
- Assumes waste is aqueous, with no separate organic phase.

Input Information:

A area of impoundment ($m^2$)
$C_o$ initial concentration of chemical in the waste ($g/m^3$)

### 4.3.1.1 Procedure

1. **Emission Rate.** For VOC emission estimates from waste water treatment systems, refer to Industrial Waste Water VOC Emissions -Background from BACT/LAER, EPA-450/3-90-004, NTIS PB90-194754. This document is available from the EPA Control Technology Center, (919) 541-0800.

   The emission rate can be calculated as follows:

$$Q_m \text{ (g/s)} = K\text{(m/s)}\ C_o\text{(g/m}^3\text{)}\ A\text{(m}^2\text{)} \qquad (4.3.1\text{-}1)$$

   where: $K = 4 \times 10^{-6}$(m/s) for the quiescent case
   $K = 8 \times 10^{-4}$ (m/s) for the aerated case

2. Run the SCREEN dispersion model for an area source.

### 4.3.1.2 Example: Emission of benzene

Discussion:

One-hour concentration estimates of benzene are desired from a quiescent impoundment with an area of 1500$m^2$ and a fenceline 200 m from source.

The following input information will be required:

A area of impoundment (1500 $m^2$)
$C_o$ initial concentration of the chemical in the waste (1000 $g/m^3$)

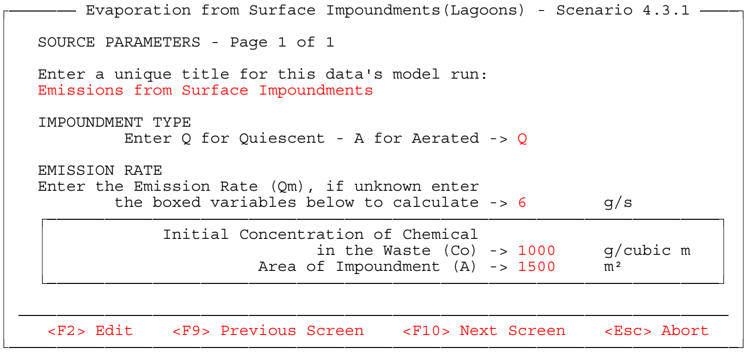
Procedure:

1. **Emission Rate.** Calculate the emission rate using Equation (4.3.1-1):

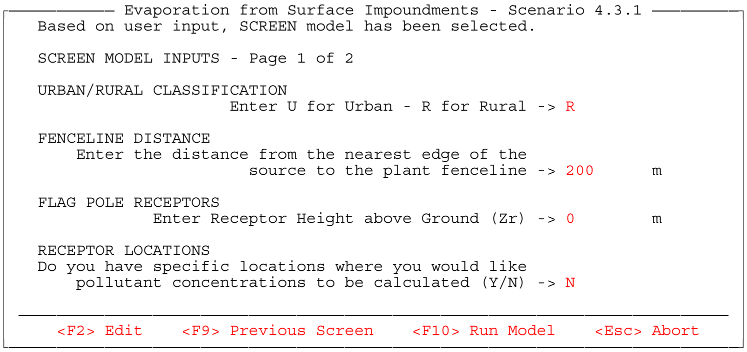
$$Q_m (g/s) = 4x10^{-6} (m/s) \bullet 1000 (g/m^3) \; 1500 (m^2) = 6 (g/s)$$

2. TSCREEN will run the SCREEN model for an area source.

Data entry in the TSCREEN model for this example is shown below:



```
 Evaporation from Surface Impoundments(Lagoons) - Scenario 4.3.1

SOURCE PARAMETERS - Page 1 of 1

Enter a unique title for this data's model run:
Emissions from Surface Impoundments

IMPOUNDMENT TYPE
         Enter Q for Quiescent - A for Aerated -> Q

EMISSION RATE
Enter the Emission Rate (Qm), if unknown enter
        the boxed variables below to calculate -> 6        g/s

             Initial Concentration of Chemical
                             in the Waste (Co) -> 1000     g/cubic m
                       Area of Impoundment (A) -> 1500     m²

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

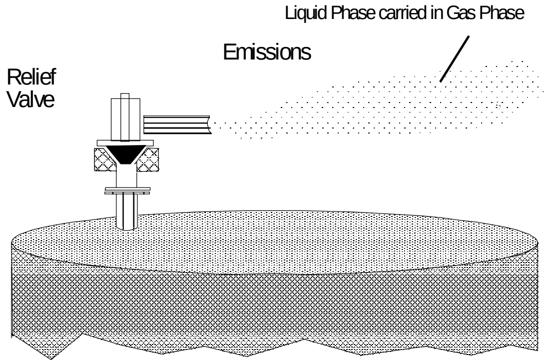


```
 Evaporation from Surface Impoundments - Scenario 4.3.1
Based on user input, SCREEN model has been selected.

SCREEN MODEL INPUTS - Page 1 of 2

URBAN/RURAL CLASSIFICATION
                    Enter U for Urban - R for Rural -> R

FENCELINE DISTANCE
    Enter the distance from the nearest edge of the
                      source to the plant fenceline -> 200      m

FLAG POLE RECEPTORS
            Enter Receptor Height above Ground (Zr) -> 0        m

RECEPTOR LOCATIONS
Do you have specific locations where you would like
    pollutant concentrations to be calculated (Y/N) -> N

    <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

A summary of the SCREEN model's output for this example is shown below:

```
      ***************************************
      *** SUMMARY OF SCREEN MODEL RESULTS ***
      ***************************************

 CALCULATION        MAX CONC    DIST TO   TERRAIN
  PROCEDURE        (UG/M**3)    MAX (M)    HT (M)
--------------    -----------   -------   -------
SIMPLE TERRAIN      .2944E+05     200.         0.

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
```

## 4.3.2 Continuous (Two-Phase) Release Rate Estimates: Saturated Liquid from Pressurized Storage



Similar Releases: Saturated liquid leak from a pressurized tank (possibly through a relief valve) or a saturated liquid leak from a pipe.

Discussion:

Materials which are stored under pressure will depressurize when released to the atmosphere. This depressurization results in the formation of two contaminant phases (saturated liquid and vapor) for: gases which cool so that condensation occurs during the depressurization process; and high volatility liquids (liquids whose normal boiling point is below the ambient temperature) which are typically stored at above ambient pressure. (So called saturated liquids are liquids stored at a pressure equal to their vapor pressure for the storage temperature; subcooled liquids are liquids stored at a pressure above their vapor pressure for the storage temperature; and superheated liquids are liquids stored at a pressure below their vapor pressure for the storage temperature. For a preliminary estimate, the temperature of superheated liquid releases should be set to the saturation temperature.) In this scenario, the terms gas, saturated liquid, and subcooled liquid all refer to the state of the tank contents. The scenario considers the release from a tank (or reservoir) and includes a provision for the effect of a pressure drop (piping) between the tank and the hole or opening.

This procedure applies to a continuous release of pressurized liquid stored under saturated conditions. The release occurs from (constant pressure and temperature) contaminant (reservoir) through a hole or opening; a provision is made for the effect of a pressure drop (piping) between the tank and the hole or opening.

Limitations and Assumptions:

The hole or opening size must be sufficiently small, otherwise the reservoir temperature and pressure may no longer be constant. For the case of a leak from a tank, the assumption of constant reservoir temperature and pressure may be violated if a significant percentage of the tank contents is released. If the reservoir temperature and pressure are not constant, the release rate may vary with time, but the maximum release rate is generally obtained from the initial reservoir temperature and pressure. For the case of a leak from a pipeline, the initial pipeline conditions can be used to estimate the release rate, but this may greatly overpredict the actual release rate as the hole size approaches the pipe diameter.

The vapor phase of the released material must be an ideal gas at the reservoir conditions, during the depressurization process, and after depressurization to the atmosphere; for the case of a tank containing vapor and liquid, the hole must be in the liquid space of the tank (Spicer, 1992).

Input Information:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($m^2$) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (J/kg·°K) (For contaminant mixtures, see Appendix B) |
| $C_{pl}$ | liquid (contaminant) heat capacity at $T_1$ (J/kg·°K) (For contaminant mixtures, see Appendix B) |
| $D_0$ | (equivalent) diameter of hole or opening ($D_0=2\cdot\sqrt{A_0/\pi}$) (m) |
| $D_p$ | pipe diameter (as appropriate) (m) |
| $L_p$ | pipe length (appropriate) (m) |
| $M_w$ | gas (contaminant) molecular weight (kg/kmol) (For contaminant mixtures, see Appendix B) |
| $P_a$ | ambient pressure (Pa) |
| $P_1$ | reservoir pressure (Pa) |
| Q | total amount of material released (kg) |
| $T_a$ | ambient temperature (°K) |
| $T_b$ | contaminant normal boiling point (°K) |
| $T_1$ | reservoir temperature (°K) |
| $\lambda$ | heat of vaporization at the normal boiling point (J/kg) |
| $\rho_1$ | contaminant liquid density at the normal boiling point ($kg/m^3$) |
| R | gas constant (8314 J/kg-mole°K or 8314 $Pa.m^3$/kg-mole.°K) |

4.3.2.1 Procedure:

1. **Estimate Discharge Temperature.** For pure components, estimate the discharge temperature $T_2$ from the vapor pressure (Clausius-Clapeyron) equation:

$$P_a = 101325 \exp\left( \frac{\lambda\ M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_2} \right) \right) \qquad (4.3.2\text{-}1)$$

which can be rewritten as:

$$T_2 = \frac{1}{\frac{1}{T_b} - \frac{R}{\lambda\ M_w} \cdot \ln\left( \frac{P_a}{M_w} \right)}$$

2. **Vapor Fraction after Depressurization.** Estimate the vapor mass fraction (or quality) after depressurization $X_2$ as:

$$X_2 = C_{pl}\ (\ T_1 - T_2\ )\ /\ \lambda \qquad (4.3.2\text{-}2)$$

If $1 > X_2 > 0$, then this estimate is valid; go to step 3. If $X_2 \leq 0$ then the release should be modeled like a high volatility liquid release; the case of $X_2 \geq 1$ is unlikely on physical grounds.

3. **Release Rate.** As recommended by Fauske and Epstein (1987), estimate the emission rate $Q_m$ (kg/s) depending on the pipe length $L_p$ as follows: If $L_p/L_e \leq 1$ (where $L_e$=0.1 m),

$$Q_m\ (\text{kg/s}) = A_0 \left( \frac{\lambda\ M_w\ P_1}{R\ T_1^2} \right) \left( \frac{T_1}{N\ C_{pl}} \right)^{1/2} \qquad (4.3.2\text{-}3)$$

where

$$N = \frac{R\ (\lambda\ M_w\ P_1)^2}{2\ (P_1 - P_a)\ \rho_1\ C^2\ (R\ T_1)^3\ C_{pl}} + L_p/L_e \qquad (4.3.2\text{-}4)$$

where C is the discharge coefficient (here, $C \approx 0.6$). (Note that if $L_p/L_e = 0$, Equations (4.3.2-3) and (4.3.2-4) reduce to the standard orifice equation for incompressible flow.) If $L_p/L_e > 1$,

$$Q_m\ (\text{kg/s}) = A_0\ F \left( \frac{\lambda\ M_w\ P_1}{R\ T_1^2} \right) \left( \frac{T_1}{C_{pl}} \right)^{1/2} \qquad (4.3.2\text{-}5)$$

where F represents the effect of friction in the pipe (here,

$F^2 \simeq 1/(1+4fL_p/D_p)$; for a Reynold's number typical of liquid flow, $f \simeq 0.0015$ can be used as an estimate).

4. **Discharge Density.** Estimate the density after depressurization $\rho_2$ as:

$$\rho_2\ (\mathrm{kg/m^3}) = \left[ X_2 \left( \frac{R\ T_2}{P_a\ M_w} \right) + \left( \frac{1 - X_2}{\rho_1} \right) \right]^{-1} \qquad (4.3.2\text{-}6)$$

5. **Buoyancy Check.** Estimate release buoyancy as a first check.

   A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\ M_a}{R\ T_a} \qquad (4.3.2\text{-}7)$$

   where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

   B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 6. If the buoyancy is zero or positive, the SCREEN model for a point source should be used. (See Section 2.4 for more information on model selection.)

6. **Release Duration.** The release duration is used as an input into the RVD and Britter-McQuaid models. The release duration can be used to determine if the release is continuous or instantaneous (see Section 2.5). Calculate the release duration $T_d$ using the equation below:

$$T_d\ (\mathrm{min}) = \frac{Q\ (\mathrm{kg})}{Q_m\ (\mathrm{kg/s}) \cdot 60\ (\mathrm{s/min})} \qquad (4.3.2\text{-}8)$$

### 4.3.2.2 Example: Saturated Liquid Chlorine Leak

Discussion:

In this example, saturated chlorine liquid is discharged from a heated pressurized tank through a 10.16 cm diameter hole well below the liquid level in the tank (the pressure and temperature were chosen to illustrate that the release rates from the vapor space are generally much smaller than release rates from the liquid space); the chlorine vapor temperature is that of the tank, 349.2 °K. The fenceline is 100 m from the tank

The following information will be required:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening (0.008107 $m^2$) |
| $C_{pl}$ | liquid (contaminant) heat capacity at $T_1$ (920 J/kg·°K) |
| $D_0$ | diameter of hole or opening (0.1016 m) |
| $M_w$ | gas (contaminant) molecular weight (70.9 kg/kmol) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_1$ | reservoir pressure ($2.586\text{x}10^6$ Pa) |
| Q | total amount of material released (50,000 kg) |
| $T_a$ | ambient temperature (293 °K) |
| $T_b$ | contaminant normal boiling point (239.05 °K) |
| $T_1$ | reservoir temperature (349.2 °K) |
| $\lambda$ | heat of vaporization at the normal boiling point ($2.870\text{x}10^5$ J/kg) |
| $\rho_1$ | contaminant density at reservoir conditions (1574 $kg/m^3$) |

Procedure:

1. **Estimate Discharge Temperature.** Estimate the discharge temperature $T_2$ from Equation (4.3.2-1):

$$T_2 = \frac{1}{\dfrac{1}{239.05} - \dfrac{8314}{2.879\times10^5 \cdot 70.9} \cdot \ln\left(\dfrac{101325}{101325}\right)} = 239.05\ ^\circ K$$

(This temperature is also the normal boiling point since $P_a$ = 101325 Pa).

2. **Vapor Fraction after Depressurization.** Estimate the vapor fraction after depressurization $X_2$ from Equation (4.3.2-2)

$$X_2 = 920\ (\ 349.2 - 239.05\ )\ /\ 2.879\times10^5 = 0.352$$

Since $1 > X_2 > 0$, then this estimate is valid; go to step 3.

3. **Release Rate.** Since $L_p/L_e \leq 1$ (where $L_p = 0$ and $L_e = 0.1$ m), estimate the release rate from Equation (4.3.2-3):

$$Q_m(kg/s) = 0.008107\left(\frac{2.879\times10^5 \cdot 70.9 \cdot 2.586\times10^6}{(8314)\cdot(349.2)^2}\right)\left(\frac{349.2}{0.365 \cdot 920}\right)^{1/2}$$

$$Q_m = 430\ kg/s$$

where N is calculated from Equation (4.3.2-4):

$$N = \frac{8314\ (2.879\times10^5 \cdot 2.586\times10^6)^2}{2\ (2.586\times10^6 - 101325)\ 1574 \cdot 0.6^2\ (8314\ 349.2)^3\ 920} + 0/1 = 0.365$$

(Note that at this rate a "ton" container would be emptied in 2 to 3 seconds.)

4. **Discharge Density.** Estimate the density after depressurization $\rho_2$ from Equation (4.3.2-6):

$$\rho_2\ (\mathrm{kg/m^3}) = \left[ 0.352 \left( \frac{8314 \cdot 239.05}{101325 \cdot 70.9} \right) + \left( \frac{1 - 0.187}{1574} \right) \right]^{-1} = 10.23\ \mathrm{kg/m^3}$$

5. **Buoyancy Check.** Estimate release buoyancy as a first check.

   A. Calculate the density of air using the following:

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 293} = 1.20\ \mathrm{kg/m^3}$$

   where 28.9 kg/kmol is the molecular weight of air.

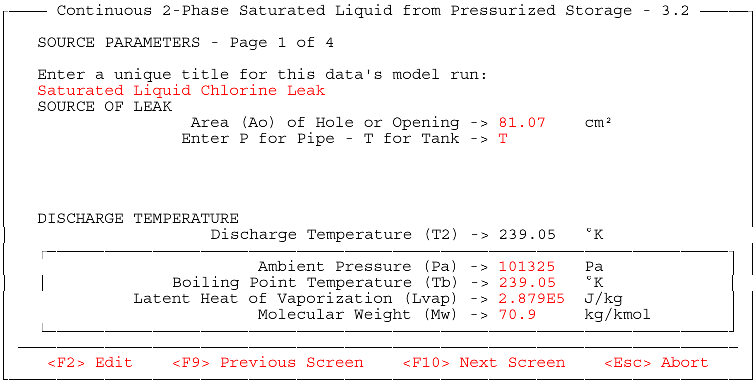
   B. $\rho_2/\rho_{air}$ >1 therefore, buoyancy is negative.

6. **Release Duration.** Calculate the release duration $T_d$ using the equation below:

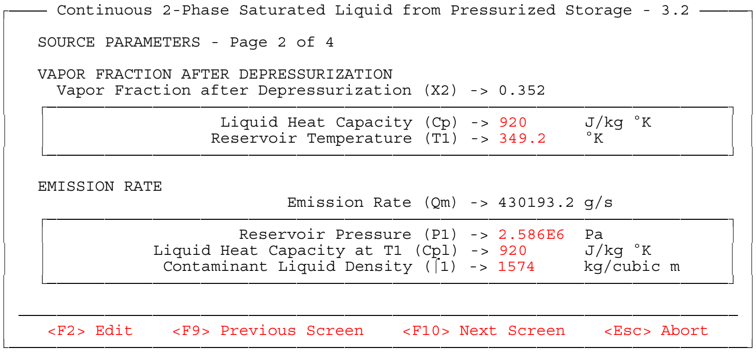
$$T_d\ (\mathrm{min}) = \frac{50{,}000\ (\mathrm{kg})}{430\ (\mathrm{kg/s}) \cdot 60\ (\mathrm{s/min})} = 1.94\ \mathrm{min}$$

   After this calculation run the Britter-McQuaid model since the release is assumed not to be vertically directed jet. (See Section 5.4 for more information on the Britter-McQuaid model.)

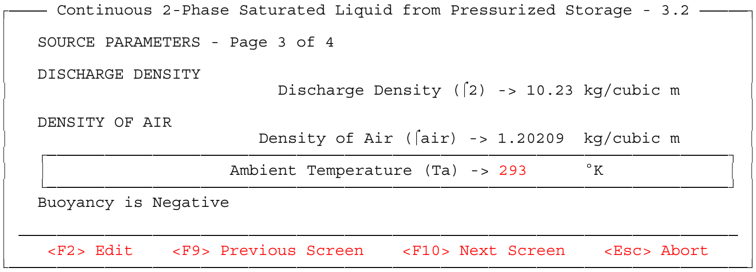
Data entry in the TSCREEN model for this example is shown below:



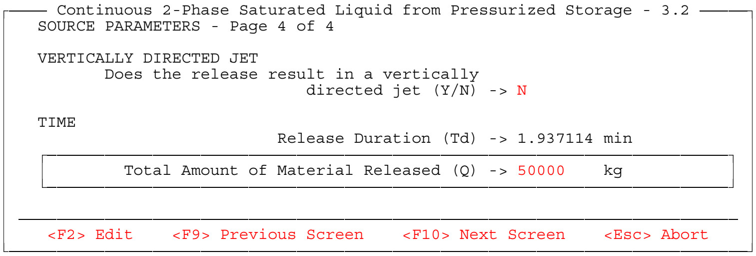
```
Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Saturated Liquid Chlorine Leak
SOURCE OF LEAK
                Area (Ao) of Hole or Opening -> 81.07     cm²
               Enter P for Pipe - T for Tank -> T



DISCHARGE TEMPERATURE
                  Discharge Temperature (T2) -> 239.05    °K

                       Ambient Pressure (Pa) -> 101325    Pa
              Boiling Point Temperature (Tb) -> 239.05    °K
          Latent Heat of Vaporization (Lvap) -> 2.879E5   J/kg
                       Molecular Weight (Mw) -> 70.9      kg/kmol

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



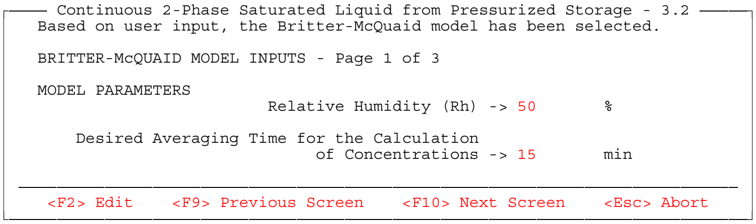
```
 Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2
 SOURCE PARAMETERS - Page 2 of 4

 VAPOR FRACTION AFTER DEPRESSURIZATION
   Vapor Fraction after Depressurization (X2) -> 0.352

                     Liquid Heat Capacity (Cp) -> 920      J/kg °K
                    Reservoir Temperature (T1) -> 349.2    °K

 EMISSION RATE
                             Emission Rate (Qm) -> 430193.2 g/s

                       Reservoir Pressure (P1) -> 2.586E6  Pa
               Liquid Heat Capacity at T1 (Cpl) -> 920      J/kg °K
                Contaminant Liquid Density (⌠1) -> 1574     kg/cubic m

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



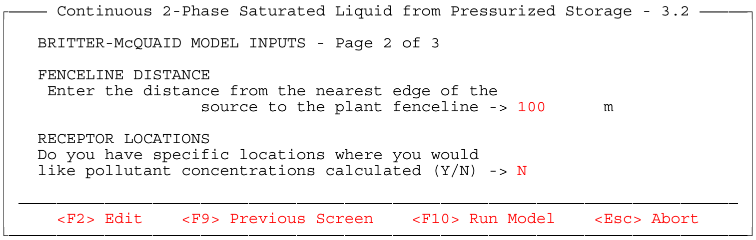
```
 Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2
 SOURCE PARAMETERS - Page 3 of 4

 DISCHARGE DENSITY
                          Discharge Density (⌠2) -> 10.23 kg/cubic m

 DENSITY OF AIR
                          Density of Air (⌠air) -> 1.20209  kg/cubic m

                      Ambient Temperature (Ta) -> 293      °K

 Buoyancy is Negative

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2
 SOURCE PARAMETERS - Page 4 of 4

 VERTICALLY DIRECTED JET
        Does the release result in a vertically
                             directed jet (Y/N) -> N

 TIME
                          Release Duration (Td) -> 1.937114 min

         Total Amount of Material Released (Q) -> 50000    kg

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2
 Based on user input, the Britter-McQuaid model has been selected.

 BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

 MODEL PARAMETERS
                          Relative Humidity (Rh) -> 50       %

     Desired Averaging Time for the Calculation
                          of Concentrations -> 15       min

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Continuous 2-Phase Saturated Liquid from Pressurized Storage - 3.2
 BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

 FENCELINE DISTANCE
  Enter the distance from the nearest edge of the
                source to the plant fenceline -> 100      m

 RECEPTOR LOCATIONS
 Do you have specific locations where you would
 like pollutant concentrations calculated (Y/N) -> N

  <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

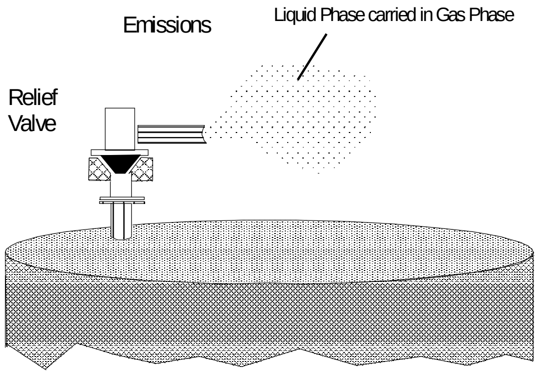
A summary of the Britter-McQuaid model's output is displayed below:

```
          ***************************************
          ***   SUMMARY OF B&M MODEL RESULTS  ***
          ***************************************

        MAX CONC      MAX CONC    DIST TO    WIND SPEED
        (UG/M**3)      (PPM)      MAX (M)      (M/S)
        ---------    ---------    -------    ----------
        .3535E+09    .1199E+06      200.          1.

