RISK-INTEGRATED
RISC
SOFTWARE FOR CLEAN-UPS

RISC$_4$

User's Manual

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bp

FORWARD

BACKGROUND

In 1993, BP made a business decision in the U.S. to develop a standardized approach for conducting soil and groundwater risk assessments across all ‘downstream’ activities (service stations through refineries). The rationale was that the company needed to ensure that the latest thinking on fate and transport, exposure, statistical analyses and toxicological criteria were adopted and applied uniformly its businesses. It would also help ensure that BP spoke with a consistent voice when approaching regulators and the community on this vital issue.

Eventually it became clear that a software package containing embedded fate and transport models with intuitive user inputs offered the most convenient and flexible means of implementing this objective. This would enable the process to be readily standardized, communicated and transferred, while still allowing a risk application to be individually tailored to the regulatory regime of the particular business or country. By developing the code in-house, BP would also be able to rapidly adopt new algorithms or approaches (e.g. indoor air models), thus keeping the process *evergreen*.

Versions 1.0 and 2.0 of the code were released in January, 1994 and August, 1995, respectively, with the former pre-dating the publication of the ASTM standard *Risk-Based Corrective Action Applied at Petroleum Release Sites*, commonly known as RBCA. Version 3.0, released in September, 1997, was a major upgrade that allowed *back-calculations* to be performed, i.e. soil and groundwater clean-up targets to be calculated for an input value of acceptable risk.

While similar to the *RBCA Toolkit* marketed by Groundwater Services Inc., RISC is more functional, flexible and user-friendly. The major differences are:

- RISC has a more intuitive graphical interface

- RISC allows for pathway, compound and receptor additivity
- The fate and transport models in RISC can be used in the presence of phase-separated product
- There is a vadose zone model in RISC
- The groundwater models are transient
- Probabilistic (Monte Carlo) exposure capabilities are provided in RISC
- RISC includes a critical pathway - indoor showering - missing in the *Toolkit*

VERSION 4.0 NEW FEATURES

Version 4.0 of RISC has new features that give it even greater flexibility in assessing risk for the following scenarios:

- Irrigation pathways, i.e. water used for gardening but not for indoor usage
- Vegetables grown in contaminated soil
- Two new vapor models , where the vapors are allowed to biodegrade during transport through the unsaturated zone