***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
***************************************************
```

### 4.3.2.3 Considerations for Time-Varying and Time-Limited Releases

See Section 2.5 for a discussion of considerations for time-varying and time-limited releases.

## 4.3.3 Instantaneous (Two-Phase) Release Rate Estimates: Saturated Liquid from Pressurized Storage



Similar Releases: Saturated liquid leak from a pressurized tank or a saturated liquid leak from a pipe.

Discussion:

This procedure applies to an instantaneous release of pressurized liquid stored under saturated conditions. The release occurs (at constant pressure and temperature) from a containment (reservoir) through a hole or opening; a provision is made for the effect of a pressure drop (piping) between the tank and the hole or opening. See Section 4.3.2 for further discussion.

Limitations and Assumptions:

Same as Section 4.3.2.

Input Information:

Same as Section 4.3.2.

### 4.3.3.1 Procedure:

1-4. Same as Section 4.3.2.

5. **Buoyancy Check.** Perform buoyancy check as a first check.

   A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\ M_a}{R\ T_a} \tag{4.3.3-1}$$

   where $M_a$ is the molecular weight of air (assumed to equal 28.9 g/g-mole).

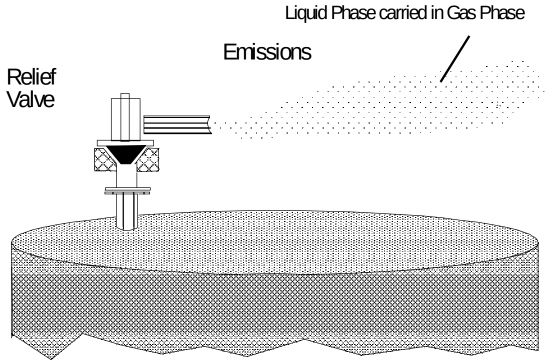
   B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 6. If the buoyancy is positive, the PUFF model for a point source should be used. (See Section 2.4 for more information on model selection.)

6. Same as Section 4.3.2.

#### 4.3.3.2 Examples

See the examples in Section 4.3.2.

## 4.3.4 Continuous (Two-Phase) Release Rate Estimates: Subcooled Liquid from Pressurized Storage



Similar Releases: Subcooled liquid leak from a pressurized tank (possibly through a relief valve) or a subcooled liquid leak from a pipe.

Discussion:

Materials which are stored under pressure will depressurize when released to the atmosphere. This depressurization results in the formation of two contaminant phases (saturated liquid and vapor) for: gases which cool so that condensation occurs during the depressurization process; and high volatility liquids (liquids whose normal boiling point is below the ambient temperature) which are typically stored at above ambient pressure. (So called saturated liquids are liquids stored at a pressure equal to their vapor pressure for the storage temperature; subcooled liquids are liquids stored at a pressure above their vapor pressure for the storage temperature; and superheated liquids are liquids stored at a pressure below their vapor pressure for the storage temperature. For a preliminary estimate, the temperature of superheated liquid releases should be set to the saturation temperature.) In this scenario, the terms gas, saturated liquid, and subcooled liquid all refer to the state of the tank contents. The scenario considers the release from a tank (or reservoir) and includes provision for the effect of a pressure drop (piping) between the tank and the hole or opening.

This procedure applies to a continuous release of a pressurized liquid stored above its saturation pressure. This release occurs (at constant pressure and temperature) from a containment (reservoir) through a hole or opening; a provision is made for the effect of pressure drop (piping) between the tank and the hole or opening.

## Limitations and Assumptions:

The hole or opening size must be sufficiently small, otherwise the reservoir temperature and pressure may no longer be constant. For the case of a leak from a tank, the assumption of constant reservoir temperature and pressure may be violated if a significant percentage of the tank contents is released. If the reservoir temperature and pressure are not constant, the release rate may vary with time, but the maximum release rate is generally obtained from the initial reservoir temperature and pressure. For the case of a leak from a pipeline, the initial pipeline conditions can be used to estimate the release rate, but this may greatly overpredict the actual release rate as the hole size approaches the pipe diameter.

The vapor phase of the released material must be an ideal gas at the reservoir conditions, during the depressurization process, and after depressurization to the atmosphere; for the case of a tank containing vapor and liquid, the hole must be in the liquid space of the tank (Spicer, 1992).

## Input Information:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening ($m^2$) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ ($J/kg \cdot {}^\circ K$) (For contaminant mixtures, see Appendix B) |
| $C_{pl}$ | liquid (contaminant) heat capacity at $T_1$ ($J/kg \cdot {}^\circ K$) (For contaminant mixtures, see Appendix B) |
| $D_0$ | (equivalent) diameter of hole or opening ($D_0 = 2 \cdot \sqrt{A_0/\pi}$) (m) |
| $D_p$ | pipe diameter (as appropriate) (m) |
| $L_p$ | pipe length (appropriate) (m) |
| $M_w$ | gas (contaminant) molecular weight (kg/kmol) (For contaminant mixtures, see Appendix B) |
| $P_a$ | ambient pressure (Pa) |
| $P_1$ | reservoir pressure (Pa) |
| R | gas constant (8314 $J/kg\text{-}mole \cdot {}^\circ K$ or 8314 $Pa \bullet m^3/kg\text{-}mole \bullet {}^\circ K$) |
| Q | total amount of material released (kg) |
| $T_a$ | ambient temperature (°K) |
| $T_b$ | contaminant normal boiling point (°K) |
| $T_1$ | reservoir temperature (°K) |
| $\lambda$ | heat of vaporization at the normal boiling point (J/kg) |
| $\rho_1$ | contaminant density at the normal boiling point ($kg/m^3$) |

### 4.3.4.1 Procedure:

1. **Estimate Discharge Temperature.** For pure components, estimate the discharge temperature $T_2$ from the Clausius-Clapeyron equation:

$$P_a = 101325 \exp\left( \frac{\lambda M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_2} \right) \right) \qquad (4.3.4\text{-}1)$$

which can be rewritten as:

$$T_2 = \frac{1}{\dfrac{1}{T_b} - \dfrac{R}{\lambda M_w} \cdot \ln\left( \dfrac{P_a}{101325} \right)}$$

2. **Vapor Fraction after Depressurization.** Estimate the vapor mass fraction (or quality) after depressurization $X_2$ as:

$$X_2 = C_{pl} \, ( T_1 - T_2 ) \, / \, \lambda \qquad (4.3.4\text{-}2)$$

If $1 > X_2 > 0$, then this estimate is valid; go to step 3. If $X_2 \leq 0$ then the release should be modeled like a high volatility liquid release; the case of $X_2 \geq 1$ is unlikely on physical grounds.

3. **Release Rate.** As recommended by Fauske and Epstein (1987), estimate the emission rate $Q_m$ (kg/s) as follows:

$$Q_m(\text{kg/s}) = A_0 \left( 2\, C^2 \, (P_1 - P_{1v}) \, \rho_1 + \frac{F^2}{C_{pl} \, T_1} \left( \frac{\lambda \, M_w \, P_1}{R T_1} \right)^2 \right)^{1/2} \qquad (4.3.4\text{-}3)$$

where

$$P_{1v} \text{ (Pa)} = 101325 \exp\left( \frac{\lambda M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_1} \right) \right) \qquad (4.3.4\text{-}4)$$

where C is the discharge coefficient (here, $C \simeq 0.6$) and F represents the effect of friction in the pipe (here, $F^2 \simeq 1/(1+4fL_p/D_p)$; for a Reynold's number typical of liquid flow, $f \simeq 0.0015$ can be used as an estimate).

4. **Discharge Density.** Estimate the density after depressurization $\rho_2$ as:

$$\rho_2 \; (\text{kg/m}^3) = \left[ X_2 \left( \frac{R \, T_2}{P_a \, M_w} \right) + \left( \frac{1 - X_2}{\rho_1} \right) \right]^{-1} \qquad (4.3.4\text{-}5)$$

5. **Buoyancy Check.** Perform buoyancy check as a first check.

A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\ M_a}{R\ T_a} \qquad (4.3.4\text{-}6)$$

where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 6. If the buoyancy is positive, the SCREEN model for a point source should be used. (See Section 2.4 for more information on model selection.)

6. **Release Duration.** The release duration is used as an input into the RVD and Britter-McQuaid models. The release duration can be used to determine if the release is continuous or instantaneous (see Section 2.5). Calculate the release duration $T_d$ using the equation below:

$$T_d\ (\text{min}) = \frac{Q\ (\text{kg})}{Q_m\ (\text{kg/s}) \cdot 60\ (\text{s/min})} \qquad (4.3.4\text{-}7)$$

4.3.4.2 Example: Subcooled Liquid Chlorine Leak

Discussion:

In this example, subcooled chlorine liquid is discharged through a 10.16 cm diameter hole in a tank (the pressure and temperature were chosen to illustrate that the release rates from the vapor space are generally much smaller than release rates from the liquid space); the chlorine vapor temperature is estimated to be 349.2 °K using the Clausius-Clapeyron equation and the normal boiling point of chlorine (239.05 °K). The fenceline is 100 m from the tank.

The following information will be required:

| | |
|---|---|
| $A_0$ | area of reservoir hole or opening (0.008107 $m^2$) |
| $C_p$ | gas (contaminant) heat capacity at $T_1$ (489 J/kg·°K) |
| $C_{pl}$ | liquid (contaminant) heat capacity at $T_1$ (920 J/kg·°K) |
| $D_0$ | diameter of hole or opening (0.1016 m) |
| $M_w$ | gas (contaminant) molecular weight (70.9 kg/kmol) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_1$ | reservoir pressure ($2.586\times10^6$ Pa) |
| Q | total amount of material released (50,000 kg) |
| $T_a$ | ambient temperature (293 °K) |
| $T_b$ | contaminant normal boiling point (239.05 °K) |
| $T_1$ | reservoir temperature (298.15 °K) |

$\lambda$ heat of vaporization at the normal boiling point ($2.879\text{x}10^5$ J/kg)

$\rho_1$ contaminant density at reservoir conditions (1574 kg/m$^3$)

Procedure:

1. **Estimate Discharge Temperature.** Estimate the discharge temperature $T_2$ from Equation (4.3.4-1):

$$T_2 = \frac{1}{\dfrac{1}{239.05} - \dfrac{8314}{2.879\times10^5\cdot70.9}\cdot\ln\left(\dfrac{101325}{101325}\right)} = 239.05\ ^\circ\text{K}$$

(This temperature is also the normal boiling point since $P_a$ = 101325 Pa).

2. **Vapor Fraction after Depressurization.** Estimate the vapor fraction after depressurization $X_2$ from Equation (4.3.4-2)

$$X_2 = 920\ (\ 298.15 - 239.05\ )\ /\ 2.879\times10^5 = 0.1888$$

Since $1 > X_2 > 0$, then this estimate is valid; go to step 3.

3. **Release Rate.** Using $L_p$=0 (and F = 1) , estimate the release rate from Equation (4.3.4-3):

$$Q_m(\text{kg/s}) = .008107\left(2C^2(2.586\times10^6 - P_{1v})1574 + \frac{F^2\left(\dfrac{2.879\times10^5\cdot70.9\cdot2.586\times10^6}{8314\ 298.15}\right)^2}{920\cdot298.15}\right)^{\frac{1}{2}}$$

$$Q_m\ (\text{kg/s}) = 493\ (\text{kg/s})$$

where C = 0.6 and

$$P_{1v}\ (\text{Pa}) = 101325\ \exp\left(\frac{2.879\times10^5\cdot70.9}{8314}\left(\frac{1}{239.05} - \frac{1}{298.15}\right)\right) = 7.76\times10^5\ \text{Pa}$$

4. **Discharge Density.** Estimate the density after depressurization $\rho_2$ from Equation (4.3.4-5):

$$\rho_2\ (\text{kg/m}^3) = \left[\ 0.1888\left(\frac{8314\cdot239.05}{101325\cdot70.9}\right) + \left(\frac{1 - 0.100}{1574}\right)\right]^{-1} = 18.96\ \text{kg/m}^3$$

5. **Buoyancy Check.** Perform buoyancy check as a first check.

A. Calculate the density of air using the following:

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 293} = 1.20\ kg/m^3$$

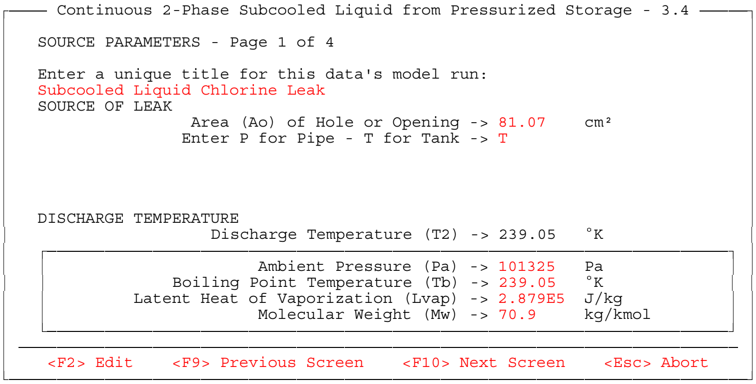
B. $\rho_2/\rho_{air} > 1$, therefore, buoyancy is negative.

6. **Release Duration.** Calculate the release duration $T_d$ using the equation below:

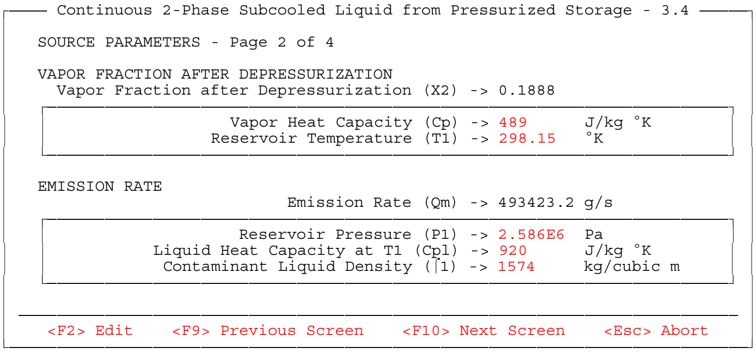
$$T_d\ (min) = \frac{50{,}000\ (kg)}{493\ (kg/s) \cdot 60\ (s/min)} = 1.69\ min$$

After this calculation run the Britter-McQuaid model since the release is not from a vertically directed jet. (See Section 5.4 for more information on the Britter-McQuaid model.)

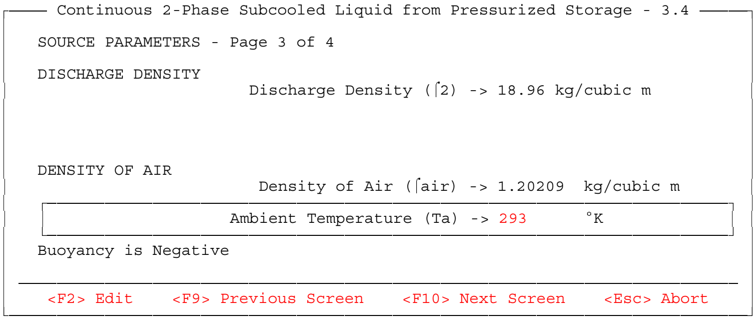
Data entry in the TSCREEN model for this example is shown below:



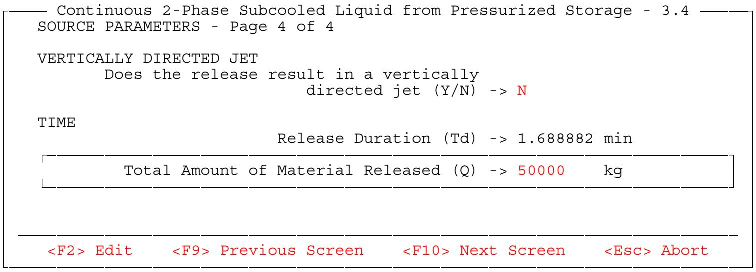
```
Continuous 2-Phase Subcooled Liquid from Pressurized Storage - 3.4

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Subcooled Liquid Chlorine Leak
SOURCE OF LEAK
                Area (Ao) of Hole or Opening -> 81.07     cm²
               Enter P for Pipe - T for Tank -> T



DISCHARGE TEMPERATURE
                  Discharge Temperature (T2) -> 239.05    °K

                       Ambient Pressure (Pa) -> 101325    Pa
              Boiling Point Temperature (Tb) -> 239.05    °K
          Latent Heat of Vaporization (Lvap) -> 2.879E5   J/kg
                       Molecular Weight (Mw) -> 70.9      kg/kmol
```



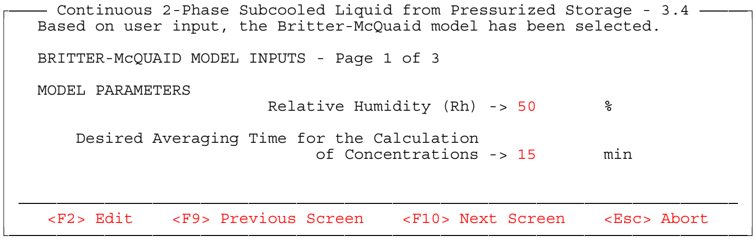
```
Continuous 2-Phase Subcooled Liquid from Pressurized Storage - 3.4

SOURCE PARAMETERS - Page 2 of 4

VAPOR FRACTION AFTER DEPRESSURIZATION
  Vapor Fraction after Depressurization (X2) -> 0.1888

                    Vapor Heat Capacity (Cp) -> 489       J/kg °K
                  Reservoir Temperature (T1) -> 298.15    °K


EMISSION RATE
                          Emission Rate (Qm) -> 493423.2 g/s

                     Reservoir Pressure (P1) -> 2.586E6   Pa
         Liquid Heat Capacity at T1 (Cpl) -> 920       J/kg °K
          Contaminant Liquid Density (⌈1) -> 1574      kg/cubic m
```



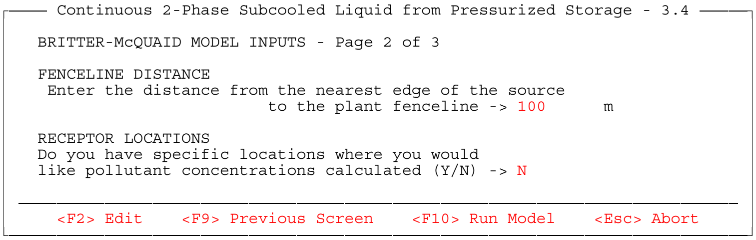
```
Continuous 2-Phase Subcooled Liquid from Pressurized Storage - 3.4

SOURCE PARAMETERS - Page 3 of 4

DISCHARGE DENSITY
                      Discharge Density (⌈2) -> 18.96 kg/cubic m



DENSITY OF AIR
                       Density of Air (⌈air) -> 1.20209  kg/cubic m

                   Ambient Temperature (Ta) -> 293      °K

Buoyancy is Negative

 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous 2-Phase Subcooled Liquid from Pressurized Storage - 3.4
SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET
       Does the release result in a vertically
                            directed jet (Y/N) -> N

TIME
                         Release Duration (Td) -> 1.688882 min

         Total Amount of Material Released (Q) -> 50000    kg


 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous 2-Phase Subcooled Liquid from Pressurized Storage - 3.4
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS
                        Relative Humidity (Rh) -> 50       %

    Desired Averaging Time for the Calculation
                           of Concentrations -> 15       min


 <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous 2-Phase Subcooled Liquid from Pressurized Storage - 3.4

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE
 Enter the distance from the nearest edge of the source
                        to the plant fenceline -> 100      m

RECEPTOR LOCATIONS
Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

  <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

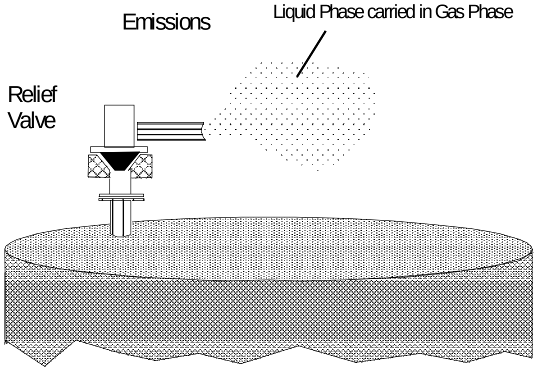
A summary of the Britter-McQuaid model's output is displayed below:

```
       ***************************************
       ***   SUMMARY OF B&M MODEL RESULTS  ***
       ***************************************

     MAX CONC      MAX CONC     DIST TO    WIND SPEED
     (UG/M**3)      (PPM)       MAX (M)      (M/S)
     ---------    ---------     -------    ----------
     .3535E+09    .1199E+06      200.          1.

  ***************************************************
  ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
  ***************************************************
```

### 4.3.4.3 Considerations for Time-Varying and Time-Limited Releases

See Section 2.5 for a discussion of considerations for time-varying and time-limited releases.

## 4.3.5 Instantaneous (Two-Phase) Release Rate Estimates: Subcooled Liquid from Pressurized Storage



Similar Releases: Subcooled liquid leak from a pressurized tank or a subcooled liquid leak from a pipe.

Discussion:

This procedure applies to an instantaneous release of a pressurized liquid stored above its saturation pressure. This release occurs (at constant pressure and temperature) from a containment (reservoir) through a hole or opening; a provision is made for the effect of pressure drop (piping) between the tank and the hole or opening. See Section 4.3.4 for further discussion.

Limitations and Assumptions:

Same as Section 4.3.4.

Input Information:

Same as Section 4.3.4.

### 4.3.5.1 Procedure:

1-4. Same as Section 4.3.4

5. **Buoyancy Check.** Perform buoyancy check as a first check.

A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\ M_a}{R\ T_a} \qquad (4.3.5\text{-}1)$$

where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

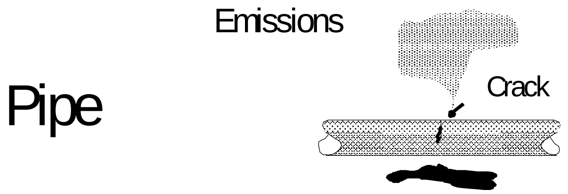
B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 8. If the buoyancy is positive, the PUFF model for a point source should be used. (See Section 2.4 for more information on model selection.)

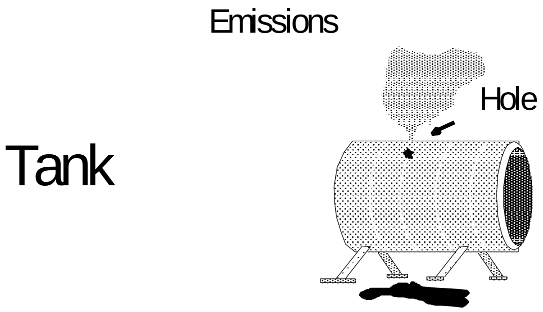
6. Same as Section 4.3.4.

#### 4.3.5.2 Examples

See the examples in Section 5.4.4.

### 4.3.6 Continuous High Volatility Leaks





Similar Releases: High-volatility liquid leak from a tank or a high volatility liquid leak from a pipe (when the ratio of the hole diameter to the pipe diameter is less than 0.2).

Discussion:

A high-volatility liquid is considered to be a material (liquid) whose normal boiling point is below the ambient temperature; a high-volatility material will be released as a liquid if the storage pressure is near ambient pressure whereas release from high pressure storage will result in aerosol formation. The following considers the problem of estimating the release rate of a high-volatility liquid when the diameter of the hole or opening is less than the diameter of the containment (e.g., a pipe or a reservoir). (When considering hole sizes which approach the pipe diameter, the release rate should be taken as the maximum of the pipe flow rate and the estimated release rate.) For high-volatility liquid releases, the (conservative) assumption is that the liquid boils off instantaneously so that the liquid release rate is equal to the (gas) evolution rate.

This procedure applies to a continuous release of a high volatility liquid (at constant temperature and pressure) from a containment (reservoir) through a hole or opening.

Limitations and Assumptions:

For this screening procedure, the following assumptions are applied:

- The pressure and temperature of the liquid in the reservoir are essentially constant.
- The hole or opening is located in the liquid space (as opposed to the vapor space).
- The gas evolution rate is assumed to be equal to the liquid release rate (i.e., vaporization is instantaneous).

The hole or opening size must be sufficiently small, otherwise considerations other than those outlined below may determine the release rate. For the case of a leak from a pipe, $\beta$ (defined below) should be less than 0.2; if $\beta>0.2$, the release rate should be taken to be the normal flow rate in the pipe. In either case, the gas evolution rate is assumed to be equal to the liquid release rate (i.e., vaporization is instantaneous). If the reservoir temperature, pressure, and liquid level are not constant, the release rate may vary with time, but the maximum release rate is generally obtained for the initial reservoir conditions (Spicer, 1992).

Input Information:

| | |
|---|---|
| $A_0$ | area of hole or opening ($m^2$) |
| $A_1$ | flow area representing reservoir conditions ($m^2$) (In the case of a leak from a tank, $A_1 \rightarrow \infty$ (and $\beta=0$); in the case of a leak from a pipe, $A_1$ is the cross-sectional area of the pipe.) |
| $D_0$ | (equivalent) diameter of hole or opening ($D_0=2\cdot\sqrt{A_0/\pi}$) (m) |
| g | acceleration due to gravity (9.81 $m^2/s$) |
| $H_L$ | distance between the hole or opening and the top of the liquid level (m) (In the case of a leak from a pipe, $H_L=0$.) |
| $M_w$ | contaminant molecular weight (kg/kmol) |
| $P_a$ | ambient pressure (Pa) |
| $P_v$ | vapor pressure as a function of temperature (Pa) |
| $P_1$ | reservoir pressure (Pa) |
| R | gas constant (8314 J/kg-mole·°K or 8314 $Pa\bullet m^3/kg\text{-}mole\bullet{}^\circ K$) |
| Q | total amount of material released (kg) |
| $T_a$ | ambient temperature (°K) |
| $T_b$ | contaminant normal boiling point (°K) |
| $T_1$ | reservoir temperature (°K) |
| $\beta$ | $\sqrt{A_0/A_1}$ (dimensionless) |
| $\gamma$ | heat of vaporization at the normal boiling point (J/kg) |

$\rho_1$ contaminant (liquid) density at reservoir conditions ($T_1$ and $P_1$) (kg/m$^3$)

4.3.6.1 Procedure:

1. **Pressure at the Hole or Opening.** Estimate the liquid pressure at the hole or opening $P_*$ as:

$$P_* = \max(P_a, P_1) + \rho_1 g H_L \qquad (4.3.6\text{-}1)$$

where $P_1 \geq P_v(T_1)$ which is estimated using the Clausius-Clapeyron Equation:

$$P_v = 101325 \exp\left( \frac{\lambda M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_1} \right) \right) \qquad (4.3.6\text{-}2)$$

2. **Emission Rate.** Estimate the emission rate $Q_m$ (kg/s) as follows from Perry et al. (1984):

$$Q_m \text{ (kq/s)} = K A_0 \left[ 2 \rho_1 \left( P_* - P_a \right) \right]^{1/2} \qquad (4.3.6\text{-}3)$$

where

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

where $C \simeq 0.65$ (although C can be larger if $\beta > 0.2$)

3. **Discharge Density.** Calculate the discharge density as follows:

$$\rho_2 = \frac{P_a M_w}{R T_1} \qquad (4.3.6\text{-}4)$$

4. **Buoyancy Check.** Perform buoyancy check as a first check.

   A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a M_a}{R T_a} \qquad (4.3.6\text{-}5)$$

   where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

   B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 5. If the buoyancy is positive, the SCREEN model for a point source should be used. (See Section 2.4 for more information on model selection.)

5. **Release Duration.** The release duration is used as an input

into the RVD and Britter-McQuaid models. The release duration can be used to determine if the release is continuous or instantaneous (see Section 2.5). Calculate the release duration $T_d$ using the equation below:

$$T_d \text{ (min)} = \frac{Q \text{ (kg)}}{Q_m \text{ (kg/s)} \cdot 60 \text{ (s/min)}} \qquad (4.3.6\text{-}6)$$

### 4.3.6.2 Example: Refrigerated Liquid Chlorine Leak

Discussion:

In this example, liquid chlorine presently at 101325 Pa is released from a tank through a 2.54 cm hole in the tank. The tank is 1.6 m long with a diameter of 0.8 m; the tank is half full and laying on its side. The fenceline is located 100 m from the tank.

The following information is required:

| | |
|---|---|
| $A_0$ | area of hole or opening ($\pi D_0^2/4 = 0.0005067\ m^2$) |
| $A_1$ | flow area representing reservoir conditions ($A_1 \rightarrow \infty\ m^2$) |
| $D_0$ | diameter of hole or opening (0.0254 m) |
| g | acceleration due to gravity ($9.81\ m^2/s$) |
| $H_L$ | distance between the hole or opening and the top of the liquid level (0.8 m/2 = 0.4 m) |
| $M_w$ | contaminant molecular weight (70.9 kg/kmol) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_1$ | reservoir pressure (101325 Pa) |
| R | gas constant (8314 J/kg-mole·°K or 8314 $Pa \bullet m^3/kg\text{-}mole \bullet {}^\circ K$) |
| Q | total amount of material released (200 kg) |
| $T_a$ | ambient temperature (293 °K) |
| $T_b$ | contaminant normal boiling point (239.05 °K) |
| $T_1$ | reservoir temperature (239.05 °K) |
| $\beta$ | $2 \cdot \sqrt{A_0/\pi}$ (0.0) |
| $\lambda$ | heat of vaporization at the normal boiling point ($2.879 \times 10^5$ J/kg) |
| $\rho_1$ | contaminant (liquid) density at reservoir conditions ($1574\ kg/m^3$) |

Procedure:

1. **Pressure at the Hole or Opening.** Estimate the liquid pressure $P_*$ at the hole or opening from Equation (4.3.6-1). In this case, liquid chlorine is being released as a saturated liquid at ambient pressure, so $P_a$=$P_1$=101325 Pa, and $P_*$ is estimated as:

$$P_* = \max(101325,\ 101325) + 1574 \cdot 9.81 \cdot 0.4 = 1.075\times10^5 \text{ Pa}$$

which is greater than $P_v$ calculated from Equation (4.3.6-2):

$$P_v = 101325 \exp\left( \frac{2.879\times10^5 \cdot 70.9}{8314} \left( \frac{1}{239.05} - \frac{1}{239.05} \right) \right) = 101325 \text{ Pa}$$

2. **Emission Rate.** Estimate the emission rate $Q_m$ from Equation (4.3.6-3) as follows:

$$Q_m = K\ 0.0005067 \left[ 2 \cdot 1574 \left( 1.075\times10^5 - 101325 \right) \right]^{1/2} = 1.45 \text{ kg/s}$$

where

$$K = 0.65 \,/ \sqrt{1 - 0.0^4} = 0.65$$

At this (maximum) rate, the tank will be emptied in 436 s; the actual time would be longer since $Q_m$ will decrease with time (because $H_L$ decreases with time). (Note that this situation can be compared to the earlier two-phase chlorine examples if the hole diameter is changed to agree with the earlier examples; if the hole diameter is changed to 10.16 cm, the emission rate for this case would be 23.2 kg/s. This liquid release rate is even smaller than the example pressurized vapor release rate of Section 2.3.)

3. **Discharge Density.** Calculate the discharge density using Equation (4.3.6-4) as follows:

$$\rho_2 = \frac{101325 \cdot 70.9}{8314 \cdot 239.05} = 3.61 \text{ kg/m}^3$$

4. **Buoyancy Check.** Perform buoyancy check as a first check.

   A. Calculate the density of air using Equation (4.3.6-5):

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 293} = 1.20 \text{ kg/m}^3$$

   where 28.9 kg/kmol is the molecular weight of air.

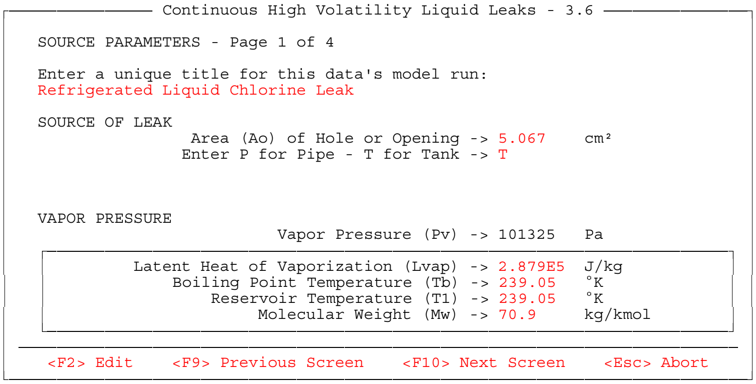
   B. Since $\rho_2/\rho_{air} > 1$, the buoyancy is negative.

5. **Release Duration.** Calculate the release duration $T_d$ using the equation below:

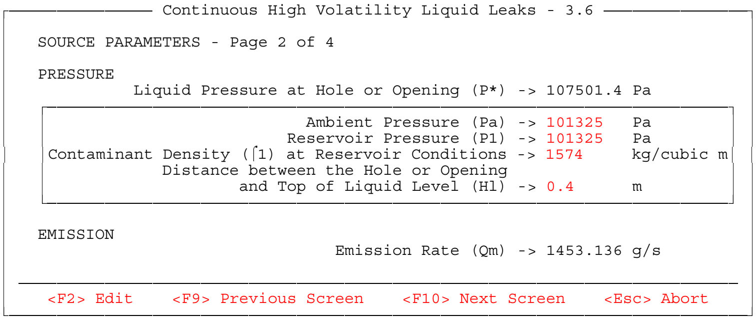
$$T_d\ (\mathrm{min}) = \frac{200\ (\mathrm{kg})}{1.45\ (\mathrm{kg/s}) \cdot 60\ (\mathrm{s/min})} = 2.30\ \mathrm{min}$$

After this calculation run the Britter-McQuaid model since the release is not from a vertically directed jet. (See Section 5.4 for more information on the Britter-McQuaid model.)

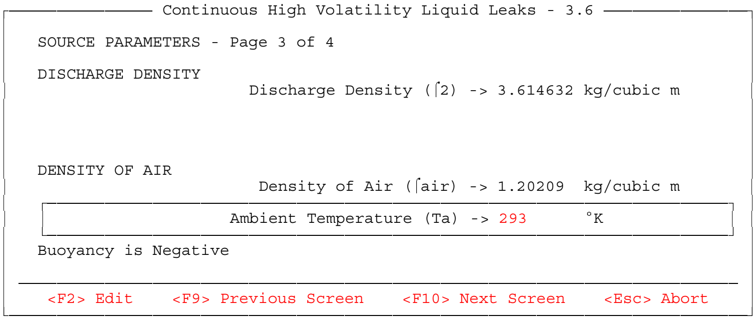
Data entry in the TSCREEN model for this example is shown below:



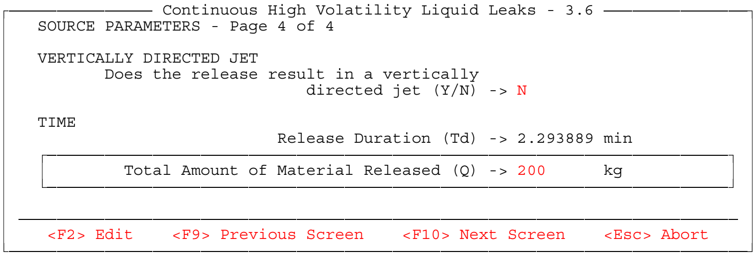
```
            Continuous High Volatility Liquid Leaks - 3.6

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Refrigerated Liquid Chlorine Leak

SOURCE OF LEAK
                Area (Ao) of Hole or Opening -> 5.067    cm²
               Enter P for Pipe - T for Tank -> T


VAPOR PRESSURE
                         Vapor Pressure (Pv) -> 101325   Pa

          Latent Heat of Vaporization (Lvap) -> 2.879E5  J/kg
              Boiling Point Temperature (Tb) -> 239.05   °K
                  Reservoir Temperature (T1) -> 239.05   °K
                       Molecular Weight (Mw) -> 70.9     kg/kmol
```



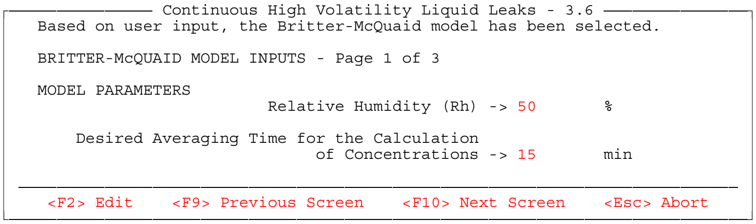
```
            Continuous High Volatility Liquid Leaks - 3.6

SOURCE PARAMETERS - Page 2 of 4

PRESSURE
          Liquid Pressure at Hole or Opening (P*) -> 107501.4 Pa

                            Ambient Pressure (Pa) -> 101325   Pa
                          Reservoir Pressure (P1) -> 101325   Pa
 Contaminant Density (ρ1) at Reservoir Conditions -> 1574     kg/cubic m
             Distance between the Hole or Opening
                     and Top of Liquid Level (Hl) -> 0.4      m

EMISSION
                               Emission Rate (Qm) -> 1453.136 g/s
```



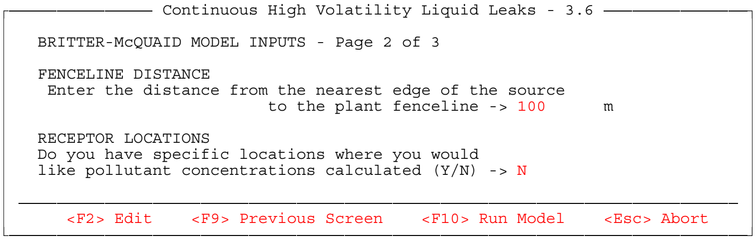
```
            Continuous High Volatility Liquid Leaks - 3.6

SOURCE PARAMETERS - Page 3 of 4

DISCHARGE DENSITY
                      Discharge Density (ρ2) -> 3.614632 kg/cubic m



DENSITY OF AIR
                       Density of Air (ρair) -> 1.20209  kg/cubic m

                    Ambient Temperature (Ta) -> 293      °K

Buoyancy is Negative
```



```
Continuous High Volatility Liquid Leaks - 3.6
SOURCE PARAMETERS - Page 4 of 4

VERTICALLY DIRECTED JET
       Does the release result in a vertically
                            directed jet (Y/N) -> N

TIME
                         Release Duration (Td) -> 2.293889 min

        Total Amount of Material Released (Q) -> 200      kg

<F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous High Volatility Liquid Leaks - 3.6
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS
                        Relative Humidity (Rh) -> 50       %

    Desired Averaging Time for the Calculation
                             of Concentrations -> 15       min

<F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Continuous High Volatility Liquid Leaks - 3.6

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE
 Enter the distance from the nearest edge of the source
                        to the plant fenceline -> 100      m

RECEPTOR LOCATIONS
Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

   <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

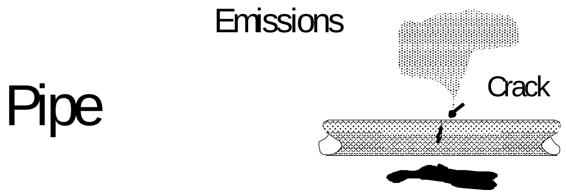
A summary of the Britter-McQuaid model's results is displayed below:

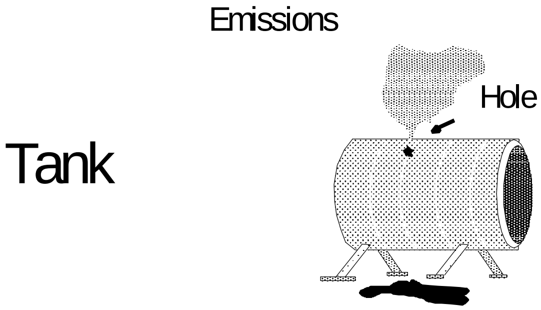
```
     ***************************************
     ***   SUMMARY OF B&M MODEL RESULTS  ***
     ***************************************

   MAX CONC      MAX CONC     DIST TO    WIND SPEED
   (UG/M**3)      (PPM)       MAX (M)      (M/S)
   ---------    ---------     -------    ----------
   .2865E+08    9716.          100.          3.

****************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
****************************************************
```

### 4.3.6.3 Considerations for Time-Varying and Time-Limited Releases

See Section 2.5 for a discussion of considerations for time-varying and time-limited releases.

## 4.3.7 Instantaneous High Volatility Leaks





Similar Releases: (High volatility) liquid leak from a tank or a liquid leak from a pipe (when the ratio of the hole diameter to the pipe diameter is less than 0.2).

Discussion:

This procedure applies to an instantaneous release of a high volatility liquid (at constant temperature and pressure) from a ment (reservoir) through a hole or opening. See Section 4.3.6 for further discussion.

Limitations and Assumptions:

Same as Section 4.3.6.

Input Information:

Same as Section 4.3.6.

### 4.3.7.1 Procedure:

1-3. Same as Section 4.3.6

4. **Buoyancy Check.** Perform buoyancy check as a first check.

A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\ M_a}{R\ T_a} \qquad (4.3.7\text{-}1)$$

where $M_a$ is the molecular weight of air (assumed to equal 28.9 k/kmol).

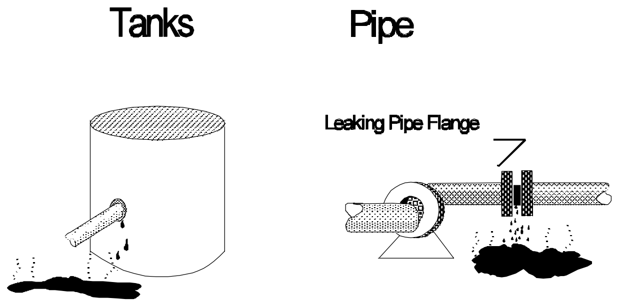
B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the RVD model should be used if the release is from a vertically directed jet; otherwise, the Britter-McQuaid model should be used; go to step 8. If the buoyancy is positive, the PUFF model for a point source should be used. (See Section 2.4 for more information on model selection.)

5. Same as Section 4.3.6.

#### 4.3.7.2 Examples

See the examples in Section 4.3.6.

### 4.3.8 Continuous Low Volatility Liquids from Tanks and Pipes



Similar Releases: Possible applications include a (low volatility) liquid leak from a tank or a pipe.

Discussion:

Low volatility liquid is considered to be a material whose normal boiling point is above the ambient temperature; a low volatility material stored at moderate to low pressure (and so that the boiling point is above the storage temperature) will typically be released as a liquid and form a pool or puddle on the ground. For low-volatility liquid releases, the (conservative) assumption is that the liquid evaporates at the same rate it is spilled (except when the puddle is confined by a bund or dike from which liquid does not overflow).

Limitations and Assumptions:

- The liquid level, pressure, and temperature in the reservoir are essentially constant. If these parameters are not constant, the release rate may vary with time, but the maximum release rate is generally obtained for the initial reservoir conditions.
- The hole or opening is located in the liquid space (as opposed to the vapor space).
- The gas evolution (evaporation) rate is assumed to be equal to the liquid release rate (except when the puddle is confined by a dike or bund from which liquid does not overflow). See Spicer, 1992.

Input Information:

$A_0$ area of hole or opening ($m^2$)
$A_p$ puddle area ($m^2$) (For unbounded puddles, $A_p$ is to be determined; for releases within dikes or bunds, $A_p$ is the dike or bund area from which liquid would

| | |
|---|---|
| | evaporate.) |
| $A_1$ | flow area representing reservoir conditions ($m^2$) (In the case of a leak from a tank, $A_1 \rightarrow \infty$ (and $\beta=0$); in the case of a leak from a pipe, $A_1$ is the cross-sectional area of the pipe.) |
| $D_0$ | (equivalent) diameter of hole or opening ($D_0=2 \cdot \sqrt{A_0/\pi}$) (m) |
| g | acceleration due to gravity (9.81 $m^2/s$) |
| $H_L$ | distance between the hole or opening and the top of the liquid level (where the pressure is $P_1$) (m) (In the case of a leak from a pipe, $H_L=0$.) |
| $M_w$ | contaminant molecular weight (kg/kmol) |
| $P_a$ | ambient pressure (Pa) |
| $P_v$ | vapor pressure as a function of temperature (Pa) |
| $P_1$ | reservoir pressure (Pa) |
| R | gas constant (8314 J/kg-mole·°K or 8314 Pa•$m^3$/kg-mole•°K) |
| Q | total amount of material released (kg) |
| $T_a$ | ambient temperature (°K) |
| $T_b$ | contaminant normal boiling point (°K) |
| $T_1$ | liquid storage temperature (°K) |
| $U_r$ | ambient windspeed (typically considered to be at 10 m elevation) (m/s) |
| $\beta$ | $\sqrt{A_0/A_1}$ (dimensionless) |
| $\lambda$ | heat of vaporization at the normal boiling point (J/kg) |
| $\rho_1$ | contaminant density at reservoir conditions ($T_1$ and $P_1$) ($kg/m^3$) |

4.3.8.1 Procedure:

1. **Pressure at the Hole or Opening.** Estimate the liquid pressure at the hole or opening $P_*$ as:

$$P_* = \max(P_a, P_1) + \rho_1 g H_L \qquad (4.3.8\text{-}1)$$

2. **Emission Rate.** Estimate the emission rate $Q_m$ (kg/s) as follows from Perry et al. (1984):

$$Q_m \text{ (kg/s)} = K A_0 \left[ 2 \rho_1 \left( P_* - P_a \right) \right]^{1/2} \qquad (4.3.8\text{-}2)$$

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

where $C \approx 0.65$ (although C can be larger if $\beta > 0.2$)

3. **Puddle Area.** For unconfined puddles, estimate the puddle area $A_p$ required for the emission rate $Q_m$ as follows from Clewell (1983):

$$Q_m \text{(kg/s)} = 6.94 \times 10^{-7} \left(1 + 0.0043 \left[T_2 - 273.15\right]^{\ast 2}\right) U_r^{0.75} A_p M_w P_v / P_{vh}$$

(4.3.8-3)

where $T_2 = \max(T_1, T_a)$ and $[T_2 - 273.15]^*$ is taken to be zero if $T_2 - 273.15 < 0$; $P_v$ (in Pa) is evaluated at $T_2$ using the Clausius-Clapeyron Equation:

$$P_v = 101325 \exp\left( \frac{\lambda\, M_w}{R} \left( \frac{1}{T_b} - \frac{1}{T_2} \right) \right) \tag{4.3.8-4}$$

where $P_{vh}$ is the vapor pressure (in Pa) of hydrazine evaluated at $T_2$ as follows:

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

For (potentially) confined puddles where $A_p$ is known <u>a priori</u>, Equation (4.3.8-3) must be solved for $Q_m$ using the known value to $A_p$. If $Q_m$ from Equation (4.3.8-3) is less than $Q_m$ from Equation (4.3.8-2), the estimate of $Q_m$ from Equation (4.3.8-3) and the <u>a priori</u> value of $A_p$ best represent the release conditions. However if $Q_m$ from Equation (4.3.8-3) is greater than $Q_m$ from Equation (4.3.8-2), the estimate of $Q_m$ from Equation (4.3.8-2) and $A_p$ estimated from Equation (4.3.8-3) best represent the release conditions. ($A_p$ is so estimated in this case because the puddle size from Equation (4.3.8-3) is smaller than the confining area for the release conditions.)

4. **Discharge Density.** Calculate the discharge density as follows:

$$\rho_2 = \frac{P_a\, M_w}{R\, T_2} \tag{4.3.8-5}$$

5. **Buoyancy Check.** Perform buoyancy check as a first check.

   A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\, M_a}{R\, T_a} \tag{4.3.8-6}$$

   where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

   B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the Britter-McQuaid model should be used; go to step 6. If the buoyancy is positive, the SCREEN model for an area source should be used. (See Section 2.4 for more information on model selection.)

6. **Release Duration.** The release duration is used as an input into the Britter-McQuaid model. Calculate the release duration $T_d$ using the equation below:

$$T_d \text{ (min)} = \frac{Q \text{ (kg)}}{Q_m \text{ (kg/s)} \cdot 60 \text{ (s/min)}} \qquad (4.3.8\text{-}7)$$

### 4.3.8.2 Example: Continuous Leak of Liquid Unsymmetrical Dimethlhydrazine (UDMH)

Discussion:

For this example, consider a liquid UDMH (101325 Pa and 283 °K) leak from a 3.2 cm diameter hole in a tank; the hole is 1.0 m below the liquid surface. The tank is located in a bund with a floor area of 2500 m$^2$. The distance to the fenceline is 100 m.

The following information will be required:

| | |
|---|---|
| $A_0$ | area of hole or opening ($\pi D_0^2/4 = 0.0008042$ m$^2$) |
| $A_p$ | (maximum) puddle area (2500 m$^2$) |
| $A_1$ | flow area representing reservoir conditions ($A_1 \rightarrow \infty$ m$^2$) |
| $D_0$ | (equivalent) diameter of hole or opening (0.032 m) |
| g | acceleration due to gravity (9.81 m$^2$/s) |
| $H_L$ | distance between the hole or opening and the top of the liquid level (where the pressure is $P_1$) (1.0 m) |
| $M_w$ | contaminant molecular weight (60.1 kg/kmol) |
| $P_a$ | ambient pressure (101325 Pa) |
| $P_v$ | vapor pressure as a function of temperature (Pa) |
| $P_1$ | reservoir pressure (101325 Pa) |
| R | gas constant (8314 J/kg-mole·°K or 8314 Pa•m$^3$/kg-mole•°K) |
| Q | total amount of material released (500 kg) |
| $T_a$ | ambient temperature (283 °K) |
| $T_b$ | contaminant normal boiling point (335.5 °K) |
| $T_1$ | liquid storage temperature (283 °K) |
| $U_r$ | ambient windspeed (typically considered to be at a 10 m elevation) (2.0 m/s) |
| $\beta$ | $\sqrt{A_0/A_1}$ (0.0) |
| $\lambda$ | heat of vaporization at the normal boiling point (5.44x10$^5$ J/kg) |
| $\rho_1$ | contaminant density at reservoir conditions ($T_1$ and $P_1$) (800 kg/m$^3$) |

With this information, the procedure discussed above determines the release rate and puddle area.

Procedure:

1. **Pressure at the Hole or Opening.** Estimate the liquid pressure $P_*$ at the hole or opening using Equation (4.3.8-1).

In this case, the UDMH is released as a liquid at the ambient pressure and temperature, so $P_a=P_1=101325$ Pa:

$$P_* = \max(101325,\ 101325) + 800 \cdot 9.81 \cdot 1.0 = 1.09 \times 10^5 \text{ Pa}$$

2. **Emission Rate.** Estimate the emission rate $Q_m$ using Equation (4.3.8-2) with C = 0.65 as follows:

$$Q_m(\text{kg/s}) = K \cdot 0.0008042 \cdot \left[\, 2 \cdot 800 \cdot \left( 1.09 \times 10^5 - 101325 \right) \right]^{1/2} = 1.83 \text{ kg/s}$$

where

$$K = 0.65 \,/\, \sqrt{1 - 0.0^4} = 0.65$$

3. **Puddle Area.** Since this puddle could be bounded, use the known $A_p$ = 2500 $m^2$ in Equation (4.3.8-3) to determine $Q_m$ as follows:

$$Q_m = 6.94 \times 10^{-7} \left(1 + 0.0043 \left[\, 283 - 273.15 \right]^2\right) 2.0^{0.75} \cdot 2500 \cdot 60.1 \cdot P_v / P_{vh}$$

$$Q_m = 3.9 \text{ kg/s}$$

where $T_2 = \min(283\ ^\circ K, 283\ ^\circ K) = 283\ ^\circ K$ and $P_v$ (in Pa) is evaluated at $T_2$ using the Clausius-Clapeyron Equation (4.3.8-4):

$$P_v = 101325 \exp\left( \frac{5.44 \times 10^5 \cdot 60.1}{8314} \left( \frac{1}{335.5} - \frac{1}{283} \right) \right) = 1.15 \times 10^4 \text{ Pa}$$

where $P_{vh}$ is the vapor pressure (in Pa) of hydrazine evaluated at $T_2$ as follows:

$$P_{vh} = \exp\left( 76.8580 - \frac{7245.2}{283} - 8.22 \cdot \ln(283) + 0.0061557 \cdot 283 \right) = 730 \text{ Pa}$$

So $Q_m$ (3.9 kg/s) from Equation (4.3.8-3) is greater than $Q_m$ (1.83 kg/s) from Equation (4.3.8-2), and the estimate of $Q_m$ (1.83 kg/s) from Equation (4.3.8-2) is accepted. Using 1.83 kg/s in Equation (4.3.8-3) $A_p$ is calculated as follows:

$$A_p = \frac{1.83 \cdot 730}{6.94 \times 10^{-7} \left(1 + 0.0043 \left[\, 283 - 273.15 \right]^2\right) 2.0^{0.75} \cdot 60.1 \cdot 1.15 \times 10^4}$$

$$A_p = 1170 \text{ m}^2$$

4. **Discharge Density.** Calculate the discharge density using Equation (4.3.8-5) as follows:

$$\rho_2 = \frac{101325 \cdot 60.1}{8314 \cdot 283} = 2.59 \text{ kg/m}^3$$

5. **Buoyancy Check.** Perform buoyancy check as a first check.

   A. Calculate the density of air using Equation (4.3.8-6):

$$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 283} = 1.24 \text{ kg/m}^3$$

   where 28.9 kg/kmol is the molecular weight of air.

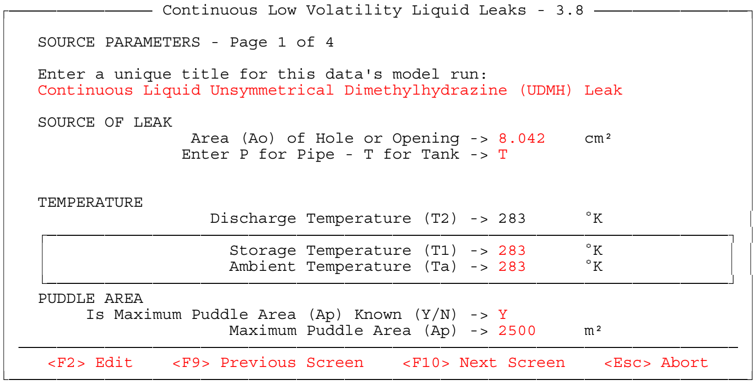
   B. Since $\rho_2/\rho_{air} > 1.02$, then the buoyancy is negative.

6. **Release Duration.** Calculate the release duration $T_d$ using the equation below:

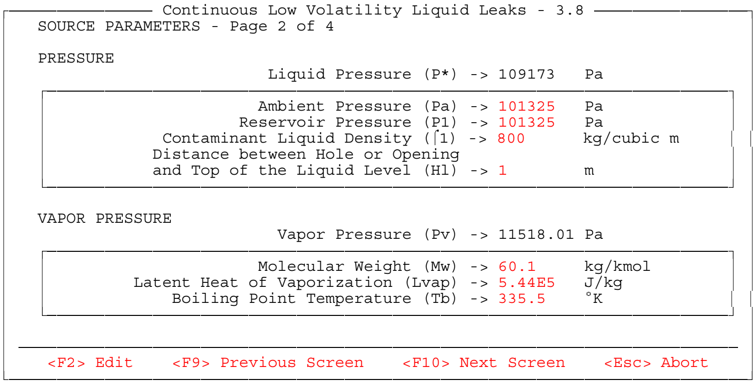
$$T_d \text{ (min)} = \frac{500 \text{ (kg)}}{1.83 \text{ (kg/s)} \cdot 60 \text{ (s/min)}} = 4.55 \text{ min}$$

   After this calculation run the Britter-McQuaid model. (See Section 5.4 for more information on the Britter-McQuaid model.)

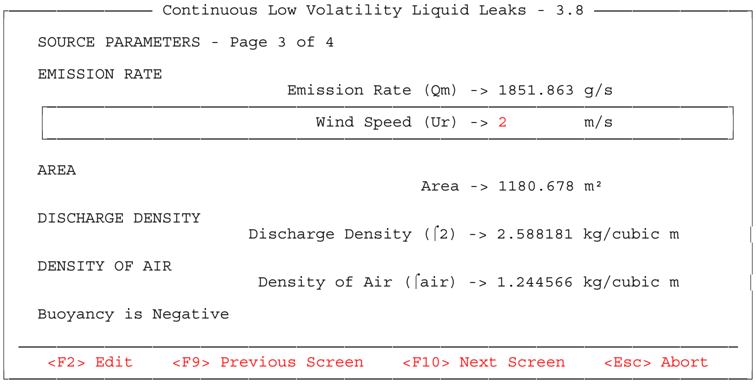
Data entry in the TSCREEN model for this example is shown below:



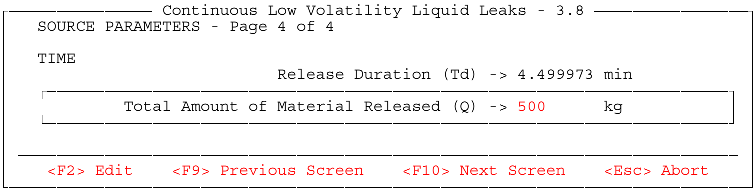
```
Continuous Low Volatility Liquid Leaks - 3.8

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Continuous Liquid Unsymmetrical Dimethylhydrazine (UDMH) Leak

SOURCE OF LEAK
                Area (Ao) of Hole or Opening -> 8.042     cm²
               Enter P for Pipe - T for Tank -> T


TEMPERATURE
                  Discharge Temperature (T2) -> 283       °K

                    Storage Temperature (T1) -> 283       °K
                    Ambient Temperature (Ta) -> 283       °K

PUDDLE AREA
     Is Maximum Puddle Area (Ap) Known (Y/N) -> Y
                    Maximum Puddle Area (Ap) -> 2500      m²

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



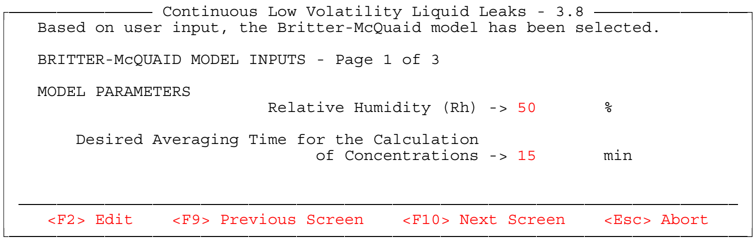
```
Continuous Low Volatility Liquid Leaks - 3.8
SOURCE PARAMETERS - Page 2 of 4

PRESSURE
                        Liquid Pressure (P*) -> 109173    Pa

                       Ambient Pressure (Pa) -> 101325    Pa
                     Reservoir Pressure (P1) -> 101325    Pa
              Contaminant Liquid Density (⌠1) -> 800       kg/cubic m
             Distance between Hole or Opening
             and Top of the Liquid Level (Hl) -> 1         m


VAPOR PRESSURE
                         Vapor Pressure (Pv) -> 11518.01 Pa

                       Molecular Weight (Mw) -> 60.1      kg/kmol
              Latent Heat of Vaporization (Lvap) -> 5.44E5    J/kg
                  Boiling Point Temperature (Tb) -> 335.5     °K


   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



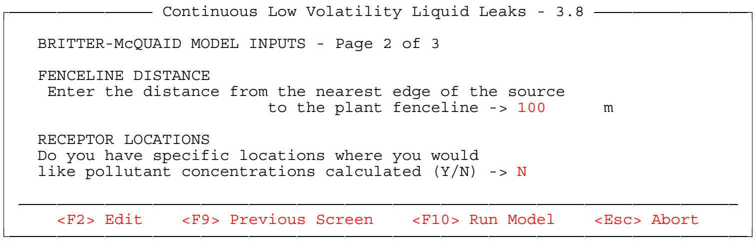
```
                Continuous Low Volatility Liquid Leaks - 3.8
   SOURCE PARAMETERS - Page 3 of 4

   EMISSION RATE
                              Emission Rate (Qm) -> 1851.863 g/s

                                 Wind Speed (Ur) -> 2        m/s

   AREA
                                            Area -> 1180.678 m²

   DISCHARGE DENSITY
                          Discharge Density (⌠2) -> 2.588181 kg/cubic m

   DENSITY OF AIR
                           Density of Air (⌠air) -> 1.244566 kg/cubic m

   Buoyancy is Negative

      <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
                Continuous Low Volatility Liquid Leaks - 3.8
   SOURCE PARAMETERS - Page 4 of 4

   TIME
                             Release Duration (Td) -> 4.499973 min

             Total Amount of Material Released (Q) -> 500      kg

      <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
                Continuous Low Volatility Liquid Leaks - 3.8
   Based on user input, the Britter-McQuaid model has been selected.

   BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

   MODEL PARAMETERS
                            Relative Humidity (Rh) -> 50       %

       Desired Averaging Time for the Calculation
                                 of Concentrations -> 15       min

      <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
                Continuous Low Volatility Liquid Leaks - 3.8

   BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

   FENCELINE DISTANCE
    Enter the distance from the nearest edge of the source
                            to the plant fenceline -> 100      m

   RECEPTOR LOCATIONS
   Do you have specific locations where you would
   like pollutant concentrations calculated (Y/N) -> N

       <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

A summary of the Britter-McQuaid model's output is displayed below:

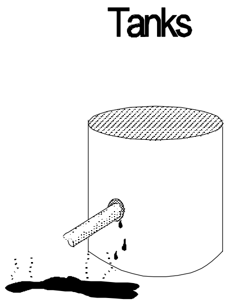
```
       ***************************************
       ***   SUMMARY OF B&M MODEL RESULTS  ***
       ***************************************

     MAX CONC      MAX CONC     DIST TO     WIND SPEED
     (UG/M**3)      (PPM)       MAX (M)       (M/S)
     ---------    ---------     -------     ----------
     .3518E+08    .1359E+05      100.           3.

  ***************************************************
  ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
  ***************************************************
```

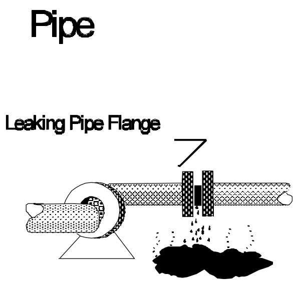
### 4.3.8.3 Considerations for Time-Varying and Time Limited Releases

A release is considered time varying if the release rate varies with time. Typically, this behavior might be expected because the reservoir pressure and temperature or the liquid level vary with time. If, for example, the release rate was very large in comparison with the reservoir volume. For these conditions, the release rate decreases with time so that the maximum release rate would be determined from initial reservoir conditions. Therefore, a screening method which uses the initial reservoir conditions would be expected to overestimate the release rate; this overestimation could be quite large depending on the situation.

A release is considered (only) time limited if the liquid release rate is constant over the duration of the release, but the release duration is short in comparison with other important time scales (e.g., the averaging time used to assess the toxicity, the cloud travel time to a downwind position of interest, or the time required to evaporate the released liquid puddle). For liquid releases of short duration (including instantaneous liquid releases), the procedure outlined above can be used to estimate the vapor evolution rate $Q_m$ if the puddle area for screening purposes, the puddle area can be estimated if a liquid depth of, say 1 cm is assumed. (While an equilibrium depth of 1 cm may be justified strictly on the grounds it is a reasonable estimate for screening purposes, more extensive modeling efforts have used a 1 cm equilibrium depth to fit experimental data e.g., Moorehouse and Carpenter (1986) and Webber and Jones (1987).) With this assumption, an unconfined puddle size can be determined. Finally, the (vapor) release duration $T_d$ can be calculated as $T_d = Q/Q_m$ where Q is the total mass of liquid released. (Note that $T_d$ may be sufficiently large enough to consider the vapor release as being continuous even for an instantaneous liquid release.)

## 4.3.9 Instantaneous Low Volatility Liquids from Tanks and Pipes





Similar Releases: Possible applications include a (low-volatility) liquid leak from a tank or a pipe.

Discussion:

Low-volatility liquid is considered to be a material whose normal boiling point is above the ambient temperature; a low-volatility material stored at moderate to low pressure (and so that the boiling point is above the storage temperature) will typically be released as a liquid and form a pool or puddle on the ground. For low-volatility liquid releases, the (conservative) assumption is that the liquid evaporates at the same rate it is spilled (except when the puddle is confined by a bund or dike from which liquid does not overflow). Possible applications include a (low-volatility) liquid leak from a tank or a pipe.

In contrast to scenario 4.3.8, pressure at the hole or opening is not applicable to an instantaneous liquid release. Although determination of the liquid release rate is not applicable to an instantaneous liquid release, determination of whether the liquid puddle will be confined or not is necessary to know how to proceed.

Limitations and Assumptions:

- The liquid level, pressure, and temperature in the reservoir are essentially constant. If these parameters are not constant, the release rate may vary with time, but the maximum release rate is generally obtained for the initial reservoir conditions.
- The hole or opening is located in the liquid space (as opposed to the vapor space).

- The gas evolution (evaporation) rate is assumed to be equal to the liquid release rate (except when the puddle is confined by a dike or bund from which liquid does not overflow). See Spicer, 1992.

Input Information:

| | |
|---|---|
| $A_p$ | puddle area ($m^2$) (For unbounded puddles, $A_p$ is to be determined; for releases within dikes or bunds, $A_p$ is the dike or bund area from which liquid would evaporate.) |
| $M_w$ | contaminant molecular weight (kg/kmol) |
| R | gas constant (8314 J/kg-mole·°K or 8314 Pa•$m^3$/kg-mole•°K) |
| Q | total amount of material released (kg) |
| $T_a$ | ambient temperature (°K) |
| $T_b$ | contaminant normal boiling point (°K) |
| $T_1$ | liquid storage temperature (°K) |
| $U_r$ | ambient windspeed (typically considered to be at 10 m elevation) (m/s) |
| V | volume of liquid spilled ($m^3$) |
| $\lambda$ | heat of vaporization at the normal boiling point (J/kg) |
| $\rho_1$ | contaminant density at reservoir conditions ($T_1$ and $P_1$) (kg/$m^3$) |

4.3.9.1 Procedure:

1. **Puddle Area.** Calculate the area of liquid spilled based on volume of liquid spilled assuming a 1 cm puddle depth.

$$A_p\ (m^2) = \frac{V\ (m^3)}{0.01\ (m)} \qquad (4.3.9\text{-}1)$$

If the area from Equation (4.3.9-1) is smaller than the bund area (which is the maximum possible puddle area), then the area from Equation (4.3.9-1) is used as the puddle area ($A_p$). Otherwise, if the bund size is smaller than the area calculated in Equation (4.3.9-1), then the bund area is used as the puddle size ($A_p$).

2. **Emission Rate.** The puddle area is used to calculate the emission rate $Q_m$ (kg/s) as follows:

$$Q_m = 6.94\times10^{-7}\left(1 + 0.0043\left[T_2 - 273.15\right]^{*2}\right) U_r^{0.75} A_p M_w P_v / P_{vh} \qquad (4.3.9\text{-}2)$$

where $T_2 = \max(T_1, T_a)$ and $[T_2 - 273.15]^*$ is taken to be zero if $T_2 - 273.15 < 0$; $P_v$ (in atm) is evaluated at $T_2$ using the Clausius-Clapeyron Equation:

$$P_v = 101325 \exp\left(\frac{\lambda\ M_w}{R}\left(\frac{1}{T_b} - \frac{1}{T_2}\right)\right) \qquad (4.3.9\text{-}3)$$

where $P_{vh}$ is the vapor pressure (in Pa) of hydrazine evaluated at $T_2$ as follows:

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

3. **Discharge Density.** Calculate the discharge density as follows:

$$\rho_2 = \frac{P_a\ M_w}{R\ T_2} \qquad (4.3.9\text{-}4)$$

4. **Buoyancy Check.** Perform buoyancy check as a first check.

   A. Calculate the density of air using the following:

$$\rho_{air} = \frac{P_a\ M_a}{R\ T_a} \qquad (4.3.9\text{-}5)$$

   where $M_a$ is the molecular weight of air (assumed to equal 28.9 kg/kmol).

   B. If $\rho_2/\rho_{air} > 1$, then the buoyancy is negative. For negative buoyancy, the Britter-McQuaid model should be used. If the buoyancy is positive, the PUFF should be used. (See Section 2.4 for more information on model selection.)

5. **Release Duration.** The release duration is used as an input into the PUFF and Britter-McQuaid models. Calculate the release duration $T_d$ using the equation below:

$$T_d\ (\text{min}) = \frac{Q\ (\text{kg})}{Q_m\ (\text{kg/s}) \cdot 60\ (\text{s/min})} \qquad (4.3.9\text{-}6)$$

### 4.3.9.2 Example: Instantaneous Liquid UDMH Leak

Discussion:

For this example, consider an instantaneous spill of 20 $m^3$ liquid UDMH from storage at 1 atm and 283 °K. The spill occurs in a bund with a floor area of 2500 $m^2$. The fenceline is 100 m away.

The following information will be required:

| | |
|---|---|
| $A_p$ | maximum puddle area (2500 $m^2$) |
| $M_w$ | contaminant molecular weight (60.1 g/g-mole) |
| R | gas constant |
| Q | total amount of material released (16,000 kg) |

| | |
|---|---|
| $T_a$ | ambient temperature (283 °K) |
| $T_b$ | contaminant normal boiling point (335.5 °K) |
| $T_1$ | liquid storage temperature (283 °K) |
| $U_r$ | ambient windspeed (typically considered to be at 10 m elevation) (2.0 m/s) |
| V | volume of liquid spilled (20 $m^3$) |
| $\lambda$ | heat of vaporization at the normal boiling point ($5.44 \times 10^5$ J/kg) |
| $\rho_1$ | contaminant density at reservoir conditions ($T_1$ and $P_1$) (800 $kg/m^3$) |

Procedure:

1. **Puddle Area.** Calculate the area of liquid spilled based on the volume of liquid spilled assuming a 1 cm puddle depth from Equation (4.3.9-1) as follows:

$$A_p\ (m^2) = \frac{20\ m^3}{0.01\ m} = 2000\ m^2$$

The area from Equation (4.3.9-1) is smaller than the bund area (which is the maximum possible puddle area); therefore, the area from Equation (4.3.9-1) is used as the puddle area ($A_p$).

2. **Emission Rate.** The puddle area is used to calculate the emission rate ($Q_m$) from Equation (4.3.9-2) as follows:

$$Q_m = 6.94 \times 10^{-7} \left(1 + 0.0043 \left[283 - 273.15\right]^2\right) 2.0^{0.75} \cdot 2000 \cdot 60.1 \cdot P_v / P_{vh}$$

$$Q_m = 3.13\ kg/s$$

where $T_2$ = min(283 °K,283 °K) = 283 °K and $P_v$ (in atm) is evaluated at $T_2$ using the Clausius-Clapeyron Equation (4.3.9-3):

$$P_v = 101325 \exp\left( \frac{5.44 \times 10^5}{8315} \left( \frac{1}{335.5} - \frac{1}{283} \right) \right) = 1.15 \times 10^4\ Pa$$

where $P_{vh}$ is the vapor pressure (in Pa) of hydrazine evaluated at $T_2$ as follows:

$$P_{vh} = \exp\left( 76.8580 - \frac{7245.2}{283} - 8.22 \ln(283) + 0.0061557 \cdot 283 \right) = 730\ Pa$$

3. **Discharge Density.** Calculate the discharge density using Equation (4.3.9-4) as follows:

$$\rho_2 = \frac{101325 \cdot 60.1}{8314 \cdot 283} = 2.59\ \mathrm{kg/m^3}$$

4. **Buoyancy Check.** Perform buoyancy check as a first check.

   A. Calculate the density of air using Equation (4.3.9-:

   $$\rho_{air} = \frac{101325 \cdot 28.9}{8314 \cdot 283} = 1.24\ \mathrm{kg/m^3}$$

   where 28.9 kg/kmol is the molecular weight of air.

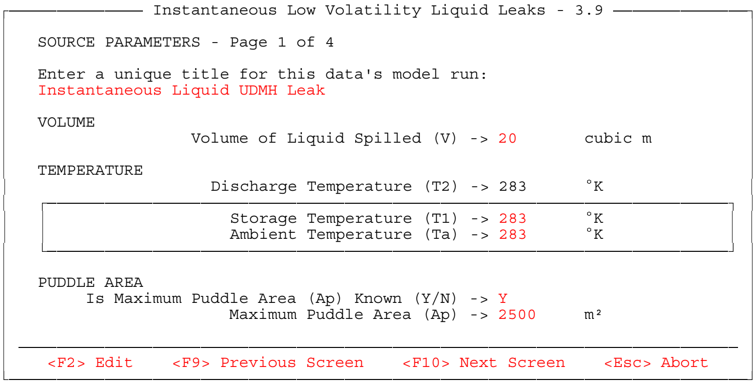
   B. Since $\rho_2/\rho_{air} > 1$, the buoyancy is negative.

5. **Release Duration.** Calculate the release duration $T_d$ using the equation below:

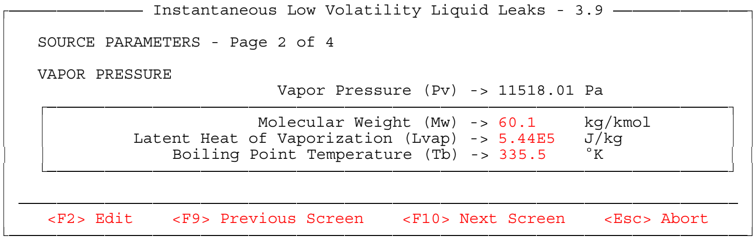
   $$T_d\ (\mathrm{min}) = \frac{16{,}000\ (\mathrm{kg})}{3.13\ (\mathrm{kg/s}) \cdot 60\ (\mathrm{s/min})} = 85\ \mathrm{min}$$

   After this calculation run the Britter-McQuaid. (See Section 5.4 for more information on the Britter-McQuaid model.)

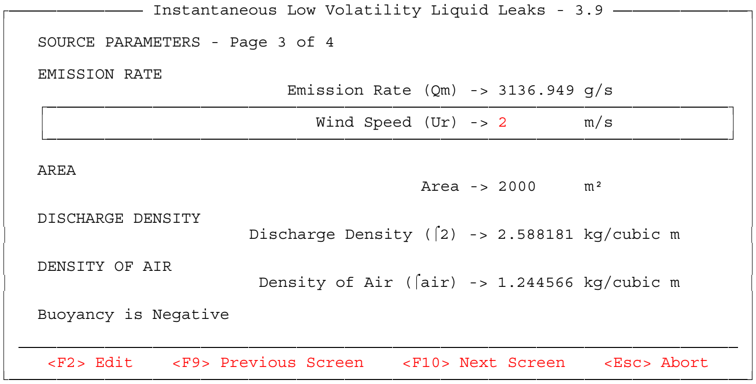
Data entry in the TSCREEN model for this example is shown below:



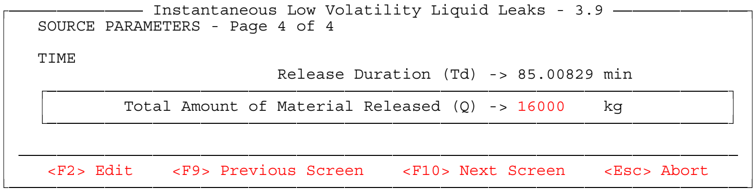
```
Instantaneous Low Volatility Liquid Leaks - 3.9

SOURCE PARAMETERS - Page 1 of 4

Enter a unique title for this data's model run:
Instantaneous Liquid UDMH Leak

VOLUME
                Volume of Liquid Spilled (V) -> 20       cubic m

TEMPERATURE
                  Discharge Temperature (T2) -> 283      °K

                    Storage Temperature (T1) -> 283      °K
                    Ambient Temperature (Ta) -> 283      °K


PUDDLE AREA
     Is Maximum Puddle Area (Ap) Known (Y/N) -> Y
                    Maximum Puddle Area (Ap) -> 2500     m²
```



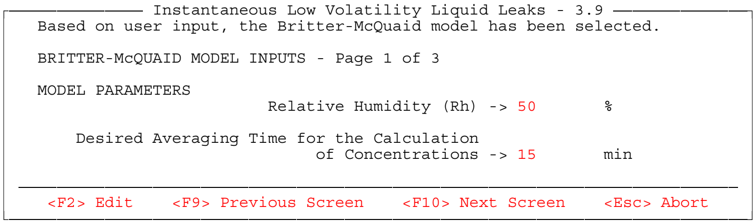
```
Instantaneous Low Volatility Liquid Leaks - 3.9

SOURCE PARAMETERS - Page 2 of 4

VAPOR PRESSURE
                         Vapor Pressure (Pv) -> 11518.01 Pa

                       Molecular Weight (Mw) -> 60.1     kg/kmol
          Latent Heat of Vaporization (Lvap) -> 5.44E5   J/kg
              Boiling Point Temperature (Tb) -> 335.5    °K
```



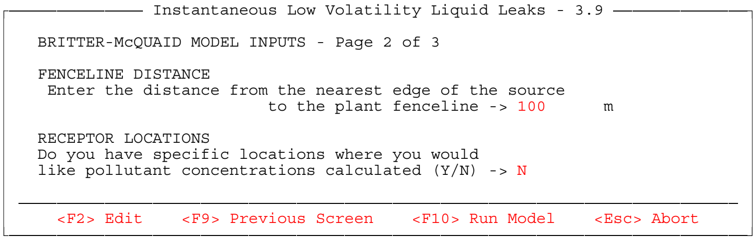
```
 Instantaneous Low Volatility Liquid Leaks - 3.9

SOURCE PARAMETERS - Page 3 of 4

EMISSION RATE
                          Emission Rate (Qm) -> 3136.949 g/s
                             Wind Speed (Ur) -> 2        m/s

AREA
                                        Area -> 2000     m²

DISCHARGE DENSITY
                      Discharge Density (⌠2) -> 2.588181 kg/cubic m

DENSITY OF AIR
                       Density of Air (⌠air) -> 1.244566 kg/cubic m

Buoyancy is Negative

  <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Instantaneous Low Volatility Liquid Leaks - 3.9
SOURCE PARAMETERS - Page 4 of 4

TIME
                         Release Duration (Td) -> 85.00829 min
          Total Amount of Material Released (Q) -> 16000    kg

  <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Instantaneous Low Volatility Liquid Leaks - 3.9
Based on user input, the Britter-McQuaid model has been selected.

BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

MODEL PARAMETERS
                        Relative Humidity (Rh) -> 50       %

    Desired Averaging Time for the Calculation
                             of Concentrations -> 15       min

  <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
 Instantaneous Low Volatility Liquid Leaks - 3.9

BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

FENCELINE DISTANCE
 Enter the distance from the nearest edge of the source
                        to the plant fenceline -> 100      m

RECEPTOR LOCATIONS
Do you have specific locations where you would
like pollutant concentrations calculated (Y/N) -> N

   <F2> Edit    <F9> Previous Screen    <F10> Run Model    <Esc> Abort
```

A summary of the Britter-McQuaid model's output is displayed below:

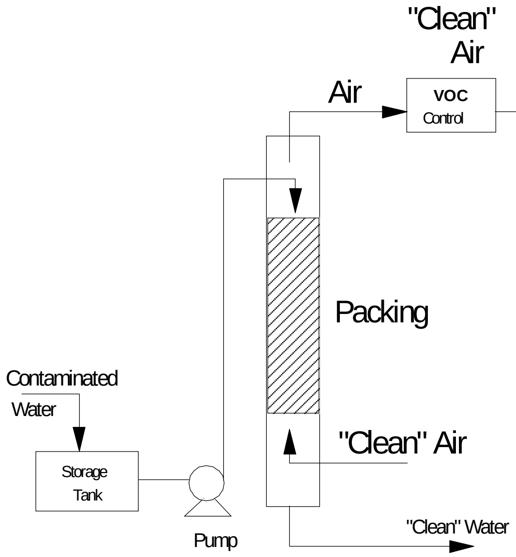
```
      ***************************************
      ***   SUMMARY OF B&M MODEL RESULTS  ***
      ***************************************

    MAX CONC      MAX CONC      DIST TO     WIND SPEED
    (UG/M**3)       (PPM)       MAX (M)       (M/S)
    ---------     ---------     -------     ----------
    .4904E+08     .1895E+05       100.          4.

 ***************************************************
 ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
 ***************************************************
```

#### 4.3.9.3 Considerations for Time-Varying and Time Limited Releases

See Section 4.3.8.3 for a discussion of considerations of time-varying and time-limited releases.

## 4.4 Superfund Releases

### 4.4.1 Air Strippers



Discussion:

Air stripping is a widely used technique for removing volatile organic compounds (VOC) from contaminated water. Procedures are given to evaluate the effect of the concentration of contaminants in water and the effect of the stripping rate on the emission rates and on the ambient air concentrations at distances from the air stripper.

Limitations and Assumptions:

None.

References:

For further information see: Air/Superfund National Technical Guidance Study Series - Air Stripper Design Manual, EPA-450/1-90-003, U.S. Environmental Protection Agency, Research Triangle Park, NC, May 1990, NTIS PB91-125997, pp 51-52.

Input Information:

In addition to the SCREEN model input (see Secion 5.1.1), the following is needed:

$C$ concentration of contaminant (mg/L)
$Q$ incoming water flow rate (L/min)

#### 4.4.1.1 Procedure

1. **Emission Rate.** Calculate emission rate ($Q_m$) (g/s) using the concentration of the contaminant (C) and the incoming water flow rate (Q). VOC concentrations in ground water typically range from 0.1 to 1 ppmw. Typical values for an air stripper are shown in Table 4.4.1-1.

$$Q_m(g/s) = C(mg/L)\ Q(L/minute)\ 1.67\times10^{-5} \qquad (4.4.1\text{-}1)$$

**TABLE 4.4.1-1**
**TYPICAL VALUES FOR AN AIR STRIPPER**

| Parameter | Units | Typical Value<br>Small | Medium | Large |
|---|---|---|---|---|
| Incoming Water Flow | L/min | 570 | 2840 | 5700 |
| Stack Height | m | 7.6 | 9 | 14 |
| Stack Diameter | m | 0.31 | 0.61 | 0.91 |
| Structure Dimensions | m | 7.6x1.2x1.2 | 9x3.6x3.6 | 13x3.6x3.6 |
| Exit Gas Velocity | m/sec | 6.4 | 8.0 | 7.3 |
| Exit Gas Temperature | °K | 293 | 293 | 293 |
| Ambient Temperature | °K | 293 | 293 | 293 |

2. TSCREEN will run the SCREEN model for a point source.

### 4.4.1.2 Example: Air stripper example

Discussion:

This example uses the default values provided by TSCREEN for a large air stripper. The fenceline is 100 m from the air stripper.

The following input information will be required:

C concentration of contaminant 0.5 (mg/L)
Q incoming water flow (L/min) 4700 (default)

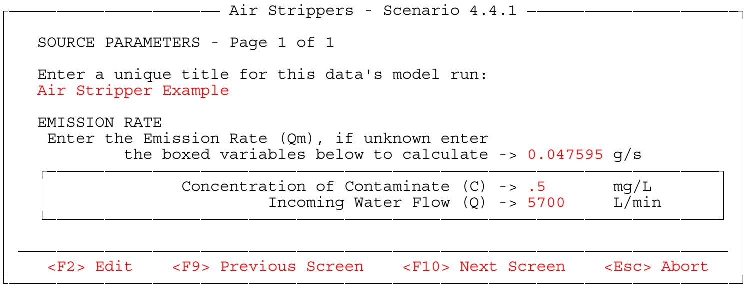
Procedure:

1. **Emission Rate.** Calculate emission rate ($Q_m$) (g/s) using Equation (4.4.1-1):

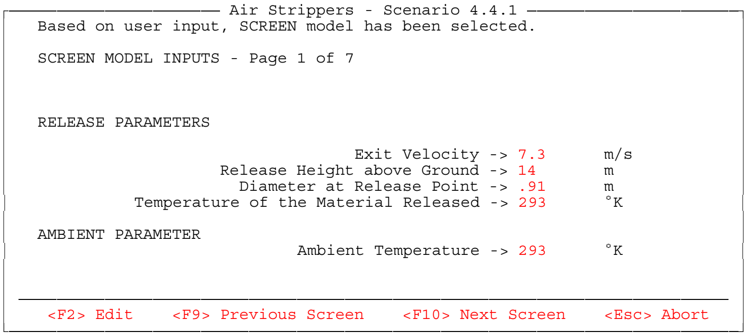
$$Q_m(g/s) = .5(mg/L)\ 5700(L/minute)\ 1.67\times10^{-5} = 0.048(g/s)$$

2. TSCREEN will run the SCREEN model for a point source. For an explanation of inputs for the SCREEN model see Section 5.1.1.

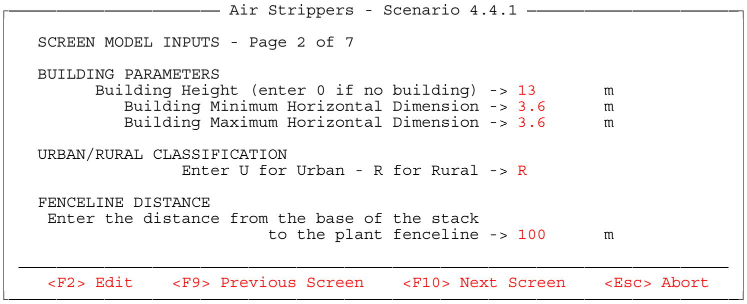
Data entry in the TSCREEN model for this example is shown below:



```
Air Strippers - Scenario 4.4.1

SOURCE PARAMETERS - Page 1 of 1

Enter a unique title for this data's model run:
Air Stripper Example

EMISSION RATE
 Enter the Emission Rate (Qm), if unknown enter
         the boxed variables below to calculate -> 0.047595 g/s

               Concentration of Contaminate (C) -> .5       mg/L
                        Incoming Water Flow (Q) -> 5700     L/min

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Air Strippers - Scenario 4.4.1
Based on user input, SCREEN model has been selected.

SCREEN MODEL INPUTS - Page 1 of 7


RELEASE PARAMETERS

                                 Exit Velocity -> 7.3      m/s
                   Release Height above Ground -> 14       m
                     Diameter at Release Point -> .91      m
          Temperature of the Material Released -> 293      °K

AMBIENT PARAMETER
                           Ambient Temperature -> 293      °K

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```



```
Air Strippers - Scenario 4.4.1

SCREEN MODEL INPUTS - Page 2 of 7

BUILDING PARAMETERS
      Building Height (enter 0 if no building) -> 13       m
         Building Minimum Horizontal Dimension -> 3.6      m
         Building Maximum Horizontal Dimension -> 3.6      m

URBAN/RURAL CLASSIFICATION
               Enter U for Urban - R for Rural -> R

FENCELINE DISTANCE
 Enter the distance from the base of the stack
                        to the plant fenceline -> 100      m

   <F2> Edit    <F9> Previous Screen    <F10> Next Screen    <Esc> Abort
```

A summary of the SCREEN model's output for this example is one other input screen shown below.

```
      ***************************************
      *** SUMMARY OF SCREEN MODEL RESULTS ***
      ***************************************

 CALCULATION         MAX CONC     DIST TO   TERRAIN
  PROCEDURE          (UG/M**3)    MAX (M)    HT (M)
 --------------     -----------   -------   -------
SIMPLE TERRAIN        7.276         104.        0.

BUILDING CAVITY-1   678.0            12.       --   (DIST = CAVITY LENGTH)
BUILDING CAVITY-2   678.0            12.       --   (DIST = CAVITY LENGTH)


***************************************************
** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **

 ***************************************************
```

### 4.4.2 Soil Vapor Extraction (SVE)

This scenario is listed in the TSCREEN model, but is not discussed here at this time.

## 5.0 ATMOSPHERIC DISPERSION ESTIMATES

Maximum short-term ground level concentrations in TSCREEN are based on current EPA screening models (SCREEN, RVD, and PUFF) which are embedded in the TSCREEN model. In addition, TSCREEN implements the Britter-McQuaid method for estimating maximum concentration from denser-than-air continuous (plume) and instantaneous (puff) releases. This section lists the TSCREEN model inputs needed. Sources of additional information about the models are referenced, where appropriate.

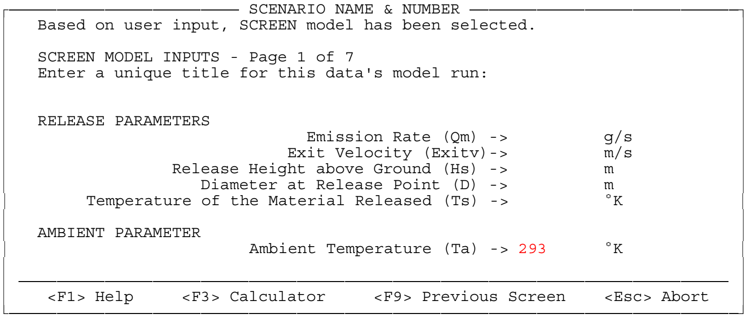
## 5.1 SCREEN

The SCREEN model implements most of the single source, short term procedures contained in the revised EPA screening procedure document (EPA, 1988c). This includes providing estimated maximum ground-level concentrations and distances to the maximum based on a pre-selected range of meteorological conditions. SCREEN is a Gaussian dispersion model applicable to continuous releases of particulate matter and non-reactive, non-dense gases that are emitted from point, area, and flared sources. In addition, SCREEN has the option of incorporating the effects of building downwash, as described in the Industrial Source Complex (ISC2) model user's guide (EPA, 1992). Refer to the document referenced above for more information about the implementation of the SCREEN model.

### 5.1.1 Point Sources

#### 5.1.1.1 Model Inputs

This section contains a complete listing of the inputs TSCREEN will request for the SCREEN point source. Some of these inputs may have already been entered from the scenario input section.



```
                    SCENARIO NAME & NUMBER
 Based on user input, SCREEN model has been selected.

 SCREEN MODEL INPUTS - Page 1 of 7
 Enter a unique title for this data's model run:


 RELEASE PARAMETERS
                            Emission Rate (Qm) ->          g/s
                          Exit Velocity (Exitv)->          m/s
                  Release Height above Ground (Hs) ->      m
                     Diameter at Release Point (D) ->      m
      Temperature of the Material Released (Ts) ->         °K

 AMBIENT PARAMETER
                        Ambient Temperature (Ta) -> 293    °K

  <F1> Help     <F3> Calculator     <F9> Previous Screen     <Esc> Abort
```

RELEASE PARAMETERS

1 Emission Rate ($Q_m$) (g/s) -
Enter the source specific emission rate. EPA recommends that emission rates from sources be determined through source testing using EPA References Methods (40 CFR Part 60 Appendix A) or process calculations. If source specific emissions are not available, representative emission factors can be substituted. Emission factors are available for individual toxic compounds. For some sources of applicable emissions factors for individual toxic compounds see Appendix A items 1-4 of this workbook.

2 Exit Velocity ($Exit_v$) (m/s) -
This value can be calculated from the following equation:

$$Exit_v = 4\ V/(\pi D^2)$$

where:

D = inside diameter of stack (m)
V = volumetric flow rate ($m^3/s$)

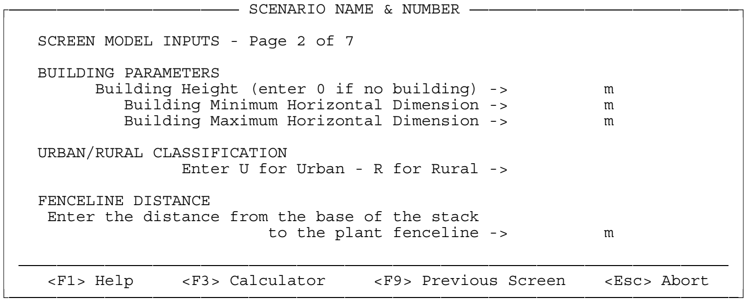
3 <u>Release Height above Ground ($H_s$) (m) -</u>
Enter the height of the stack or of the release point above the ground.

4 <u>Diameter at Release Point (D) (m) -</u>
Enter the inside diameter of the stack or release point in meters.

5 <u>Temperature of the Material Released ($T_s$) (K) -</u>
Enter the temperature of the material released in degrees Kelvin.

AMBIENT PARAMETER

6 <u>Ambient Temperature ($T_a$) (K) -</u>
The default if 293 °K.



```
SCENARIO NAME & NUMBER

  SCREEN MODEL INPUTS - Page 2 of 7

  BUILDING PARAMETERS
        Building Height (enter 0 if no building) ->          m
           Building Minimum Horizontal Dimension ->          m
           Building Maximum Horizontal Dimension ->          m

  URBAN/RURAL CLASSIFICATION
                  Enter U for Urban - R for Rural ->

  FENCELINE DISTANCE
   Enter the distance from the base of the stack
                          to the plant fenceline ->          m

   <F1> Help     <F3> Calculator     <F9> Previous Screen     <Esc> Abort
```

BUILDING PARAMETERS

7 <u>Building Height (m) -</u>
Enter the buildings maximum height above ground in meters. Building parameters are needed for calculating downwash for a stack due to a "nearby" building. "Nearby" includes structures within a distance of five times the lesser of the height or width of the structure, but not greater than 0.8 km (0.5 mile). If more than one building is involved, each building/stack configuration must be modeled separately. For information about complex structures, refer to the Guideline for <u>Determination of Good Engineering Practice Stack Height (Technical Support Document for Stack Height Regulations), Revised</u>, EPA 450/4-80-023R. For these complex configurations, a refined model such as the Industrial Source Complex (ISC) model is recommended. Wake effects are included. Cavity calculations are made for two building dimensions alongwind. The cavity calculations are summarized in the SCREEN model output at the distance-dependent calculations. Building downwash effects are not considered in the SCREEN model in either the VALLEY or simple terrain component of the complex terrain screening procedures (see description Terrain Type below), even if the building downwash option is selected by entering a building height.

- If the building height is 0 the next two parameters are not requested and the user will proceed to step 10.

8 <u>Building Minimum Horizontal Dimension (m) -</u>
Enter the alongwind minimum horizontal dimension of the "nearby" structure in meters. A simple rectangular building is assumed. (See the description of Building Height above.)

9 <u>Building Maximum Horizontal Dimension (m) -</u>
Enter the alongwind maximum horizontal dimension of the "nearby" structure in meters. A simple rectangular building is assumed. (See the description of Building Height.)

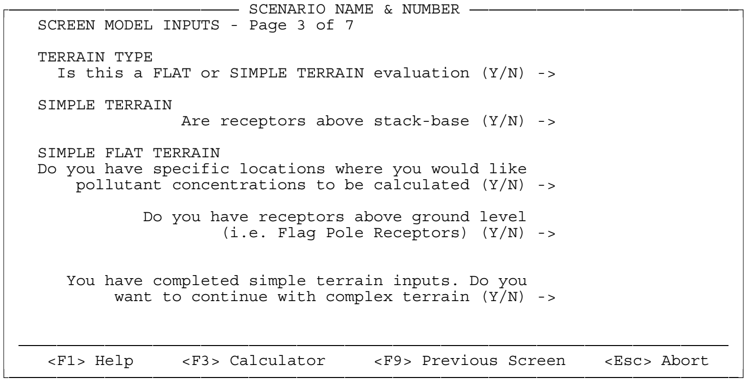
URBAN/RURAL CLASSIFICATION

10 <u>Enter U for Urban - R for Rural -</u>
The classification of a site as urban or rural is based on the procedures described in Section 8.2.8 of the <u>Guideline on Air Quality Models (Revised)</u>, EPA-450/2-78-027R.

FENCELINE DISTANCE

11 <u>Enter the distance from the base of the stack to the plant fenceline (m) -</u>
Enter the distance from the base of the stack to the plant fenceline in meters. SCREEN calculates the maximum concentrations across a range of meteorological conditions for the minimum distance given (> 1 m) and then for each

distance in a built-in array of distances. Thus, the user can input the minimum fenceline distance as the minimum distance for calculation and obtain a concentration at the site boundary and beyond. Distances less than the fenceline are ignored. Receptors beyond the fenceline are defined as ambient air.



```
────────────────────── SCENARIO NAME & NUMBER ──────────────────────────
 SCREEN MODEL INPUTS - Page 3 of 7

 TERRAIN TYPE
   Is this a FLAT or SIMPLE TERRAIN evaluation (Y/N) ->

 SIMPLE TERRAIN
                Are receptors above stack-base (Y/N) ->

 SIMPLE FLAT TERRAIN
 Do you have specific locations where you would like
     pollutant concentrations to be calculated (Y/N) ->

            Do you have receptors above ground level
                    (i.e. Flag Pole Receptors) (Y/N) ->


    You have completed simple terrain inputs. Do you
         want to continue with complex terrain (Y/N) ->

────────────────────────────────────────────────────────────────────────
  <F1> Help     <F3> Calculator     <F9> Previous Screen    <Esc> Abort
```

TERRAIN TYPE

12 <u>Is this a FLAT or SIMPLE TERRAIN elevation (Y/N) -</u>
Terrain type is determined according to whether it is above or below stack-top. Simple terrain is an area where terrain features are all lower in elevation than the top of the stack of the source. Complex terrain is defined as terrain exceeding the height of the stack being modeled. In TSCREEN, the user is given the option of modeling simple elevated terrain heights where terrain heights exceed stack base but are below stack height, or simple flat terrain, where terrain heights are assumed not to exceed stack base elevation. Answer "N" if there are no flat or simple terrain receptors; a "N" answer will bring up the COMPLEX TERRAIN screen. Answer "Y" if one or more receptors are located in terrain which is below stack-top. Answer "Y" if your evaluation involves both simple and complex terrain receptors. You will have another opportunity following completion of the simple terrain inputs to evaluate the complex terrain receptor. In summary:

"Y" selects FLAT or SIMPLE TERRAIN
"N" selects COMPLEX TERRAIN

- If "Y" was entered above, TSCREEN proceeds to step 13.

- If "N" was entered above, TSCREEN proceeds to step 15.

SIMPLE TERRAIN

13 <u>Are receptors above stack-base (Y/N) -</u>
Simple terrain is an area where terrain features are all

lower in elevation than the top of the stack of the source. Answer "Y" if one or more receptors are located in simple terrain. "N" if all receptors are in FLAT terrain. In summary:

"Y" selects SIMPLE TERRAIN
"N" selects FLAT TERRAIN

- If "Y" was entered, TSCREEN proceeds to step 15.

- If "N" was entered, TSCREEN proceeds to step 14.

SIMPLE FLAT TERRAIN

14 Do you have specific locations where you would like pollutant concentrations to be calculated (Y/N) -
The entry of "Y" will allow the user to input any number of specific distances (>1 m) and the maximum concentration for each distance will be calculated. Note that SCREEN has an automated distance array which calculates maximum concentrations at a pre-selected array of 50 distances ranging from 100 m to 50 km. Increments of 100 m are used out to 3 km, increments of 500 m are used from 3 km to 10 km, increments of 5 km from 10 km to 30 km, and increments of 10 km are used out to 50 km. For example, a specific location of interest may be a school 117 m from the source.

15 Do you have receptors above ground level (i.e. Flag Pole Receptors) (Y/N) -
A flag pole receptor is any receptor which is located above local ground level, e.g., on the roof of a building. Flag pole receptors are useful for estimating concentrations on rooftops or similar exposed locations and are most often used in urban modeling evaluations. Note, flag pole receptors should NOT be used to evaluate impacts on hilltops or on other exposed terrain features; the latter should be evaluated using the TSCREEN options for simple or complex terrain. Answer "Y" if you want to use flag pole receptors. A "Y" response will invoke a request for the receptor (i.e., flag pole) height. Answer "N" if you do not want to use flag pole receptors. The receptor height defaults to zero for a "N" response.

- If there is Simple terrain (response of "Y" at step 13) then, TSCREEN proceeds to step 17.

- If there is no Simple or Flat terrain (response of "N" at step 12) then, TSCREEN assumes that there is Complex terrain and proceeds to step 19.

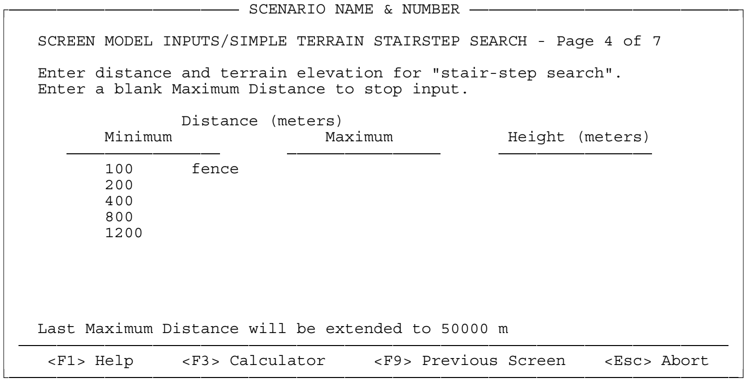
- If there is Flat terrain and specific locations of interest (response of "N" at step 13 and response of "Y" at step 14) then, TSCREEN proceeds to step 18.

- If there is Flat terrain but no specific locations of interest (response of "N" at step 13 and response of "N" at step 14) then, TSCREEN proceeds to step 16.

16 You have completed simple terrain inputs. Do you want to continue with complex terrain (Y/N) -
Complex terrain is terrain exceeding the height of the stack being modeled. Enter "Y" to model complex terrain. SCREEN has no automated distance array for Complex Terrain. Distances must be specified by the user.

- If "Y" was entered, TSCREEN proceeds to step 19.

- If "N" was entered, TSCREEN runs the SCREEN model.



```
──────────────────── SCENARIO NAME & NUMBER ────────────────────

  SCREEN MODEL INPUTS/SIMPLE TERRAIN STAIRSTEP SEARCH - Page 4 of 7

  Enter distance and terrain elevation for "stair-step search".
  Enter a blank Maximum Distance to stop input.

                 Distance (meters)
         Minimum                Maximum            Height (meters)
     ________________       ________________     ________________
         100      fence
         200
         400
         800
         1200




  Last Maximum Distance will be extended to 50000 m
 ________________________________________________________________________
    <F1> Help     <F3> Calculator     <F9> Previous Screen     <Esc> Abort
```

SIMPLE TERRAIN STAIR-STEP SEARCH

17 Enter distance and terrain elevation for "stair-step search"-
The SCREEN model assumes that terrain elevation either remains the same or increases with distance from the source, i.e., incremental steps, as in an ascending staircase or on a terraced hillside. "Stair-step search" describes how the SCREEN model searches for the maximum concentration in simple terrain. The user should enter the distance to and the elevation (above stack-base) of each stair-tread or terrace. SCREEN assumes that the first stair-tread begins at the fenceline. Thus, the user must begin by entering the

elevation and the distance to the end of the first stair-tread. This is repeated for each succeeding stair-tread. The distance to the end of the last stair-tread defaults to 50 km.

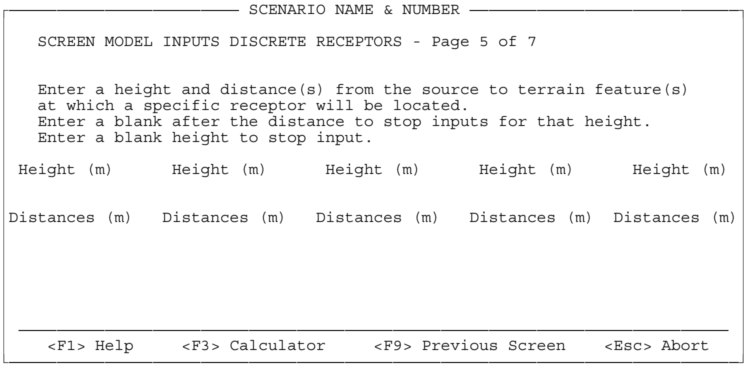
After finishing inputs for this section, TSCREEN will ask if there are specific locations of interest (See step 13).

- If "Y", TSCREEN proceeds to step 18.

- If "N", TSCREEN will ask the if there is Complex terrain (See step 16).

- If there is Complex terrain, TSCREEN proceeds to step 19.

- If there is no Complex terrain, TSCREEN runs the SCREEN model.



```
                          SCENARIO NAME & NUMBER

   SCREEN MODEL INPUTS DISCRETE RECEPTORS - Page 5 of 7

   Enter a height and distance(s) from the source to terrain feature(s)
   at which a specific receptor will be located.
   Enter a blank after the distance to stop inputs for that height.
   Enter a blank height to stop input.

 Height (m)      Height (m)      Height (m)      Height (m)      Height (m)

Distances (m)   Distances (m)   Distances (m)   Distances (m)  Distances (m)

    <F1> Help     <F3> Calculator     <F9> Previous Screen    <Esc> Abort
```

DISCRETE RECEPTORS

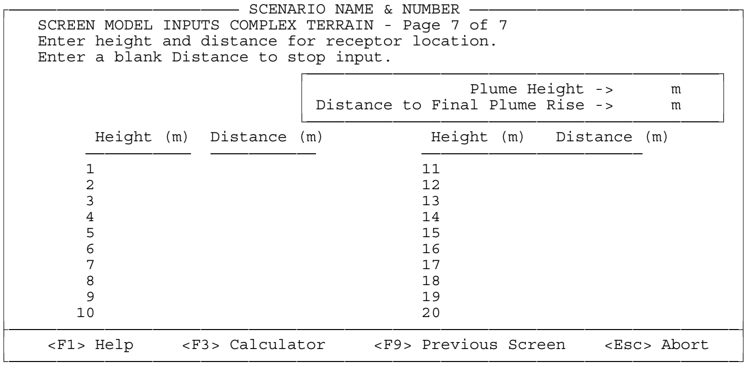
18 Enter a height and distance(s) from the source to terrain feature(s) at which a specific receptor will be located - The program will calculate concentrations at receptors for a specified distance from their release. In the case of simple terrain, a terrain height can be specified from these receptors. This height must be ≤ the stack height. For the case of flat terrain, a terrain height is not requested.

- If 5 heights are entered, TSCREEN will ask if the user wants to enter more discrete receptors. If the response is "Y" a Page 6 of 7, which looks the same as Page 5 of 7, will appear.

After finishing inputs for DISCRETE RECEPTOR section, TSCREEN will ask if the user wants to proceed with complex terrain (See step 17).

- If response is "Y" then TSCREEN proceeds to step 19.

- If response in "N" then, TSCREEN runs the SCREEN model.



```
SCENARIO NAME & NUMBER
SCREEN MODEL INPUTS COMPLEX TERRAIN - Page 7 of 7
Enter height and distance for receptor location.
Enter a blank Distance to stop input.

                                    Plume Height ->      m
                  Distance to Final Plume Rise ->      m

    Height (m)  Distance (m)          Height (m)   Distance (m)

     1                                 11
     2                                 12
     3                                 13
     4                                 14
     5                                 15
     6                                 16
     7                                 17
     8                                 18
     9                                 19
    10                                 20

  <F1> Help     <F3> Calculator     <F9> Previous Screen     <Esc> Abort
```

COMPLEX TERRAIN

19 Enter height and distance from receptor locations -
Enter the terrain height and distance in meters for the receptor of interest. The terrain height must be greater than the stack height.

- After finishing inputs for this section, TSCREEN runs the SCREEN model.

### 5.1.1.2 Model Output

For a complete example of the SCREEN model for a point source, see Section 4.1.1. See Appendix E - Running TSCREEN for output options after model is run. The following shows the format of the output file that SCREEN would generate for a point source if the user has chosen to show the maximum concentration in parts per million (PPM) in addition to µg/$m^3$ and shows the maximum concentration for additional averaging times.

```
1                                                                        02-05-92
                                                                         09:50:06
  *** SCREEN-1.2 MODEL RUN ***
  *** VERSION DATED  90XXX ***

 Particulate Stack Release

 COMPLEX TERRAIN INPUTS:
    SOURCE TYPE          =    POINT
    EMISSION RATE (G/S) =
    STACK HT (M)         =
    STACK DIAMETER (M)  =
    STACK VELOCITY (M/S)=
    STACK GAS TEMP (K)  =
    AMBIENT AIR TEMP (K)=
    RECEPTOR HEIGHT (M) =
    IOPT (1=URB,2=RUR)  =
1                                                                        02-05-92
                                                                         09:50:06
  *** SCREEN-1.2 MODEL RUN ***
  *** VERSION DATED  91/10 ***


 SIMPLE TERRAIN INPUTS:
    SOURCE TYPE             =    POINT
    EMISSION RATE (G/S)     =
    STACK HEIGHT (M)        =
    STK INSIDE DIAM (M)     =
    STK EXIT VELOCITY (M/S)=
    STK GAS EXIT TEMP (K)  =
    AMBIENT AIR TEMP (K)   =
    RECEPTOR HEIGHT (M)    =
    IOPT (1=URB,2=RUR)     =
    BUILDING HEIGHT (M)    =
    MIN HORIZ BLDG DIM (M) =
    MAX HORIZ BLDG DIM (M) =

      **************************************
```

```
      *** SUMMARY OF SCREEN MODEL RESULTS ***
      ***************************************

  CALCULATION        MAX CONC       MAX CONC     DIST TO   TERRAIN
   PROCEDURE        (UG/M**3)         (PPM)       MAX (M)    HT (M)
 --------------    -----------    -----------    -------   -------

 SIMPLE TERRAIN

 COMPLEX TERRAIN                                   (24-HR CONC)

 BUILDING CAVITY-1                             --  (DIST = CAVITY LENGTH)
 BUILDING CAVITY-2                             --  (DIST = CAVITY LENGTH)


 ***************************************************
 ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
 ***************************************************


 BUOY. FLUX =         M**4/S**3;  MOM. FLUX =         M**4/S**2.


 FINAL STABLE PLUME HEIGHT (M) =
 DISTANCE TO FINAL RISE (M)    =

                          *VALLEY 24-HR CALCS*   **SIMPLE TERRAIN 24-HR CALCS**
  TERR         MAX 24-HR              PLUME HT              PLUME HT
   HT    DIST    CONC        CONC    ABOVE STK    CONC    ABOVE STK    U10M UST
  (M)     (M)   (UG/M**3)   (UG/M**3)  BASE (M)  (UG/M**2)  HGT (M)  SC   (M/S)
 ----- ------- ----------  ----------  ------   ----------  ------  -- ---- ----




 BUOY. FLUX =         M**4/S**3;  MOM. FLUX =         M**4/S**2.

 *** FULL METEOROLOGY ***

 **********************************
 *** SCREEN AUTOMATED DISTANCES ***
 **********************************

 *** TERRAIN HEIGHT OF       M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

   DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
    (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
 -------  ----------  ----  -----  -----  ------  ------  ------  ------  -----
    100.
    200.

MAXIMUM 1-HR CONCENTRATION AT OR BEYOND        M:


 **********************************
 *** SCREEN AUTOMATED DISTANCES ***
 **********************************

 *** TERRAIN HEIGHT OF       M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

   DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
    (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
 -------  ----------  ----  -----  -----  ------  ------  ------  ------  -----
    200.
    300.
    400.

 MAXIMUM 1-HR CONCENTRATION AT OR BEYOND        M:


 **********************************
 *** SCREEN AUTOMATED DISTANCES ***
 **********************************

 *** TERRAIN HEIGHT OF       M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

   DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
    (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
 -------  ----------  ----  -----  -----  ------  ------  ------  ------  -----




 MAXIMUM 1-HR CONCENTRATION AT OR BEYOND        M:


 **********************************
 *** SCREEN AUTOMATED DISTANCES ***
 **********************************

 *** TERRAIN HEIGHT OF       M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

   DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
    (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
 -------  ----------  ----  -----  -----  ------  ------  ------  ------  -----
    900.                                                                          1000.
   1100.
   1200.
   1300.
   1400.
   1500.
   1600.
   1700.
```

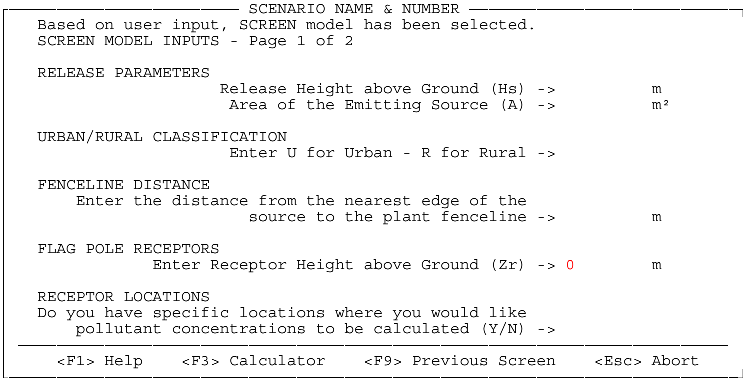
```
  1800.
  1900.
  2000.
  2100.
  2200.
  2300.
  2400.
  2500.
  2600.
  2700.
  2800.
  2900.
  3000.
  3500.
  4000.
  4500.
  5000.
  5500.
  6000.
  6500.
  7000.
  7500.
  8000.
  8500.
  9000.
  9500.
 10000.
 15000.
 20000.
 25000.
 30000.
 40000.
 50000.

MAXIMUM 1-HR CONCENTRATION AT OR BEYOND        M:


 DIST    = DISTANCE FROM THE SOURCE
 CONC    = MAXIMUM GROUND LEVEL CONCENTRATION
 STAB    = ATMOSPHERIC STABILITY CLASS (1=A, 2=B, 3=C, 4=D, 5=E, 6=F)
 U10M    = WIND SPEED AT THE 10-M LEVEL
 USTK    = WIND SPEED AT STACK HEIGHT
 MIX HT  = MIXING HEIGHT
 PLUME HT= PLUME CENTERLINE HEIGHT
 SIGMA Y = LATERAL DISPERSION PARAMETER
 SIGMA Z = VERTICAL DISPERSION PARAMETER
 DWASH   = BUILDING DOWNWASH:
           DWASH=   MEANS NO CALC MADE (CONC = 0.0)
           DWASH=NO MEANS NO BUILDING DOWNWASH USED
           DWASH=HS MEANS HUBER-SNYDER DOWNWASH USED
           DWASH=SS MEANS SCHULMAN-SCIRE DOWNWASH USED
           DWASH=NA MEANS DOWNWASH NOT APPLICABLE, X<3*LB

*********************************
*** SCREEN DISCRETE DISTANCES ***
*********************************

*** TERRAIN HEIGHT OF       M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

  DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
   (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
-------  ----------  ----  -----  -----  ------  ------  ------  ------  -----



*********************************
*** SCREEN DISCRETE DISTANCES ***
*********************************

*** TERRAIN HEIGHT OF       M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

  DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
   (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
-------  ----------  ----  -----  -----  ------  ------  ------  ------  -----




 DWASH=   MEANS NO CALC MADE (CONC = 0.0)
 DWASH=NO MEANS NO BUILDING DOWNWASH USED
 DWASH=HS MEANS HUBER-SNYDER DOWNWASH USED
 DWASH=SS MEANS SCHULMAN-SCIRE DOWNWASH USED
 DWASH=NA MEANS DOWNWASH NOT APPLICABLE, X<3*LB

 ********************************************
 *  SUMMARY OF TERRAIN HEIGHTS ENTERED FOR  *
 *    SIMPLE ELEVATED TERRAIN PROCEDURE     *
 ********************************************

      TERRAIN        DISTANCE RANGE (M)
       HT (M)       MINIMUM     MAXIMUM
      -------      --------    --------




 *** CAVITY CALCULATION - 1 ***       *** CAVITY CALCULATION - 2 ***
```

```
   CONC (UG/M**3)      =                CONC (UG/M**3)      =
   CRIT WS @10M (M/S)  =                CRIT WS @10M (M/S)  =
   CRIT WS @ HS (M/S)  =                CRIT WS @ HS (M/S)  =
   DILUTION WS (M/S)   =                DILUTION WS (M/S)   =
   CAVITY HT (M)       =                CAVITY HT (M)       =
   CAVITY LENGTH (M)   =                CAVITY LENGTH (M)   =
   ALONGWIND DIM (M)   =                ALONGWIND DIM (M)   =

**************************************
*** USER SPECIFIED AVERAGING TIMES ***
**************************************

ESTIMATED MAXIMUM CONCENTRATION FOR 15 MIN AVERAGING TIME:
         UG/M**3                PPM

ESTIMATED MAXIMUM CONCENTRATION FOR 30 MIN AVERAGING TIME:
         UG/M**3                PPM

ESTIMATED MAXIMUM CONCENTRATION FOR 3 HR AVERAGING TIME:
      (+/-      ) UG/M**3       (+/-      ) PPM

ESTIMATED MAXIMUM CONCENTRATION FOR 8 HR AVERAGING TIME:
      (+/-      ) UG/M**3       (+/-      ) PPM

ESTIMATED MAXIMUM CONCENTRATION FOR 24 HR AVERAGING TIME:
      (+/-      ) UG/M**3       (+/-      ) PPM

**********************************
*** END OF SCREEN MODEL OUTPUT ***
**********************************
```

### 5.1.2 Area Sources

#### 5.1.2.1 Inputs

This section contains a listing of the inputs TSCREEN will request that are unique for the SCREEN area source. Some of these inputs may have already been entered from the scenario input section.



```
SCENARIO NAME & NUMBER
Based on user input, SCREEN model has been selected.
SCREEN MODEL INPUTS - Page 1 of 2

RELEASE PARAMETERS
                   Release Height above Ground (Hs) ->         m
                    Area of the Emitting Source (A) ->         m²

URBAN/RURAL CLASSIFICATION
                    Enter U for Urban - R for Rural ->

FENCELINE DISTANCE
    Enter the distance from the nearest edge of the
                      source to the plant fenceline ->         m

FLAG POLE RECEPTORS
            Enter Receptor Height above Ground (Zr) -> 0       m

RECEPTOR LOCATIONS
Do you have specific locations where you would like
    pollutant concentrations to be calculated (Y/N) ->

  <F1> Help    <F3> Calculator    <F9> Previous Screen    <Esc> Abort
```

RELEASE PARAMETERS

1 Release Height above Ground ($H_S$) -
Enter the height of the release area above the ground in meters. If the height is < 10 m, then the model assumes a ground level release. If the height is > 10 m, the release are is probably a volume source and SCREEN cannot handle this case.

2 Area of the Emitting Source (A) -
Enter the release area in square meters.

URBAN/RURAL CLASSIFICATION

3 Enter U for Urban - R for Rural -
The classification of a site as urban or rural is based on the procedures described in Section 8.2.8 of the Guideline on Air Quality Models (Revised), EPA-450/2-78-027R.

FENCELINE DISTANCE

4 Enter the distance from the nearest edge of the source to the plant fenceline -
Enter the distance from the base of the stack to the plant fenceline in meters. SCREEN calculates the maximum concentrations across a range of meteorological conditions for the minimum distance given (> 1 m) and then for each distance in the array. Thus, the user can input the minimum fenceline distance as the minimum distance for calculation and obtain a concentration at the site boundary and beyond. Distances less than the fenceline distance are ignored. Receptors beyond the fenceline are defined as ambient air.

FLAG POLE RECEPTORS

5 Enter Receptor Height above Ground ($Z_r$) -
Flag pole receptors are receptors at heights (meters) above local terrain elevation, e.g., on the roof of a building. Enter 0 if receptor heights are at ground level. Flag pole receptors are useful for estimating concentrations on rooftops or similar exposed locations and are most often used in urban modeling evaluations. The default is 0.

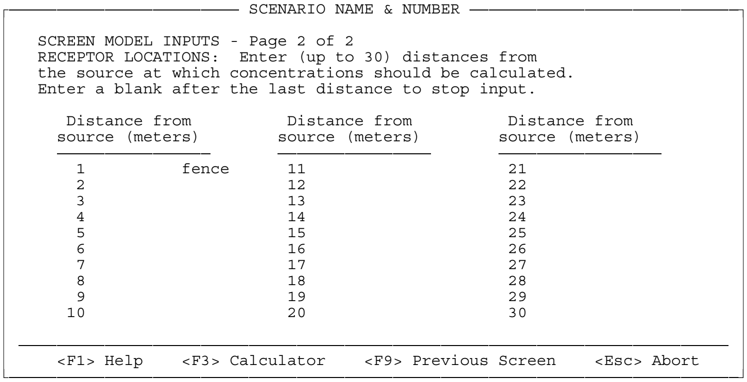
RECEPTOR LOCATIONS

Since area sources are ground level releases, there is no impact on "complex terrain"; only receptors classified as "simple terrain."

6 Do you have specific locations where you would like pollutant concentrations to be calculated (Y/N) -
The entry of "Y" will allow the user to input any number of specific distances (>1 m) and the maximum concentration for each distance will be calculated. Note that SCREEN has an automated distance array which calculates maximum concentrations at a pre-selected array of 50 distances ranging from 100 m to 50 km. For example, a specific location of interest may be a school 117 m from the source.

With the automated distance array, the SCREEN model uses an iteration routine to determine the maximum value and associated distance to the nearest meter. Note: SCREEN assumes that the overall maximum concentration occurs for the same stability class that is associated with the maximum concentration from the automated distance array, and begins iterating from that value, examining a range of wind speeds for that stability.

- If response is "Y" then TSCREEN proceeds to step 7.
- If response is "N" then TSCREEN runs the SCREEN model.



```
SCENARIO NAME & NUMBER

SCREEN MODEL INPUTS - Page 2 of 2
RECEPTOR LOCATIONS:  Enter (up to 30) distances from
the source at which concentrations should be calculated.
Enter a blank after the last distance to stop input.

   Distance from          Distance from          Distance from
 source (meters)        source (meters)        source (meters)
 _______________        _______________        _________________
   1          fence       11                     21
   2                      12                     22
   3                      13                     23
   4                      14                     24
   5                      15                     25
   6                      16                     26
   7                      17                     27
   8                      18                     28
   9                      19                     29
  10                      20                     30

    <F1> Help    <F3> Calculator    <F9> Previous Screen    <Esc> Abort
```

DISCRETE RECEPTORS

7 <u>Enter (up to 30) distances from the source at which concentrations should be calculated -</u>
Enter the Distance in meters from the release for calculating the maximum ground level concentrations.

- After all of the desired distances have been entered, TSCREEN will run the SCREEN model for an area source.

### 5.1.2.2 Model Output

For a complete example of the SCREEN model for a area source, see Section 4.1.2. (See Appendix E-Running TSCREEN for output options after the model is run.) The following shows the format of the output file that SCREEN would generate for a area source if the user has chosen to show the maximum concentration in part per million (PPM) in addition to µg/m$^3$.

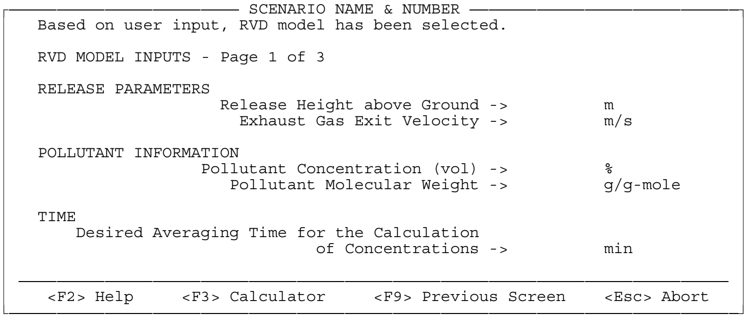
```
 1                                                                03-03-92
                                                                  10:04:59
  *** SCREEN-1.2 MODEL RUN ***
  *** VERSION DATED  90XXX ***



 SIMPLE TERRAIN INPUTS:
    SOURCE TYPE         =     AREA
    EMISSION RATE (G/S) =
    SOURCE HEIGHT (M)   =
    LENGTH OF SIDE (M)  =
    RECEPTOR HEIGHT (M) =
    IOPT (1=URB,2=RUR)  =


      ***************************************
      *** SUMMARY OF SCREEN MODEL RESULTS ***
      ***************************************

  CALCULATION        MAX CONC       MAX CONC      DIST TO   TERRAIN
   PROCEDURE        (UG/M**3)        (PPM)        MAX (M)    HT (M)
 --------------    -----------    -----------    -------   -------
 SIMPLE TERRAIN


 ***************************************************
 ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
 ***************************************************


 BUOY. FLUX =         M**4/S**3;  MOM. FLUX =         M**4/S**2.
```

```
 *** FULL METEOROLOGY ***

 **********************************
 *** SCREEN AUTOMATED DISTANCES ***
 **********************************

 *** TERRAIN HEIGHT OF    0. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

   DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
    (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
 -------  ----------  ----  -----  -----  ------  ------  ------  ------  -----
    100.
    200.
    300.
    400.
    500.
    600.
    700.
    800.
    900.
   1000.
   1100.
   1200.
   1300.
   1400.
   1500.
   1600.
   1700.
   1800.
   1900.
   2000.
   2100.
   2200.
   2300.
   2400.
   2500.
   2600.
   2700.
   2800.
   2900.
   3000.
   3500.
   4000.
   4500.
   5000.
   5500.
   6000.
   6500.
   7000.
   7500.
   8000.
   8500.
   9000.
   9500.
  10000.
  15000.
  20000.
  25000.
  30000.
  40000.
  50000.

 MAXIMUM 1-HR CONCENTRATION AT OR BEYOND        M:


  DIST    = DISTANCE FROM THE SOURCE
  CONC    = MAXIMUM GROUND LEVEL CONCENTRATION
  STAB    = ATMOSPHERIC STABILITY CLASS (1=A, 2=B, 3=C, 4=D, 5=E, 6=F)
  U10M    = WIND SPEED AT THE 10-M LEVEL
  USTK    = WIND SPEED AT STACK HEIGHT
  MIX HT  = MIXING HEIGHT
  PLUME HT= PLUME CENTERLINE HEIGHT
  SIGMA Y = LATERAL DISPERSION PARAMETER
  SIGMA Z = VERTICAL DISPERSION PARAMETER
  DWASH   = BUILDING DOWNWASH:
            DWASH=   MEANS NO CALC MADE (CONC = 0.0)
            DWASH=NO MEANS NO BUILDING DOWNWASH USED
            DWASH=HS MEANS HUBER-SNYDER DOWNWASH USED
            DWASH=SS MEANS SCHULMAN-SCIRE DOWNWASH USED
            DWASH=NA MEANS DOWNWASH NOT APPLICABLE, X<3*LB

 *********************************
 *** SCREEN DISCRETE DISTANCES ***
 *********************************

 *** TERRAIN HEIGHT OF    0. M ABOVE STACK BASE USED FOR FOLLOWING DISTANCES **

   DIST     CONC             U10M   USTK  MIX HT   PLUME   SIGMA   SIGMA
    (M)   (UG/M**3)   STAB  (M/S)  (M/S)    (M)   HT (M)   Y (M)   Z (M)  DWASH
 -------  ----------  ----  -----  -----  ------  ------  ------  ------  -----




  DWASH=   MEANS NO CALC MADE (CONC = 0.0)
  DWASH=NO MEANS NO BUILDING DOWNWASH USED
  DWASH=HS MEANS HUBER-SNYDER DOWNWASH USED
  DWASH=SS MEANS SCHULMAN-SCIRE DOWNWASH USED
  DWASH=NA MEANS DOWNWASH NOT APPLICABLE, X<3*LB

**********************************
*** END OF SCREEN MODEL OUTPUT ***
**********************************
```

## 5.2 RVD

The RVD model provides short-term ambient concentration estimates for screening pollutant sources emitting denser-than-air gases and aerosols through vertically-directed releases. The model is based on empirical equations derived from wind tunnel tests and estimates the maximum ground level concentration at plume touchdown at downwind receptor locations. For more information refer to User's Guide for RVD2.0, A Relief Valve Discharge Screening Model EPA-450/4-88-024.

### 5.2.1 Inputs



```
──────────────────── SCENARIO NAME & NUMBER ─────────────────────────
  Based on user input, RVD model has been selected.

  RVD MODEL INPUTS - Page 1 of 3

  RELEASE PARAMETERS
                     Release Height above Ground ->          m
                       Exhaust Gas Exit Velocity ->          m/s

  POLLUTANT INFORMATION
                   Pollutant Concentration (vol) ->          %
                      Pollutant Molecular Weight ->          g/g-mole

  TIME
      Desired Averaging Time for the Calculation
                               of Concentrations ->          min
─────────────────────────────────────────────────────────────────────
   <F2> Help     <F3> Calculator     <F9> Previous Screen    <Esc> Abort
```

#### RELEASE PARAMETERS

1 Release Height above Ground (m) -
Enter the height of the stack or of the release point above the ground in meters.

2 Exhaust Gas Exit Velocity (m/s) -
The exit velocity (m/s) for a two-phase mixture may be calculated from the equation:

$$\mathrm{Exit}_v(\mathrm{m/s}) = \frac{Q_m(\mathrm{g/s})}{A(\mathrm{m}^2)\ \rho_l(\mathrm{g/m}^3)}$$

where:
$Q_m$ = emission rate (g/s)
$A$ = area ($m^2$)
$\rho_l$ = liquid density of released material (g/$m^3$)

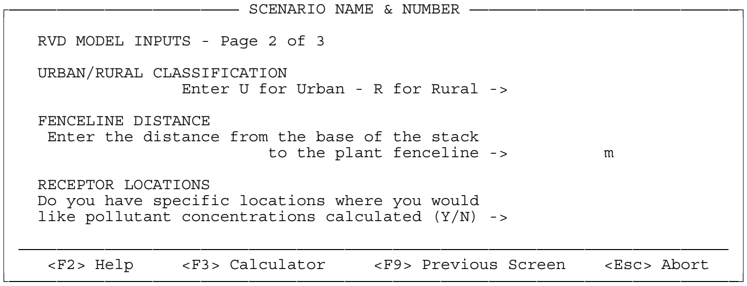
#### POLLUTANT INFORMATION

3 Pollutant Concentration (%) -
Enter the volume percent of the pollutant in the release material.

4 Pollutant Molecular Weight (g/g-mole) -
This is the individual pollutant's molecular weight, not the molecular weight of the exhaust material.

## TIME

5 Desired Averaging Time for the Calculation of Concentration (min) -
Enter the desired time span for calculating concentrations in minutes. If the release duration is less than the averaging time of interest, or if the averaging time of interest is less than 60 minutes, a correction factor is calculated within RVD.



```
────────────────────── SCENARIO NAME & NUMBER ──────────────────────────

  RVD MODEL INPUTS - Page 2 of 3

  URBAN/RURAL CLASSIFICATION
                 Enter U for Urban - R for Rural ->

  FENCELINE DISTANCE
   Enter the distance from the base of the stack
                          to the plant fenceline ->          m

  RECEPTOR LOCATIONS
  Do you have specific locations where you would
  like pollutant concentrations calculated (Y/N) ->

 ──────────────────────────────────────────────────────────────────────
   <F2> Help     <F3> Calculator     <F9> Previous Screen    <Esc> Abort
```

## URBAN/RURAL CLASSIFICATION

6 Enter U for Urban - R for Rural -
The classification of a site as urban or rural is based on the procedures described in Section 8.2.8 of the Guideline on Air Quality Models (Revised), EPA-450/2-78-927R.

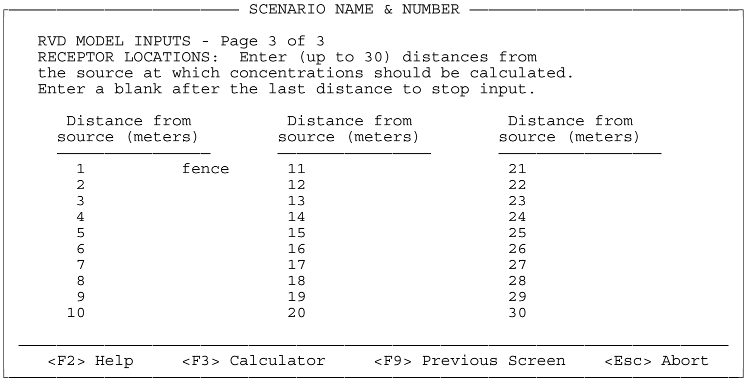
## FENCELINE DISTANCE

7 Enter the distance from the base of the stack to the plant fenceline (m) -
Enter the distance from the closest edge of the source to the fenceline in meters. The model calculates concentrations only at receptors beyond the fenceline in ambient air.

### RECEPTOR LOCATIONS

8 Do you have specific location where you would like pollutant concentrations calculated (Y/N) -
The entry of SPECIFIC LOCATIONS allows for calculating the maximum ground level concentrations at discrete, user-specified distances from the release. TSCREEN will automatically give you maximum ground level concentrations at 30 distances starting at the fenceline. The first 16 distances are in 100 m increments. The next 8 distances are in 200 m increments, and the remaining 5 distances are in 300 m increments.

- If "Y" is entered, proceed to step 9.
- If "N" is entered, TSCREEN runs the RVD model.



```
──────────────────── SCENARIO NAME & NUMBER ────────────────────────

  RVD MODEL INPUTS - Page 3 of 3
  RECEPTOR LOCATIONS:  Enter (up to 30) distances from
  the source at which concentrations should be calculated.
  Enter a blank after the last distance to stop input.

     Distance from          Distance from          Distance from
    source (meters)        source (meters)        source (meters)
    ________________       ________________       ________________
      1          fence       11                     21
      2                      12                     22
      3                      13                     23
      4                      14                     24
      5                      15                     25
      6                      16                     26
      7                      17                     27
      8                      18                     28
      9                      19                     29
     10                      20                     30
 ______________________________________________________________________
   <F2> Help     <F3> Calculator     <F9> Previous Screen     <Esc> Abort
```

### RECEPTOR LOCATIONS

9 Enter (up to 30) distances from the source at which concentrations should be calculated -
Enter the distance in meters from the release for calculating the maximum ground level concentrations.

- After the user finishes entering distances, TSCREEN runs the RVD model.

### 5.2.2 Model Output

For a complete example of the RVD model, see Section 4.2.3. (See Appendix E - Running TSCREEN for output options after model is run.) The following shows the format of the output file that RVD would generate. The output begins with a listing of model inputs. The second portion of the output identifies the maximum concentration and the distance at which it occurred, and the meteorological conditions associated with the maximum concentration. The next section lists the maximum concentration at each of the distances along with the meteorological conditions. The next portion of the output identifies those cases in which the model is applicable. In this section, a "0" indicates that the release is passive and the model is inapplicable, a "1" indicates that the gas is influenced by gravitational effects and a "2" indicates that the meteorological condition identified is not likely to occur. The determination of whether the gas is affected by gravitational effects is based initially on the Richardson number for which a table is presented. Next, the model results are presented in two forms, a table showing plume rise, touchdown distance, and touchdown concentration for each meteorological condition and a table of concentrations at specified receptors.

```
                                Input Data

Pollutant emission rate (kg/sec) =
Exit gas velocity (m/sec)=
Exit Temperature (K)=
Stack Height (m) =        Diameter (m) =
Pollutant Concentration (volume %) =
Exhaust Gas Density (kg/m3) =
Exhaust Gas Molecular Weight =
Exhaust Gas Mass Flow Rate (kg/sec) =
Pollutant Molecular Weight =
Release duration (min) =      Av. Time (min) =
Wind Speeds (m/sec) =  1.0    2.0    3.0    4.0    5.0
                       8.0   10.0   15.0   20.0
Distances (m) =  100    200    300    400    500    600    700
                 800    900    1000    1100    1200    1300    1400
                 1500    1600    1800    2000    2200    2400    2600
                 2800    3000    3200    3500    3800    4100    4400
                 4700    5000
Ambient Temperature (K) =
Rural Wind Speed Profile Exponents


*************************************************************
***             SUMMARY OF RVD MODEL RESULTS             ***
*************************************************************

Maximum offsite concentration is                ug/m3
                or equivalently             ppm
                 occurring at               m downwind
              when wind speed is     m/sec
                and stability is

*************************************************************
***      REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS    ***
*************************************************************


***********************
***  RVD DISTANCES  ***
***********************

Distance Concentration  Stability  Wind
                          Class    Speed
  (m)      (ug/m3)                (m/sec)      (ppm)
------------------------------------------------------
  100.0
  200.0
  300.0
  400.0
  500.0
  600.0
  700.0
  800.0
  900.0
 1000.0
 1100.0
 1200.0
 1300.0
 1400.0
 1500.0
 1600.0
 1800.0
 2000.0
 2200.0
 2400.0
 2600.0
 2800.0
 3000.0
 3200.0
 3500.0
 3800.0
 4100.0
 4400.0
 4700.0
 5000.0


          Dense Gas Behavior
```

```
           Stability  Class

 Wind    A   B   C   D   E   F
Speed
  1.0
  2.0
  3.0
  4.0
  5.0
  8.0
 10.0
 15.0
 20.0

(0=Non-Dense Behavior   1=Dense Gas Behavior
     2=Combinations that cannot occur)

             Release Richardson Numbers

                   Stability Class

   Wind       A         B         C         D         E         F
   Speed
   1.0
   2.0
   3.0
   4.0
   5.0
   8.0
  10.0
  15.0
  20.0


             Dense Plume Trajectory

Stability  Wind Plume Touchdown        Touchdown
  Class   Speed  Rise  Distance      Concentration
         (m/sec)  (m)      (m)      (ug/m3)     (ppm)
----------------------------------------------------------
    A
    A
    A
----------------------------------------------------------
    B
    B
    B
    B
    B
----------------------------------------------------------
    C
    C
    C
    C
    C
    C
    C
---------------------------------------------------------
    D
    D
    D
    D
    D
    D
    D
----------------------------------------------------------
    E
    E
    E
    E
----------------------------------------------------------
    F
    F
    F


 Concentrations at Specific Receptor Distances

Stability  Wind Distance Concentration
  Class   Speed
         (m/sec)   (m)      (ug/m3)      (ppm)
--------------------------------------------------
    A

    A
    A

    A
    A
    A

    A
    A
    A
.
.
.

--------------------------------------------------
    F

    F
    F
    F

    F
```

```
    F
    F

    F
    F
    F
.
.
.

*******************************
*** END OF RVD MODEL OUTPUT ***
*******************************
```

## 5.3 PUFF

The PUFF dispersion model provides an estimate of peak downwind concentrations for the case where the release time is finite but smaller than the travel time (i.e., an instantaneous release). The PUFF model is based on the Gaussian instantaneous puff equation and is applicable for neutrally buoyant non-reactive releases. For more information on PUFF refer to (Petersen, W., 1982: Estimating Concentrations Downwind from an Instantaneous Puff Release EPA 600/3-82-078). The following is brief summary of the model assumptions.

### 5.3.1 PUFF Model Discussion

The generalized puff equation is given as:

$$\chi_{(x,y,z,h)} = \frac{Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left[-\frac{1}{2}\left(\frac{x-ut}{\sigma_x}\right)^2\right]\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z+h}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z-h}{\sigma_z}\right)^2\right]\right\} \qquad (5.3\text{-}1)$$

Following the puff, and assuming $\sigma_x = \sigma_y$, the puff equation can be written as follows:

$$\chi_{(y,z,h)} = \frac{Q}{(2\pi)^{3/2}\sigma_y^{\,2}\sigma_z}\exp\left[-1/2\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-1/2\left(\frac{z+h}{\sigma_z}\right)^2\right]+\left[-1/2\left(\frac{z-h}{\sigma_z}\right)^2\right]\right\} \qquad (5.3\text{-}2)$$

The peak concentration at distances beyond the point where $\sigma_z$ is greater than 0.8L (mixing height) can be expressed as:

$$\chi_{(x,0,0,0)} = \frac{Q}{2\pi\sigma_y^{\,2}L} \quad \text{for } \sigma_z > 0.8L \qquad (5.3\text{-}3)$$

The concentration at the ground from an elevated release at a radical distance y from the puff center is given by Equation 5.3-4:

$$\chi_{(x,y,o,h)} = \frac{Q}{2\pi\sigma_y^{\,2}L}\exp\left[-1/2\left(\frac{y}{\sigma_y}\right)^2\right] \quad \text{for } \sigma_z > 0.8L \qquad (5.3\text{-}4)$$

Equations 5.3-3 and 5.3-4 account for reflection from the top of the mixed depth layer and are appropriate for surface level releases during neutral and unstable conditions. However, if the effective release height is small compared to the mixing height, Equations 5.3-3 and 5.3-4 are still good approximations.

Frequently, instantaneous releases are large enough in the horizontal and vertical dimensions that the initial size cannot be ignored in the concentration estimates. One approach to assessing the impact of the initial size on downwind concentrations is to introduce an initial horizontal dispersion parameter, $\sigma_{y_o}$ , and an initial vertical dispersion parameter, $\sigma_{z_o}$ . For a ground level release, $\sigma_{y_o}$ can be approximated by dividing the total initial width (W) of the puff by 4.3, $\sigma_{y_o} = W/4.3$. The second parameter, $\sigma_{z_o}$ , can be approximated by dividing the initial vertical extent of the puff (h) by 2.15, $\sigma_{z_o} = h/2.15$. For an elevated release, $\sigma_{y_o}$ can be approximated by dividing the total initial diameter (D) of the puff by 4.3, $\sigma_{y_o} = \sigma_{z_o} = D/4.3$. The total horizontal and vertical dispersion parameters are then given by:

$$\sigma_{y_t} = (\sigma_y{}^2 + \sigma_{y_o}{}^2)^{1/2} \qquad (5.3\text{-}5)$$

$$\sigma_{z_t} = (\sigma_z{}^2 + \sigma_{z_o}{}^2)^{1/2} \qquad (5.3\text{-}6)$$

Stability Parameters

The stability parameters used in the instantaneous puff model are those recommended by Slade (1968). Slade classified the data according to the broad categories of unstable, neutral, and very stable. A review of the data reveals two pertinent points: (1) There was very little data upon which to base the $\sigma_z$s during unstable conditions; (2) Much of the dispersion data during stable conditions lie closer to the Pasquill-Gifford F curve than to the curve recommended by Slade.

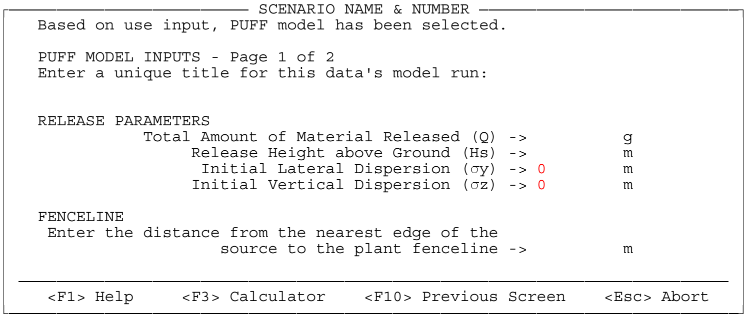
Model Applicability

Estimating concentrations at point locations is very difficult because of the deficiencies in determining the trajectory of the puff. Puff trajectory is most important if concentration estimates are to be made at specific points. However, the modeling effort is significantly simplified if the magnitudes of the concentrations are needed without regard to exactly where the concentrations will occur. Releases are seldom point sources, but are more typically small area sources. Small area source releases can be modeled to some extent by using initial dispersion parameters. The initial horizontal dispersion is typically calculated by dividing the initial horizontal dimension of the area source by 4.3. This method will give reasonable concentration estimates at downwind distances greater than about five times the horizontal dimension of the source. The initial vertical dispersion parameter is typically evaluated by dividing the initial vertical extent of the surface release by 2.15.

Many sources are not truly instantaneous. However, if the travel time is long compared to the release time, then the puff model can be used to estimate concentrations. If the travel time to a receptor is on the same order or smaller than the release time, the Gaussian plume model can be used (see Turner, 1970). For the case where the release time is finite but smaller than the travel time, the instantaneous puff model will provide a worst-case estimate of peak concentrations for the same total release. It is difficult to evaluate the effect on average concentrations over a given sampling time for a finite release using simple models, since the puff is distorted in the downwind direction. Finally, the modeling procedures are simple approaches to very complex problems. In general, these techniques will yield worst-case concentration estimates. The proper modeling of any sudden release requires the skills of an air quality specialist and a thorough understanding of the physical and chemical properties of the release.

### 5.3.2 Model Inputs

This section contains a complete listing of the inputs TSCREEN will request to run the PUFF model.



```
─────────────────────── SCENARIO NAME & NUMBER ──────────────────────────
  Based on use input, PUFF model has been selected.

  PUFF MODEL INPUTS - Page 1 of 2
  Enter a unique title for this data's model run:


  RELEASE PARAMETERS
             Total Amount of Material Released (Q) ->          g
                  Release Height above Ground (Hs) ->          m
                   Initial Lateral Dispersion (σy) -> 0        m
                  Initial Vertical Dispersion (σz) -> 0        m

  FENCELINE
   Enter the distance from the nearest edge of the
                     source to the plant fenceline ->          m

 ─────────────────────────────────────────────────────────────────────────
   <F1> Help     <F3> Calculator    <F10> Previous Screen    <Esc> Abort
```

RELEASE PARAMETERS

1 Total Amount of Material Released (Q) (g) -
Calculate total amount of material released during the duration of the release. If limited information is available in the technical literature. Conservative estimates of release amounts can be made based on transfer line rates and time from equipment shutdown and equipment capacity. A point source is assumed because no indication of initial dilution dimensions are provided in the problem.

2 Release Height above Ground ($H_s$) (m) -
Enter the height of the stack for the release point above the ground in meters. If the puff has positive buoyancy the effective height of release is release height plus the rise of the puff due to buoyancy. Screening methods are not

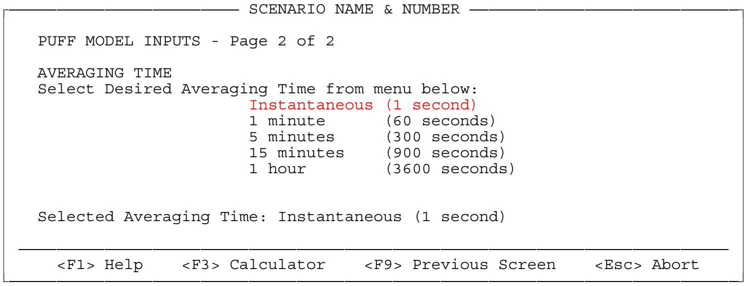
available for estimating plume rise for a PUFF release.

3 Initial Lateral Dispersion ($\sigma_y$) (m) -
Frequently, instantaneous releases are large enough in the horizontal dimension that the initial size cannot be ignored in the concentration estimates. One approach is to introduce the impact of the initial horizontal dispersion parameter, $\sigma_y$. For a ground level release, $\sigma_y$ can be approximated by dividing the total initial width (W) of the puff by 4.3, $\sigma_y$ = W/4.3. For an elevated release, $\sigma_y$ can be approximated by dividing the total initial diameter (D) of the puff by 4.3, $\sigma_y$ = D/4.3. The default in TSCREEN is 0 m.

4 Initial Vertical Dispersion ($\sigma_z$) (m) -
Frequently, instantaneous releases are large enough in the vertical dimension that the initial size cannot be ignored in the concentration estimates. One approach is to introduce the impact of the initial vertical dispersion parameter, $\sigma_z$. For a ground level release, $\sigma_z$ can be approximated by dividing the total initial vertical extent of the puff (h) by 2.15, $\sigma_z$ = h/2.15. For an elevated release, $\sigma_z$ can be approximated by dividing the total initial diameter (D) of the puff by 4.3, $\sigma_z$ = D/4.3. The default in TSCREEN is 0 m.

FENCELINE

5 Enter the distance from the nearest edge of the source to the plant fenceline (m) -
Enter the Distance from the edge of the source to the plant fenceline in meters. The fenceline distance is used only to set the minimum distance for concentration calculations.



```
SCENARIO NAME & NUMBER

PUFF MODEL INPUTS - Page 2 of 2

AVERAGING TIME
Select Desired Averaging Time from menu below:
                      Instantaneous (1 second)
                      1 minute      (60 seconds)
                      5 minutes     (300 seconds)
                      15 minutes    (900 seconds)
                      1 hour        (3600 seconds)


Selected Averaging Time: Instantaneous (1 second)

    <F1> Help    <F3> Calculator    <F9> Previous Screen    <Esc> Abort
```

AVERAGING TIME

6. Select Desired Averaging Time from menu below:

| | |
|---|---|
| Instantaneous (1 second) | |
| 1 minute | (60 seconds) |
| 5 minutes | (300 seconds) |
| 15 minutes | (900 seconds) |
| 1 hour | (3600 seconds) |

The PUFF model will calculate averaging times according to the procedure described in Appendix D. The PUFF model will calculate concentrations at all five averaging times, but only the concentrations at the selected averaging time will be plotted if the user chooses to graph the data (See Appendix E - RUNNING TSCREEN). The averaging time would normally be based on some health related standards. See Appendix D in the <u>Technical Guidance for Hazards Analysis, Emergency Planning for Extremely Hazardous Substances</u> as an example. From this document, threshold limiting values (TLV's) for averaging times and concentrations can be obtained for certain chemicals. The user can then use the model output to locate the distance or the distance range where this TLV occurs.

- ▸ After the user makes this selection, TSCREEN runs the PUFF model.

### 5.3.4 <u>Model Output</u>

For a complete example of the PUFF model, see Section 4.1.3. (Also see Appendix E - Running TSCREEN for output options after model is run). The following shows the format of the output file that PUFF would generate. This output is useful in determining: 1) sensitivity of the concentrations to the averaging time; and 2) distances to important concentrations (e.g., TLV's). The PUFF model uses three stability categories: labeled U for unstable, N for neutral, and S for stable. Unstable corresponds to stability categories 1 through 3 (for stabilities A - C) used by the SCREEN model, neutral corresponds to 4 (for D), and stable corresponds to 5 and 6 (for E and F).

```
    TOTAL AMOUNT OF MATERIAL RELEASED (G):
          RELEASE HEIGHT ABOVE GROUND (M):
 INITIAL LATERAL DISPERSION (SIGMA Y) (M):
INITIAL VERTICAL DISPERSION (SIGMA Z) (M):

 ******************************************************
 ***         SUMMARY OF PUFF MODEL RESULTS          ***
 ******************************************************

THE MAXIMUM CONCENTRATION AND THE DISTANCE TO MAXIMUM
CONCENTRATION FOR DISTANCES BEYOND FENCELINE         (KM).
FOR NEAR SURFACE RELEASE MAXIMUM CONCENTRATION WILL OCCUR AT
THE FENCELINE.

    AVERAGING           MAXIMUM             DISTANCE TO         STABILITY
    TIME (MIN)     CONCENTRATION (G/M**3)   MAX. CONC. (KM)     CLASS

*INSTANTANEOUS
       1
       5
       15
       60

 ******************************************************
 **   REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS  **
 ******************************************************


 *********************************
 ***      PUFF DISTANCES       ***
 *********************************

 THE MAXIMUM CONCENTRATION AS A FUNCTION OF DOWNWIND DISTANCE
 AND THE CONDITIONS THAT PRODUCED THE MAXIMUM AT THAT DISTANCE.


 MIXING HEIGHT (M)
 WIND SPEED (M/SEC)
```

```
 AVERAGING                          DOWNWIND DISTANCE (KM)
 TIME (MIN)   MAXIMUM CONCENTRATION (G/M**3) AT VARIOUS DOWNWIND DISTANCES.
                  STABILITY CLASS THAT PRODUCED THE MAX. LISTED BELOW
             0.01      0.03      0.05      0.07       0.1       0.5
 ==========================================================================
*INST.

 1

 5

 15

 60


 AVERAGING                          DOWNWIND DISTANCE (KM)
 TIME (MIN)   MAXIMUM CONCENTRATION (G/M**3) AT VARIOUS DOWNWIND DISTANCES.
                  STABILITY CLASS THAT PRODUCED THE MAX. LISTED BELOW
             1.0       3.0       5.0       7.0      10.0      30.0
 ==========================================================================
*INST.

 1

 5

 15

 60


 STABILITY CLASSES
 U = UNSTABLE
 N = NEUTRAL
 S = STABLE

 * INDICATES AVERAGING TIME THAT WAS SELECTED FOR PLOTTING

********************************
*** END OF PUFF MODEL OUTPUT ***
********************************
```

## 5.4 Britter-McQuaid

Britter and McQuaid (1988) report work which provides a correlation for estimating the dispersion of denser-than-air gases from area sources for continuous (plume) and instantaneous (puff) release. The objective was to produce correlations which predicted the dependent variables (distance to a given concentration level and area covered by a plume or puff) to within a factor of two. The analysis identified the dominant independent variables as: volumetric rate (or total) contaminant released; density of released material; windspeed at a standard height (taken to be 10 m); and a characteristic source dimension. Based (at least in part) on the fact that presently available field-test data for denser-than-air gases do not clearly indicate such, independent variables of lesser importance were identified as: surface roughness; atmospheric stability; atmospheric turbulence; and exact source dimension. Other effects not included in Britter and McQuaid's analysis are: source momentum; condensation of ambient humidity; and non-ideal gas behavior. (It should be noted that the effects which were not included may be of crucial importance for contaminants whose molecular weight is less than air including, for example, liquefied natural gas (LNG), ammonia, and hydrogen fluoride; some similarity models (such as DEGADIS) can take these effects into account.)

For screening purposes, the original procedure set forth by Britter and McQuaid will be simplified in two important ways:

- Other established (passive) screening methods are recommended if the release is determined to be passive from the source (i.e., the denser-than-air effects are not expected to be important).

- The influence of buildings, topography, and releases not close to the ground are not included.

In addition, the effect of initial dilution due to jetting is beyond the scope of this effort. At present, the RVD model (U.S. EPA, 1989) is used for such cases as pressure relief valve discharge where source jetting will bring about air entrainment (and resulting dilution) for the hypothesized release. For cases where the jet orientation is unknown or is not directed vertically upward, the most conservative assumption (i.e., the assumption which results in the maximum downwind distance to a given concentration level under otherwise identical circumstances) is to discount the initial dilution due to jetting; the correlations of Britter and McQuaid do not include the effects of source jetting.

### 5.4.1 Method for Cold Contaminant Releases — Heat Transfer Effects

Heat transfer effects are not included in Britter and McQuaid's correlation; two ways suggested at looking at the limiting effects associated with heat transfer:

- Assume that heat transfer is unimportant and perform the calculations using the originally estimated temperature and density ($T_2$ and $\rho_2$, respectively).

- Assume that the heat transfer is important and (for the sake of maximizing its importance) assume that all of the heat transfer occurs at the source.

The (real) effect of heat transfer should lie somewhere between these two extremes (limiting cases). So, an estimate of the downwind distance to the desired concentration level should be made for each of the limiting cases, and the greatest of the two estimates of x (distance to a given concentration level) should be reported. For the first case, the input parameters will be the same as calculated in the earlier sections. For the second case though, the initial density and temperature are modified as follows:

$$\hat{\rho}_2 \leftarrow \rho_2 \, (T_2/T_a) \qquad (5.4\text{-}1a)$$

$$\hat{T}_2 \leftarrow T_a \qquad (5.4\text{-}1b)$$

where the ^ represents the "adjusted" initial values; for this case then, these "adjusted" values should be used whenever $\rho_2$ and $T_2$ are required.

### 5.4.2 Method for Contaminant Aerosol Releases

Since Britter and McQuaid's correlations are based on the analysis of dispersing gases, the complex thermodynamic effects of an aerosol must be considered using an ad hoc argument that, near the source, sufficient air will be entrained to evaporate all of the condensed aerosol phase and raise the temperature of the air/contaminant (gas) mixture to a temperature where the contaminant vapor pressure is equal to the ambient pressure (for an aerosol release, $T_2$). For such a process, the resulting mole fractions of contaminant and air are:

$$z_c = \left[ 1 + \frac{(1-x_2)\lambda}{c_p (T_a - T_2)} \right]^{-1} \qquad (5.4\text{-}2a)$$

$$z_a = 1 - z_c \qquad (5.4\text{-}2b)$$

where (as discussed above) the effects of humidity have been ignored. This air entrainment process will also change the temperature and density of the air/contaminant mixture. Furthermore, since for most release scenarios, $T_2 \neq T_a$, the effect of heat transfer may also be important. Therefore, two cases are considered:

Case 1: Air dilution neglecting heat transfer. The initial density is modified as follows:

$$\hat{\rho}_2 \leftarrow \frac{P_a}{RT_2} (z_c M_w + z_a M_a) \qquad (5.4\text{-}3)$$

where as before the ^ represents the "adjusted" initial values; $M_a$ is the molecular weight of air (28.96 kg/kmol). In addition, the initial volume of the release is modified. For continuous releases, $Q_m$ is modified as:

$$\hat{Q}_m \leftarrow Q_m (z_c M_w + z_a M_a) / (z_c M_c) \qquad (5.4\text{-}4)$$

and for instantaneous releases, Q ($=Q_m T_d$) is modified as:

$$\hat{Q} \leftarrow Q (z_c M_w + z_a M_a) / (z_c M_c) \qquad (5.4\text{-}5)$$

Case 2: Air dilution including heat transfer. The initial density and temperature are modified as follows:

$$\hat{\rho}_2 \leftarrow \frac{P_a}{RT_a} (z_c M + z_a M_a) \qquad (5.4\text{-}6a)$$

$$\hat{T}_2 \leftarrow T_a \qquad (5.4\text{-}6b)$$

Finally, $Q_m$ and Q are modified as described earlier in Equations 5.4-4 and 5.4-5, respectively.

### 5.4.3 Continuous (Plume) Releases

To estimate the importance of denser-than-air effects on continuous releases, Britter and McQuaid recommend that denser-than-air effects be ignored if:

$$U_r \Bigg/ \left[ \frac{g\,(Q_m/\rho_2)}{D} \left(\frac{\rho_2-\rho_a}{\rho_a}\right)\right]^{1/3} > 6 \qquad (5.4\text{-}7)$$

where D is the (low-momentum) horizontal dimension of the source (m), $Q_m$ is the release rate (kg/s), $U_r$ is the windspeed at 10 m (m/s), $\rho_a$ is the ambient air density (kg/m$^3$). If the value of D is not otherwise known (such as the diameter of a liquid pool), a (screening) estimate of D can be made assuming that the ratio of the vertical source dimension to the horizontal source dimension is approximately 1/2 and the momentum of the release is inconsequential. Using this assumption,

$$D = \sqrt{2\,(Q_m/\rho_2)\;/U_r} \qquad (5.4\text{-}8)$$

(Note that D is not necessarily the same as the hole or opening diameter and may be much larger.) If denser-than-air effects are determined to be unimportant, standard passive atmospheric dispersion techniques should be applied. Finally, note that Equation 5.4-7 can be rewritten as:

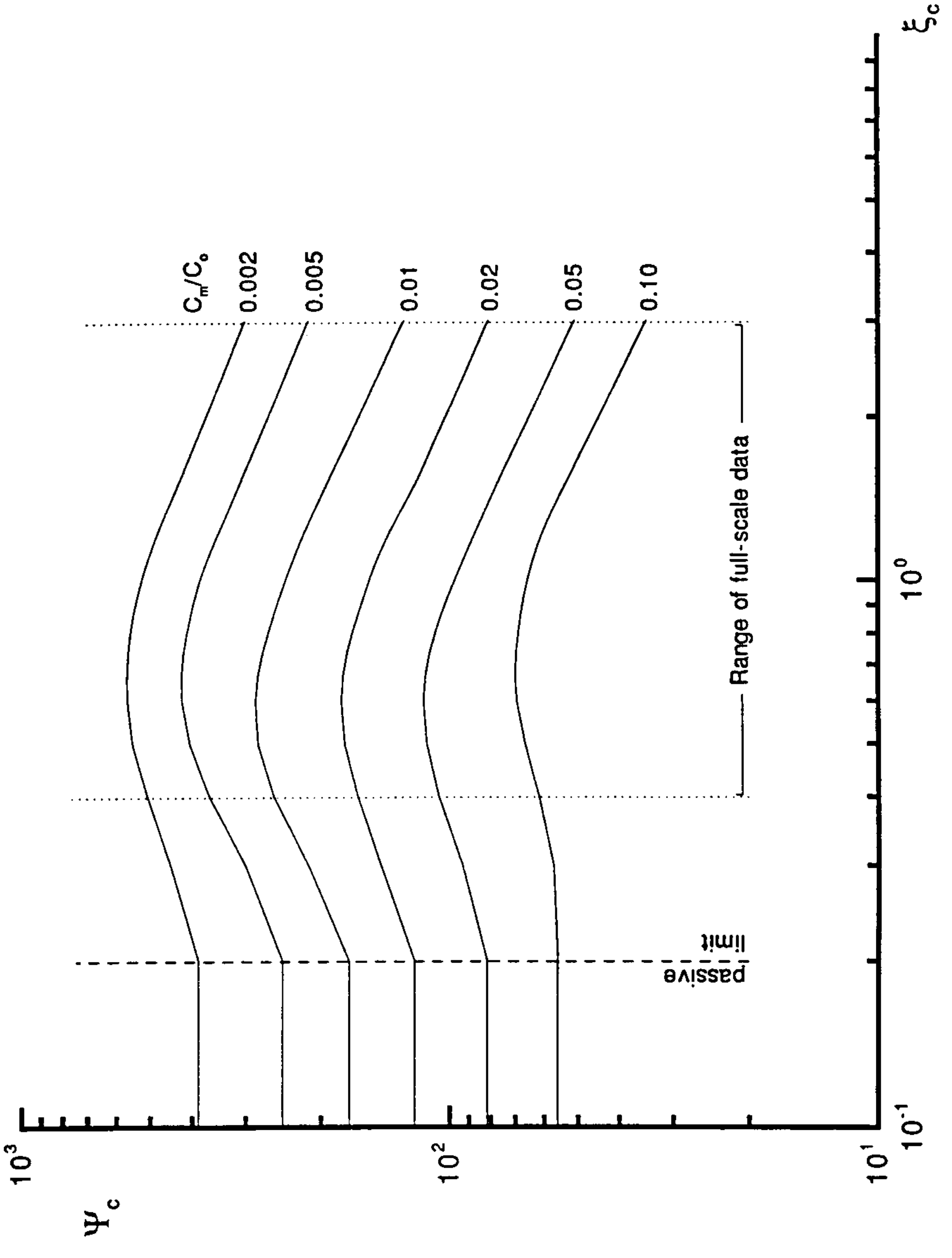
$$\left[\frac{\rho_2-\rho_a}{\rho_a}\right] \frac{g\,(Q_m/\rho_2)}{D\;U_r^3} < 1/6^3$$

where the left-hand side is a Richardson number; therefore, the criteria in Equation 5.4-7 is comparable to other Richardson number-based criteria suggested, for example, by Spicer and Havens (1989) and that $U_r/U_* \simeq 20$ to 30 for typical atmospheric flow fields (where $U_*$ is the friction velocity.)

However, if denser-than-air effects are determined to be important, the method of Britter and McQuaid can be used to determine the downwind extent of a given concentration level ($C_m/C_o$) by use of Figure 5.4-1. For simplicity, the abscissa and ordinate are given as:

$$\xi_c = \left[ \frac{g^2\;(Q_m/\rho_2)}{U_r^5} \left[\frac{\rho_2-\rho_a}{\rho_a}\right]^2 \right]^{1/5} \qquad (5.4\text{-}9a)$$

Figure 5.4-1. Britter-McQuaid (1989) Correlation for Continuous (Plume) Releases



$$\psi_c = \left[ \frac{x^2}{(Q_m/\rho_2)/U_r} \right]^{1/2} \qquad (5.4\text{-}9b)$$

respectively where x is the estimated downwind distance to the concentration level $C_m/C_o$. The choice of $C_m$ should reflect the source temperature correction and the averaging time effect discussed below. Once $C_m/C_o$ is set, Figure 5.4-1 can be used to determine the downwind distance to that ratio; interpolation for intermediate values of $C_m/C_o$ should be done using log-log interpolation (at a fixed $\zeta_c$). For $\zeta_c > 3$, $\xi_c$ should be determined by (linear) extrapolation on the log-log plot in the absence of other information since no field test data exists for $\zeta_c > c$. If the desired $C_m/C_o < 0.002$, the following equation can be used:

$$\psi_c = 22.6 \left[ \frac{C_m}{C_o} \right]^{-1/2} \xi_c^{-1/2} \qquad (5.4\text{-}10)$$

(based on extrapolation and fitting of Britter and McQuaid's Figure 9). If the desired $C_m/C_o < 0.002$ and $1 \geq \xi_c \geq 0.2$, no data exists for this region so Britter and McQuaid make no recommendation. However, the following equation can be used:

$$\psi_c = 22.6 \left[ \frac{C_m}{C_o} \right]^{-1/2} \xi_c^{-1/3} \qquad (5.4\text{-}11)$$

based on simply forcing Equation (5-10) to agree with the passive limit.

Once the distance x is determined, the release duration $T_d$ should be checked to see if steady-state conditions are expected at this distance. If $U_rT_d/x > 2.5$, then the estimate based on a continuous release is valid as recommended by Britter and McQuaid. If $0.6 < U_rT_d/x < 2.5$, then an estimate assuming the release to be instantaneous should also be made, and the greatest estimate for x should be reported. If $U_rT_d/x < 0.6$, then the release should be assumed to be instantaneous.

The effect of averaging time should be taken into account before using Figure 5.4-1 if the desired averaging time is not a long-term average (taken to be 10 minutes). Britter and McQuaid mention that shorter averaging times will produce larger concentrations with factors ranging from 1.4 (based on field-scale data) to 1.6 (based on laboratory data) over the long time-averaged concentrations. If the ratio of 1.4 is used along with a short averaging time of about one second, the following (approximate) power-law relationship would hold:

$$\left[\frac{C_m(10\mathrm{min})}{C_m(t_{av})}\right] = \left[\frac{10\mathrm{min}}{t_{av}}\right]^{-0.05} \qquad (5.4\text{-}12)$$

where $C_m$(10 min) would represent the value of $C_m$ to be used in Figure 5.4-1, and $C_m(t_{av})$ is the value of $C_m$ based on the desired averaging time $t_{av}$ (Britter, 1992).

The effect of temperature should be taken into account before using Figure 5.4-1 if the discharge (depressurized) contaminant temperature is different from ambient; Britter and McQuaid recommend using a value for $C_m$ which reflects the nonisothermal effects as follows:

$$C_m = \frac{C_{ni}}{C_{ni} + T_a(1 - C_{ni})/T_2} \qquad (5.4\text{-}13)$$

where $C_{ni}$ is the nonisothermal concentration (mole fraction), $T_a$ is the ambient temperature (K), and $T_2$ is the discharge (depressurized) contaminant temperature (K).

In summary, the following procedure should be used for continuous (plume) releases:

A. For aerosol releases, two cases must be considered for each release as outlined in Section 5.4.2. Initial conditions for the dispersion calculation for each case are based on Equations 5.4-2 through 5.4-6. Go to Step C.

B. For cold gas releases, two cases must be considered for each release as outlined in Section 5.4.1. Original initial conditions based on release calculations and modified initial conditions from Equation 5.4-1 are used in the dispersion calculation for each case.

C. For each continuous release case:

   a. Check to see if denser-than-air effects are important with Equation 5.4-7. If denser-than-air effects are unimportant, use a passive atmospheric dispersion model.
   b. Modify the desired concentration $C_m$ for averaging time using Equation 5.4.11.
   c. Modify $C_m$ from (b) for source temperature effects using Equation 5.4-12.
   d. With $C_m$ from (c), determine the downwind distance x using Figure 5.4-1 or Equation 5.4-10.
   e. Determine whether the release duration is of sufficient length to establish a steady-state plume at the distance x. As discussed earlier, depending on $U_rT_d/x$, a dispersion calculation for an instantaneous release may also be required.

Example: <u>Chlorine Gas Leak</u>

Consider the example chlorine gas leak discussed in Section 4.2.3. Based on the earlier example, the gas evolution rate $Q_m$ was 1.10 kg/s and discharged at a temperature $T_2$ of 282.5°K; the discharge density $\rho_2$ was 3.059 kg/m$^3$. For a release in 2 m/s winds (at 10 m), determine the downwind distance to 1 ppm based on a 15-minute time average. The ambient temperature and pressure are 293.15°K and 101325 Pa, respectively.

A. Since this is not an aerosol release, Step A is ignored.

B. The discharge temperature $T_2$ is 282.5°K, so heat transfer is probably unimportant since $T_a - T_2$ is not large. For the sake of illustration, though, consider two cases: (1) $\rho_2$ and $T_2$ unchanged; and (2)      = 3.059 kg/m$^3$ (282.5/293.15 = 2.948 kg/m$^3$ and      = 293.15°K.

C. For case 1 ($\rho_2$ = 3.059 kg/m$^3$ and $T_2$ = 282.5°K):

a. The left side of Equation 5.4-7 is 0.959 (with $\rho_a$ = 1.204 kg/m$^3$; D = 0.600 m, using Equation 5.4-8) so denser-than-air effects are expected to be important.
b. Using $t_{av}$ = 15 min in Equation 5.4-11, $C_m$ = 1.020 (1 ppm) = 1 ppm.
c. Using $C_{ni}$ = 1 ppm = 1 x $10^{-6}$ mole fraction in Equation 5.4-12, $C_m$ = 1 ppm.
d. Since $C_m/C_o = 1 \times 10^{-6} << 0.002$, Equation 5.4-10 is used to determine x = 8710 m $\xi_c$ = 1.21; $\zeta_c$ = 20540).
e. For this release to be considered as a steady-state release, $U_rT_dx > 2.5$; so, if $T_d > 10900$ s (182 min) then the release is a continuous plume.

C. For case 2 ($\rho_2$ = 2.948 kg/m$^3$ and $T_2$ = 293.15°K):

a. The left side of Equation 5.4-7 is 1.04 (with D = 0.611 m, using Equation 5.4-8) so denser-than-air effects are expected to be important.
b. As in case 1, using $t_{av}$ = 15 min in Equation 5.4-11, $C_m$ = 1.020 (1 ppm) = 1 ppm.
c. Also in case 1, using $C_{ni}$ = 1 ppm = 1 x $10^{-6}$ mole fraction in Equation 5.4-12, $C_m$ = 1 ppm.
d. Since $C_m/C_o = 1 \times 10^{-6} << 0.002$, Equation 5.4-10 is used to determine x = 8950 m ($\xi_c$ = 1.19; $\Psi_c$ = 20720).
e. For this release to be considered as a steady-state release, $U_rT_d/x > 2.5$; so, if $T_d > 11200$ s

(186 min), then the release is a continuous plume.

Therefore, the reported distance to the 15 minute averaged chlorine concentration is 8950 m (provided the release is of sufficient duration.)

### 5.4.4 Instantaneous (Puff) Releases

To estimate the importance of denser-than-air effects on instantaneous releases, Britter and McQuaid recommend that denser-than-air effects be ignored if:

$$\left[ \frac{g\ (Q/\rho_2)^{1/2}}{U_r^{\,2}} \left[\frac{\rho_2 - \rho_a}{\rho_a}\right]\right]^{1/2} \leq 0.2 \qquad (5.4\text{-}14)$$

where Q is the total amount of material released, $U_r$ is the windspeed at 10 m, $\rho_2$ is the discharge (depressurized) density, and $\rho_a$ is the ambient air density. If denser-than-air effects are determined to be unimportant, standard passive atmospheric dispersion techniques should be applied.

However, if denser-than-air effects are determined to be important, the method of Britter and McQuaid can be used to determine the downwind extent of a given concentration level ($C_m/C_o$) by use of Figure 5.4-2. For simplicity, the abscissa and ordinate are given as:

$$\xi_i = \left[ \frac{g\ (Q/\rho_2)^{1/3}}{U_r^{\,2}} \left[\frac{\rho_2 - \rho_a}{\rho_a}\right]\right]^{1/2} \qquad (5.4\text{-}15a)$$

and

$$\psi_i = x/(Q/\rho_2)^{1/3} \qquad (5.4\text{-}15b)$$

respectively where x is the estimated downwind distance to the concentration level $C_m/C_o$. The effect of temperature should be taken into account before using Figure 5.4-2 if the discharge (depressurized) contaminant temperature is different from ambient using Equation 5.4-12. Because Figure 5.4-2 uses concentration data based on (ensemble) short-term averaged concentrations, taking longer averaging times into account would simply shorten predicted distances to a given concentration level; in the absence of further information, the predicted concentrations will be assumed to apply regardless of averaging time (which, for screening purposes, is a conservative assumption). Once the ratio $C_m/C_o$ is set, Figure 5.4-2 can be used to determine the downwind distance to that ratio; interpolation for intermediate values of $C_m/C_o$ should be done using log-log interpolation (at a fixed $\xi_i$). For $\xi_i > 10$, $\Psi_i$ should be assigned the value of $\Psi_i(\xi_i{=}10)$. If the desired $C_m/C_o < 0.001$, the following equation can be used:

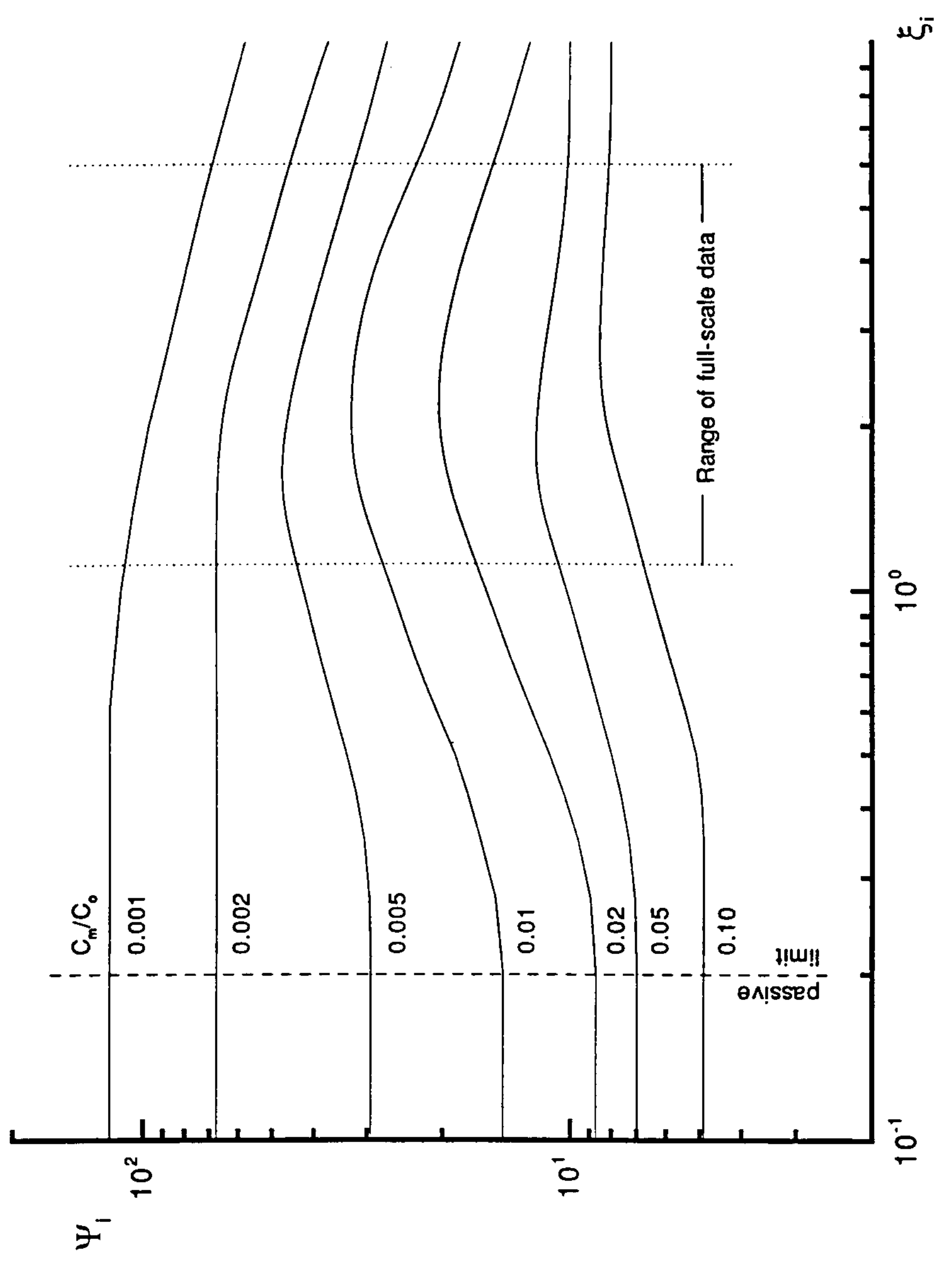
$$\psi_i = 10.2\left[\frac{C_m}{C_o}\right]^{-0.4} \xi_i^{-1/2} \qquad (5.4\text{-}16)$$

(based on extrapolation and fitting of Britter and McQuaid's Figure 12); note that for $\xi_i > 10$, a value of $\xi_i = 10$ should be used in Equation 5.4-16. If the desired $C_m/C_o < 0.001$ and $1 \geq \xi i \geq 0.2$, no data exists for this region so Britter and McQuaid make no recommendation. However, the following equation can be used:

$$\psi_i = 10.2\left[\frac{C_m}{C_o}\right]^{-0.4} \qquad (5.4\text{-}17)$$

based on simply forcing Equation (5-16) to agree with the passive limit.

Figure 5.4-2. Britter and McQuaid (1989) Correlation for Instantaneous (Puff) Releases



In summary, the following procedure should be used for instantaneous (puff) releases:

A. For aerosol releases, two cases must be considered for each release as outlined in Section 5.4.2. Initial conditions for the dispersion calculation for each case are based on Equations 5.4-2 through 5.4-6. Go to Step C.

B. For cold gas releases, two cases must be considered for each release as outlined in Section 5.4.1. Original initial conditions based on release calculations and modified initial conditions from Equation 5.4-1 are used in the dispersion calculation for each case.

C. For each instantaneous release case:

   a. Check to see if denser-than-air effects are important with Equation 5.4-13. If denser-than-air effects are unimportant, use a passive atmospheric dispersion model.
   b. Modify $C_m$ for source temperature effects using Equation 5.4-12.
   c. With $C_m$ from (b), determine the downwind distance x using Figure 5.4-2 or Equation 5.4-15.

Example: <u>Saturated Liquid Chlorine Leak (Reservoir Pressure of $2.586 \times 10^6$ Pa; 10.16 cm hole)</u>

Consider the example chlorine leak discussed in Section 3.2. Based on the earlier example, the evolution rate $Q_m$ was 430 kg/s and the discharge temperature $T_2$ was 239.05°K; the discharge density $\rho_2$ was 19.13 kg/m$^3$. For this example, assume the release came from a "ton" cylinder which was initially half full (approximately 500 kg); in this case, the release duration $T_d$ would be small and the release can be assumed to occur instantaneously (with Q = 500 kg). For a release in 2 m/s winds (at 10 m), determine the downwind distance to 1 ppm based on a 15-minute time average. The ambient temperature and pressure are 293.15°K and 101325 Pa, respectively.

A. Because this is an aerosol release, an initial amount if air is assumed to mix with the contaminant aerosol so that the liquid phase is evaporated and the mixture temperature is raised to the contaminant vapor pressure (239.05°K in this case). First, $z_c$ and $z_a$ are estimated using Equation 5.4-2 as 0.188 and 0.812, respectively (using $C_{pa}$ = 1006 J/kgK). Two cases must be considered: (1)

$_2$ = (101325) (36.8) / ((8314)(239.05)) = 1.876kg/m$^3$ ; an

$\hat{Q}$ = (500) (36.8) / ((0.188) (70.9)) = 1380 kg; and (2)

$_2$ = (101325) (36.8) / ((8314)(239.15)) = 1.530kg/m$^3$ ;

$T_2$ = 293.15°K. $\hat{Q}$ will be the same for both cases. Go to Step C.

C. For case 1 ($\rho_2$ = 1.876 kg/m$^3$; $T_2$ = 239.05°K; Q = 1380 kg):

   a. The left side of Equation 5.4-13 is 3.52 (with $\rho_a$ = 1.204 kg/m$^3$) so denser-than-air effects are expected to be important.
   b. Using $C_{ni}$ = 1 ppm = 1 x $10^{-6}$ mole fraction in Equation 5.4-12, $C_m$ = 1 ppm.
   c. Since $C_m/C_o$ = 1 x $10^{-6}$/0.188 = 5 x $10^{-6}$ < 0.001, Equation 5.4-15 is used to determine x = 6480 m ($\xi_i$ = 3.52; $\Psi_i$ = 717).

C. For case 2 ($\rho_2$ = 1.530 kg/m$^3$; $T_2$ = 293.15°K; Q = 1380 kg):

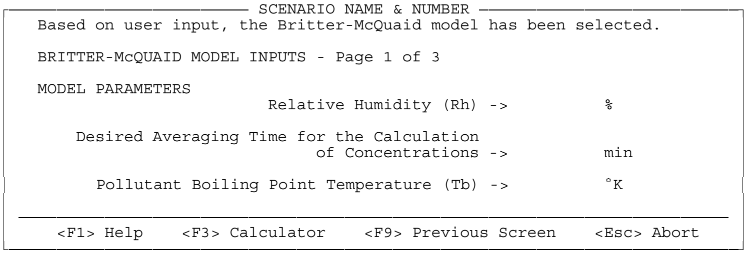
   a. The left side of Equation 5.4-13 is 2.53, so denser-than-air effects are expected to be important.
   b. As in case 1, using $C_{ni}$ = 1 ppm = 1 x $10^{-6}$ mole fraction in Equation 5.4-12, $C_m$ = 1 ppm.
   c. Since $C_m/C_o$ = 1 x $10^{-6}$/0.188 = 5 x $10^{-6}$ < 0.001, Equation 5.4-15 is used to determine x = 7550 m ($\xi_i$ = 2.97; $\Psi_i$ = 781).

Therefore, the reported distance to the 15-minute averaged chlorine concentration is 7550 m.

### 5.4.5 Assumptions in TSCREEN

In the implementation of the Britter-McQuaid model used in TSCREEN, the model calculates concentrations for an array of 9 windspeeds, for the D stability class, at each distance. Then, the model output displays the maximum concentration for each distance and the windspeed at which that concentration occurred.

### 5.4.6 Model Inputs



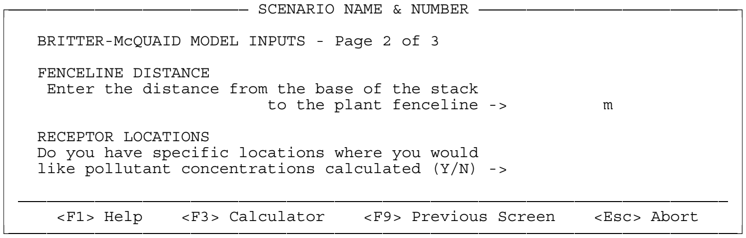
```
                        SCENARIO NAME & NUMBER
  Based on user input, the Britter-McQuaid model has been selected.

  BRITTER-McQUAID MODEL INPUTS - Page 1 of 3

  MODEL PARAMETERS
                          Relative Humidity (Rh) ->         %

      Desired Averaging Time for the Calculation
                               of Concentrations ->         min

        Pollutant Boiling Point Temperature (Tb) ->         °K

    <F1> Help    <F3> Calculator    <F9> Previous Screen    <Esc> Abort
```

MODEL PARAMETERS

1 <u>Relative Humidity (Rh) -</u>
Enter the relative humidity (%).

2 <u>Desired Averaging Time for the Calculation of Concentration (min) -</u>
The averaging time is used by the Britter and McQuaid model to correct for averaging times different from 10 min.

3 <u>Pollutant Boiling Point Temperature ($T_b$) -</u>
Enter the boiling point temperature. This value can be obtained from TSCREEN's chemical database.



```
                        SCENARIO NAME & NUMBER
  BRITTER-McQUAID MODEL INPUTS - Page 2 of 3

  FENCELINE DISTANCE
   Enter the distance from the base of the stack
                        to the plant fenceline ->         m

  RECEPTOR LOCATIONS
  Do you have specific locations where you would
  like pollutant concentrations calculated (Y/N) ->

    <F1> Help    <F3> Calculator    <F9> Previous Screen    <Esc> Abort
```

FENCELINE DISTANCE

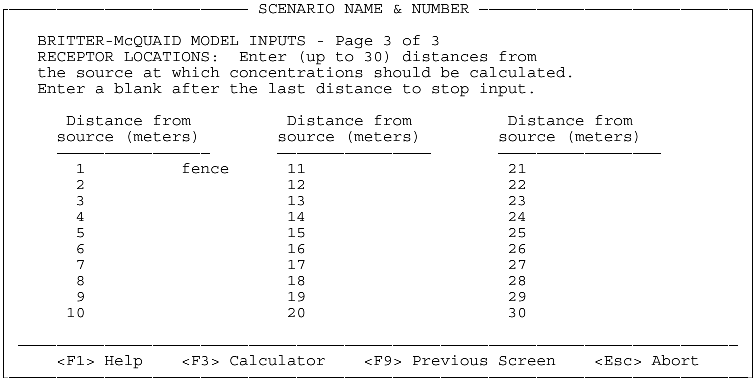
4 <u>Enter the distance from the base of the stack to the plant fenceline (m) -</u>
Enter the distance from the closest edge of the source to the fenceline in meters. The model calculates concentrations only at receptors beyond the fenceline in ambient air.

RECEPTOR LOCATIONS

5 <u>Do you have specific location where you would like pollutant concentrations calculated (Y/N) -</u>
The entry of SPECIFIC LOCATIONS allows for calculating the maximum ground level concentrations at discrete, user-specified distances from the release. TSCREEN will automatically give you maximum ground level concentrations at 30 distances starting at the fenceline. The first 16 distances are in 100 m increments. The next 8 distances are

in 200 m increments, and the remaining 5 distances are in 300 m increments.

- If "Y" is entered, proceed to step 8
- If "N" is entered, TSCREEN runs the Britter-McQuaid model.



```
────────────────────── SCENARIO NAME & NUMBER ──────────────────────

   BRITTER-McQUAID MODEL INPUTS - Page 3 of 3
   RECEPTOR LOCATIONS:  Enter (up to 30) distances from
   the source at which concentrations should be calculated.
   Enter a blank after the last distance to stop input.

      Distance from          Distance from          Distance from
     source (meters)        source (meters)        source (meters)
     ________________       ________________       _________________
       1         fence        11                     21
       2                      12                     22
       3                      13                     23
       4                      14                     24
       5                      15                     25
       6                      16                     26
       7                      17                     27
       8                      18                     28
       9                      19                     29
      10                      20                     30
 ____________________________________________________________________
     <F1> Help    <F3> Calculator    <F9> Previous Screen    <Esc> Abort
```

RECEPTOR LOCATIONS

6 <u>Enter (up to 30) distances from the source at which concentrations should be calculated -</u>
Enter the distance in meters from the release for calculating the maximum ground level concentrations.

- After the user finishes entering distances, TSCREEN runs the Britter-McQuaid model.

### 5.4.7 Model Output

For a complete example of the Britter-McQuaid model ,see Section 4.2.3. (See Appendix E-Running TSCREEN for output options after the model is run.) The following shows the format of the output file that Britter-McQuaid would generate.

```
                                               -  -92
                                                                      :  :
  *** B&M MODEL RUN ***



 INPUTS:
    AMBIENT PRESSURE (ATM)    =
    AMBIENT TEMP (K)          =
    AVERAGING TIME (MIN)      =
    BOILING PT TEMP (K)       =
    DURATION (S)              =
    EMISSION RATE (KG/S)      =
    EXIT TEMP (K)             =
    MASS (KG)                 =
    MOL. WEIGHT (G/G-MOLE)    =
    RELATIVE HUMIDITY (%)     =
    VAPOR FRACTION            =


      ***************************************
      ***   SUMMARY OF B&M MODEL RESULTS  ***
      ***************************************

    MAX CONC      MAX CONC    DIST TO    WIND SPEED
    (UG/M**3)      (PPM)      MAX (M)      (M/S)
    ---------    ---------    -------    ----------


 ***************************************************
 ** REMEMBER TO INCLUDE BACKGROUND CONCENTRATIONS **
 ***************************************************


 **********************************
 ***        B&M DISTANCES      ***
 **********************************


    DIST        CONC            CONC        WIND SPEED
     (M)      (UG/M**3)         (PPM)          (M/S)
   -------    ---------       ---------     ----------
    100.
    200.
    300.
    400.
    500.
    600.
    700.
    800.
    900.
   1000.
   1100.
   1200.
   1300.
   1400.
   1500.
   1600.
   1700.
   1900.
   2100.
   2300.
   2500.
   2700.
   2900.
   3100.
   3300.
   3600.
   3900.
   4200.
   4500.
   5000.



 CALCULATED VALUES:
    DENSITY OF DEPRESSURIZED CONTAMINANT (KG/M**3) =
    DENSITY OF AMBIENT AIR (KG/M**3)               =
    MOLE FRACTION                                  =
    MIN DIST INST (M)                              =
    MAX DIST CNST (M)                              =


 ***** NOTES & DEFINITIONS *****
(a) "inst" refers to an instantaneous release (Section 3.6 of B-M Workbook)
(b) "cnst" refers to a continuous release (Section 3.6 of B-M Workbook)
(c) "MIN DIST INST" is the minimum distance downwind at which the release
    may be treated as instantaneous
(d) "MAX DIST CNST" is the maximum distance downwind at which the release
    may be treated as continuous

 **********************************
 ***     END OF B&M OUTPUT      ***
 **********************************
```

# REFERENCES

Beilstein, 1987: Handbook of Organic Chemistry, Springer-Verlag, New York.

Beychok, M., 1979: Fundamentals of Stack Gas Dispersion, Irvine, CA.

Britter R.E. and J. McQuaid, 1989: Workbook on the Dispersion of Dense Gases, U.K. Health and Safety Executive Contract Research Report No. 17/1988.

Britter, R.E., personal communication, 1992.

Clancey, V.J., 1984: The Evaporation and Dispersion of Flammable Liquid Spillages, in Chemical Process Hazards with Special Reference to Plant Design: Proceedings of the 5th Symposium held at the University of manchester, 1974, Institution of chemical Engineers, London.

Clewell, H.J., 1983: A Simple Formula for Estimating Source Strengths from Spills of Toxic Liquids, U.S. Air Force Report ESL-TR-83-03.

Cox, A. and R. Carpenter, 1980: Further Development of a Dense Vapor Dispersion Model for Hazardous Analysis. Heavy Gas and Risk Assessment, S Hartwig (ed.) D. Reidel Publishing, Dordrecht, Holland.

EMCON Associates, 1982: Methane Generation and Recovery from Landfills, Ann Arbor Science, Ann Arbor, MI.

Environmental Protection Service, 1985: Introduction Manual, Technical Information for Problem Spills (TIPS), Technical Services Branch. Ottawa, Canada

Fauske, H.K. and M. Epstein, 1987: Source Term Considerations in Connection with Chemical Accidents and Vapor Cloud Modeling. Presented at the International Conference on Vapor Cloud Modeling, Center for Chemical Process Safety. New York, NY.

Fingas, M., I. Buist, R. Belore, D. Mackay, and P. Kawamura, 1986: The Input of Spilled Chemicals into the Environment. Hazardous Materials Spills Conference, St. Louis.

Havens, J. and T. Spicer, 1985: Development of an Atmospheric Dispersion Model for Heavier-than-Air Gas Mixtures, U.S. Dept. of Transportation CG-D-23-85.

Hoot, T., R. Meroney, and J. Peterka, 1973: Wind Tunnel Tests of Negatively Buoyant Plumes, EPA 650/3-74-003. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Hunsaker, J. and B. Rightmire, 1947: Engineering Applications of Fluid Mechanics. McGraw-Hill, New York.

Leahey, D. and M. Davies, 1984: Observations of Plume Rise from Sour Gas Flares, Atm. Envir., 18:917-922.

Lees, F.P., 1980: Loss Prevention in the Process Industries, Butterworths, London.

Levenspiel, O., 1977: The Discharge of Gases from a Reservoir through a Pipe, AIChE Journel, 23, 3, pg 402.

Lewitt, E.H., 1953: Thermodynamics Applied to Heat Engines, 5th ed, Sir Isaac Pitman and Sons, London.

List, R., 1968: Smithsonian Meteorological Tables. Smithsonian Institute, Washington, D.C.

Moorehouse, J., and R.J. Carpenter, 1986: Factors Affecting Vapour Evolution Rates from Liquefied Gas Spills, Proceedings I. Chem. E. (N.W.Branch) conference on Refinement of Estimates of the Consequences of Heavy Toxic Vapor Releases.

National Oceanographic and Atmospheric Administration, 1988: ALOHA-Areal Locations of Hazardous Atmosperes, Technical Appendix, Hazardous Materials Response Branch, Seattle, WA.

Pasquill, F., 1976: Atmospheric Diffusion (2nd ed.). John Wiley & Sons, New York.

Perry, R.H., D.W. Green, and J.O. Maloney, 1984: Perry's Chemical Engineer's Handbook, 6th Ed, McGraw-Hill, New York, pp. 5-12 through 5-15.

Petersen, W., 1982: Estimating Concentrations Downwind from an Instantaneous Puff Release, EPA 600/3-82-078. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Sandler, S.I., 1989: Chemical and Engineering Thermodynamics, 2nd ed., John Wiley and Sons, New York.

Spicer, T.O. and J. Havens, 1989: User's Guide for the DEGADIS 2.1 Dense Gas Model, EPA-450/4-89-019. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Spicer, T.O., 1992: Personal communication.

Slade, D., 1968: Meteorology and Atomic Energy, U.S. Atomic Energy Commission (T10-24190).

Thibodeaux, L. and S. Hwang, 1982: Landfarming of Petroleum Wastes - The Modeling Problem, Environmental Progress, 1 (46).

Turner, D., 1970: Workbook of Atmospheric Dispersion Estimates, Office of Air Programs Publication AP-26, U.S. Environmental Protection Agency.

U.S. Environmental Protection Agency, 1985: Compilation of Air Pollutant Emission Factors, Fourth Edition. AP-42, September 1985. And Supplement A, 1986; Supplement B, 1988; Supplement C, 1990; Supplement D, 1991.

U.S. Environmental Protection Agency, 1986: Guideline on Air Quality Models (Revised), EPA-450/2-78-027R. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1987a: Hazardous Waste Treatment, Storage, and Disposal Facilities (TSDF) - Air Emissions Models, Draft Report, U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1987b: Emission Factors for Equipment Leaks of VOC and HAP, EPA-450/3-86-002. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1987c: On-site Meteorological Program Guidance for Regulatory Modeling Applications, EPA-450/4-87-013. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1988a: A Workbook of Screening Techniques for Assessing Impacts of Toxic Air Pollutants, EPA-450/4-88-009. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1988b: Air Emissions from Municipal Solid Waste Landfills - Background Information for Proposed Standardous and Guidelines, Office of Air Quality Planning and Standards (Preliminary Draft). U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1988c: Screening Procedures for Estimating the Air Quality Impact of Stationary Sources, EPA-450/4-88-010. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1989: User's Guide for RVD 2.0 - A Relief Valve Discharge Screening Model, EPA-450/4-88-024. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1990: User's Guide to TSCREEN, A Model for Screening Toxic Air Pollutant Concentrations, EPA-450/4-90-013. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1991a: Guidance on the Application of Refined Dispersion Models for Air Toxics Releases, EPA-450/4-91-007. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1991b: Air Emissions from Municipal Solid Waste Landfills - Background Information for Proposed Standards and Guidelines, EPA-450/3-90-11a. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U.S. Environmental Protection Agency, 1992: User's Guide for the Industrial Source Complex (ISC2) Dispersion Models, Volume II - Description of Algorithms, EPA-450/4-92-008b. U.S. Environmental Protection Agency, Research Triangle Park, NC.

Van Ulden, A. 1974: On Spreading of a Heavy Gas Released Near the Ground, 1st International Loss Prevention Symposium, The Hague/Delft.

Verschueren, K., 1983: Handbook of Environmental Data on Organic Chemicals. Van Nostrand Reinhold Company, New York.

Wallis, G. 1969: One Dimensional Two-Phase Flow, McGraw-Hill, New York.

Webber, D.M., and S.J. Jones, 1987: A Model of Spreading Vaporising Pools, in International Conference on Vapor Cloud Modeling, John Woodward, ed., American Institute of Chemical Engineers, New York.

# APPENDIX A

# EMISSION FACTORS

# APPENDIX A
# EMISSION FACTORS

One alternative for estimating air toxic emissions from sources is through the use of emission factors. Emission factors have been developed for a number of processes and pollutants. Emission factors provide an estimate of emissions as a function of source activity such as process rate or some other operating parameter. Emission factors are intended to been used for making preliminary estimates of toxic air emissions. As such, they represent generic factors whose applicability to a specific source may be questionable. These factors will not likely provide exact estimates of emissions from any particular source. The source of an emission factor must be carefully evaluated to determine whether it is applicable to a particular facility. Emission factors are available for both area and point sources. Some sources of emission factors applicable to air toxics emissions are presented below.

1) U.S. Environmental Protection Agency. Locating and Estimating Air Emissions from (or of) (Source Category or Substance). EPA 450/4-84-007a-q. EPA 450/4-88-004, 450/2-89-001, 450/2-89-002, 450/2-89-006, 450/2-89-013, 450/2-89-021, 450/2-90-009, 450/4-91-029.

EPA has underway a program to compile and publish emission factors for various air toxics. To date, twenty-four reports have been published as part of this program. The substances covered by this series include: acrylonitrile, carbon tetrachloride, chloroform, ethylene dichloride, formaldehyde (revised), nickel, chromium, manganese, phosgene, epichlorohydrin, vinylidene chloride, ethylene oxide, chlorobenzenes, PCBs, POM, benzene, organic liquid storage tanks, coal and oil combustion sources, municipal waste combustors, perchloroethylene and trichloroethylene, 1,3-batadiene, and sewage sludge incinerators and styrene.

2) U.S. Environmental Protection Agency. Survey of (Substance) Emission Sources.

A second series of reports on specific air toxics has been developed by EPA as part of the National Emissions Standards for Hazardous Air Pollutants (NESHAPS) program. The substances covered by this series include: trichloroethylene (EPA 450/3-85-021), perchloroethylene (EPA 450/3-85-017), ethylene oxide (EPA 450/3-014), chloroform (EPA 450/3-85-026), ethylene dichloride (EPA 450/3-84-018), methylene chloride (EPA 450/3-85-015), and carbon tetrachloride (EPA 450/3-85-018).

3) U.S. Environmental Protection Agency. XATEF-Crosswalk/Air Toxic Emission Factors Database.

The database is available from the EPA Office of Air Quality Planning and Standards, Technology Transfer Network (TTN). Files may be downloaded by dialing (919) 541-5742. [There is no charge for access.] This database management system presents emission factors of air toxic pollutants for a variety of sources with varying activity levels. This database management system is updated and expanded periodically. The factors are associated with pollutant names and CAS numbers, process descriptions and SIC codes, emission source descriptions and SCC codes, notes on the derivation of the factors and on control measures associated with the factors, and references. The emission factors can be used to obtain quick, rough estimates of air toxic emissions. More detailed data on the emission sources can be obtained from the Notes and References Sections listed in the emission factors tables. The primary limitation of using just the emissions factors listed in this compilation is that their accuracy in application to a given source is not known. More accurate emissions estimates may require evaluation of the application of available test data to specific source characteristics. Otherwise, factors determined by compiling extensive source test results using EPA Reference Methods are reported in AP-42. Toxic components of emissions can be determined using SPECIATE database management system (see above).

4) U.S. Environmental Protection Agency. Compilation of Air Pollutant Emission Factors, Fourth Edition. AP-42, September 1985. And Supplement A 1986, Supplement B 1988; Supplement C, 1990; Supplement D, 1991.

Another tool for estimating air toxic emissions involves the use of VOC/PM factors presented in AP-42 and species profiles in SPECIATE database management system. AP-42 contains emission factors for total VOC and PM rather than for a single chemical compound. These factors can be used with profiles contained in SPECIATE to estimate the releases of specific toxic compounds based on the total amount of VOC or PM released from a source. SPECIATE shows the percent by weight and percent by volume of specific chemicals in emissions from specific chemicals in emissions from specific processes. Speciation factors are used to estimate emissions of air toxics from emission factors or estimates of total VOC or PM. Both volumes are similarly organized with speciation data presented by source category and by Source Classification Codes (SCC). Species profiles for VOCs and PM are for generic sources and may not be representative of emissions from an individual facility.

SPECIATE is updated periodically.

5) U.S. Environmental Protection Agency. Fugitive Emission Sources of Organic Compounds - Additional Information on Emissions, Emission Reductions, and Costs. EPA-450/3-82-010, 1982.

This document contains the data and methodologies which EPA believes most accurately characterize average synthetic organic chemical manufacturing industry equipment leak emission rates of VOC, effectiveness of control techniques, and control costs for selected equipment used in the processing of organic chemicals. The emission factors (on Page 1-4) can be used to estimate VOC emissions from any industrial plant which has the selected equipment and handles organic chemicals.

# APPENDIX B

# ESTIMATING SELECTED PHYSICAL PROPERTIES OF MIXTURES

# APPENDIX B
# ESTIMATING SELECTED PHYSICAL PROPERTIES OF MIXTURES

This appendix describes methods to estimate selected physical properties of mixtures using pure component physical properties. These mixture properties include:

| | |
|---|---|
| $C_p$ | gas (contaminant) heat capacity (J/kg °K) |
| $C_{pl}$ | liquid (contaminant) heat capacity (J/kg °K) |
| M | contaminant molecular weight (g/g-mole) |
| $T_c$ | pseudo-critical temperature (°K) |
| $\lambda$ | contaminant latent heat of vaporization (J/kg) |

For each of these mixture fluid properties, the corresponding fluid property for each of the mixture constituents is required. In addition, the mixture composition is required; for some calculations, the mixture composition expressed as mole fractions is required, while for other calculations, the mixture composition expressed as mass fractions is required. Because the mixture molecular weight is required when converting from mass to mole fractions, this calculation is outlined first. The calculation of mixture heat capacity and latent heat of vaporization is discussed together because these calculations all require that the mixture composition be specified as mass fractions.

## Mixture Molecular Weight

The mixture molecular weight M (g/g-mole) is calculated using mixture mass fractions as:

$$M = \left( \sum_C \omega_i / M_i \right)^{-1} \qquad \text{(B-1)}$$

where $\omega_i$ is the mass fraction of species i, $M_i$ is the molecular weight of species i (g/g-mole), and the summation is over all C components.

Using mixture mole fractions, the equation for mixture molecular weight is:

$$M = \left( \sum_C z_i \; M_i \right) \qquad \text{(B-2)}$$

where $z_i$ is the mole fraction of species i. Conversions between mass and mole fractions can be made using:

$$\omega_i M = z_i M_i \qquad \text{(B-3)}$$

for each of the i components. So, if mass fractions are known and mole fractions are desired, Equation (B-1) can be used to calculate the molecular weight, and Equation (B-3) can be used to calculate the mole fractions for each component. And, if mole fractions are known and mass fractions desired, Equation (B-2) can be used to calculate the molecular weight, and Equation (B-3) can be used to calculate the mass fractions for each component.

**Pseudo-Critical Temperature**

The equation to determine pseudo-critical temperature $T_c$ is:

$$T_c = \left( \sum_C z_i \; T_{c,i} \right) \tag{B-4}$$

where $z_i$ is the mole fraction of species i and $T_{c,i}$ is the temperature of species i.

**Mixture Heat Capacity and Latent Heat of Vaporization**

The equations to determine mixture (gas and liquid) heat capacities ($C_p$ and $C_{pl}$) and latent heat of vaporization ($\lambda$) are based on a mass-fraction weighted contribution of each pure component property. So, the equation to determine the (mixture) gas-phase contaminant heat capacity $C_p$ is:

$$C_p = \left( \sum_C \omega_i \; C_{pi} \right) \tag{B-5}$$

where $\omega_i$ is the mass fraction of species i and $C_{pi}$ is the pure component gas-phase heat capacity of species i. Likewise, the equation to determine the (mixture) liquid-phase contaminant heat capacity $C_{pl}$ is:

$$C_{pl} = \left( \sum_C \omega_i \; C_{pli} \right) \tag{B-6}$$

where $C_{pli}$ is the pure component liquid-phase heat capacity of species i. Finally, the equation to determine the (mixture) latent heat of vaporization $\lambda$ is:

$$\lambda = \left( \sum_C \omega_i \; \lambda_i \right) \tag{B-7}$$

where $\lambda_i$ is the pure component heat of vaporization of species i.

# APPENDIX C

# SELECTED CONVERSION FACTORS

# APPENDIX C
# SELECTED CONVERSION FACTORS

## Area

$1\ m^2 = 10^4\ cm^2$
$1\ ft^2 = 0.0929\ m^2$
$1\ \text{hectare} = 10^4\ m^2$
$1\ \text{acre} = 4046.86\ m^2$

## Concentration

conversions with ppm by volume:

$\frac{mg}{m^3} \cdot \frac{24.04}{M_w}$ = ppm by vol (20°C)

$\frac{mg}{m^3} \cdot 0.8347 \times 10^{-6}$
= ppm by wt

$\frac{mg}{m^3} \cdot 62.43 \times 10^{-9}$
$= lb_m\ 1\ ft^3$

for ideal gases:

vol % x 10 = ppm by vol
vol fraction x $10^6$ = ppm by vol

## Energy or Work

1 J = N · m
= $10^7$ ergs
= $10^7$ dyne · cm
= 0.23891 g-cal
= 0.7373 ft-$lb_f$
= $9.486 \times 10^{-4}$ BTU
1 ft-$lb_f$ = 0.0012861 BTU
= 1.3562 J
= $1.3562 \times 10^7$ ergs
= 0.32396 g-cal
1 cal(g) = $3.9685 \times 10^{-3}$ BTU
1 BTU = $1.0543 \times 10^{10}$ ergs
= 1054 Joules $^-$(N-m)

## Flow

$1\ m^3/h = 3600\ m^3/s$

## Force

1 N = 1 kg · m/$sec^2$
= $10^5$ dynes
= 0.2248 $lb_f$
1 dyne = 1 g · cm/$sec^2$
= $10^{-5}$ N
= $2.248 \times 10^{-6}$ $lb_p$
1 $lb_f$ = 4.448 N
= $4.448 \times 10^5$ dynes

## Gas Constant

PV = nRT
$M_{wair}$ = 29(79% $N_2$, 21% $O_2$)

| | |
|---|---|
| 8314.0 | $m^3$·Pa/kg-mole·°K |
| 0.08314 | bar·liters/g-mole·°K |
| 0.08206 | $m^3$·atm/kg-mole·°K |
| 0.08206 | liter·atm/g-mole·°K |
| 62.36 | l·mm Hg/g-mole·°K |
| 0.7302 | $ft^3$·atm/lb-mole·°R |
| 10.73 | $ft^3$·psia/lb-mole·°R |
| $8.314 \times 10^{-3}$ | J/kg-mole·°K |
| 8.314 | J/g-mole·°K |
| 1.987 | cal/g-mole·°K |
| 1.987 | BTU/lb-mole·°R |
| 5.467 | gal·atm/lb-mole °R |

1 gmole gas occupies
22.41 at 0°C
1 lb-mole gas occupies
359 $ft^3$ at 0°C
1 lb-mole gas occupies
380 $ft^3$ at 60°F

## Heat Rate

1 cal/s = $1.102 \times 10^{-6}$ BTU/h

## Length

1 m = 100 cm
= 1000 mm
= 39.37 in
= 3.2808 ft

= 1.0936 yards
= 0.0006214 mils
= $10^6$ microns ($\mu$)
= $10^{10}$ angstroms (Å)
1 ft = 12 in
= ⅓ yd
= 0.3048 m
= 30.48 cm
1 in = 2.540 cm

### Mass

1kg = 1000g
= 0.001 metric tons
= 2.20462 lbm
= 35.27392 oz

$1lb_m$ = 16 oz
= 5 x $10^{-4}$ tons
= 453.593 g
= .453593 kg

### Mass Release Rate

1 g/s = 7.9367 lb/hr
1 t/yr = 3.16 x $10^{-2}$ g/s
1 t/dy = 11.57 g/s

### Power

1 w = 1 J/sec
= 14.34 g-cal/min
= 1.341 x $10^{-3}$ hp
= 0.7376 ft-$lb_f$/sec

### Pressure

1 atm = 1.1325 x $10^5$ $N/M^2$
= 1.01325 x $10^5$ Pa
= 1.01325 x bars
= 1.01325 $dynes/cm^2$
= 760 mm Hg
= 29.9212 in Hg
= 10.33 m $H_2O$
= 33.9 ft $H_2O$
= 14.696 psi
1 millibar = 1000 $dynes/cm^2$
1 mm Hg = 1333.224 $dynes/cm^2$
1 $lb/in^2$ = 68,947.6 $dynes/cm^2$
1 in Hg = 33,863.9 $dynes/cm^2$
1 Pascal = 10 $dynes/cm^2$

### Temperature

9/5°C + 32 = °F
°F + 460 = °R
°C + 273.6 = °K

### Volume

1 $m^3$ = 1000 liters
= $10^6$ $cm^3$
= $10^6$ m 1
= 35.3145 $ft^2$
= 61, 023 $in^3$
= 220.8 imperial gal
= 264.17 gallons
= 1056.68 quarts
1 $ft^3$ = 1728 $in^3$
= 0.028317 $m^3$
= 28.317 liters
= 28,317 $cm^3$
= 7.4805 gallons
1 bbl = 42 gallons
= 158.99 liters
1 liter = $10^3$ $cm^3$
1 gallon = 3.785 $cm^3$

## Conversion Calculations

1. To convert from µg/m$^3$ to parts per million (ppm), use the following:

$$\text{concentration(ppm)} = \text{concentration}(\mu g/m^3)\left(\frac{T_0}{T_a}\right) 0.0245/M_w \quad \text{(C-1)}$$

where: $T_0$ = 273.15 (°K)
$T_a$ = ambient temperature (°K)
$M_w$ = molecular weight (g/g-mole)

Equation (C-1) is simplified in TSCREEN by assuming $T_0/T_a=1$.

2. To convert J/kg to cal/g-mole use the following:

$$J/kg\ (M_w/4184) = cal/g\text{-}mole \quad \text{(C-2)}$$

# APPENDIX D

# AVERAGING PERIOD CONCENTRATION ESTIMATES

# APPENDIX D
# AVERAGING PERIOD CONCENTRATION ESTIMATES

The purpose of this appendix is to provide some simplified techniques for converting concentrations calculated by the models to different averaging times. Methods presented are applicable to ground-level and elevated emissions of passive gases and particulate matter.

- Instantaneous Estimates

For computing ground level concentrations from an instantaneous surface release for a given stability class and sampling time, the average concentration over sampling time $\tau$ can be expressed as some fraction of the peak concentration.

$$\bar{\chi}_\tau = \chi_p \times F \qquad \text{(D-1)}$$

where:

$\bar{\chi}_\tau$ is the average concentration for a given sampling time $\tau$,
$\tau$ is the sampling time, i.e. 5 min., 1 hour etc., (expressed in seconds)
$\chi_p$ is the instantaneous peak concentration.
F is the correction factor for sampling time, which always has a value less than or equal to one.

The correction factor F can be computed using the procedure given by Petersen, 1982 for the averaging times not provided in TSCREEN.

The concentration at a given receptor location ranges from zero to a peak value as the puff moves towards the receptor. The peak instantaneous concentration is always assumed to occur at time t when the center of the puff is at the receptor location. If the growth of the puff is small as the puff passes over the receptor, then the peak average concentration for sampling time $\tau$ at a particular location occurs during the time period $t - \tau/2$ to $t + \tau/2$.

- Continuous Estimates

To obtain the estimate of the maximum concentration for a longer averaging time, multiply the 1-hour maximum concentration by the given factor:

| Averaging Time | Multiplying Factor |
|---|---|
| 3 hours | 0.9 (±0.1) |
| 8 hours | 0.7 (±0.2) |
| 24 hours | 0.4 (±0.2) |
| annual | 0.08 (±0.02) |

The numbers in parentheses are recommended limits to which one may diverge form the multiplying factors representing the general case.

For example, if aerodynamic downwash or terrain is a problem at the facility, or if the release height is very low, it may be appropriate to increase the factors up to the limits specified in parentheses. Conversely, if the stack is relatively tall and there are no terrain or downwash problems, it may be appropriate to decrease the factors. For averaging times in between the values listed above, use the multiplying factor for the shorter averaging time. For example, if a 4-hour average concentration is needed, use the multiplying factor for the 3-hour averaging time (0.9).

To obtain the estimated maximum concentration for a shorter averaging times between 30 and 60 minutes, use the 1-hour maximum concentration. For averaging times less than 30 minutes use the following equation:

$$C_t = C_{1-hr}\left(\frac{60min}{t}\right)^{.2} \tag{D-2}$$

where: $t \le 30$ minutes

TSCREEN will present a menu containing these averaging times and the 15 and 30 minute averaging times after the SCREEN model has been run. The user may select one or more of these maximum concentrations calculated by the model. The new concentrations will appear at the end of the SCREEN model output.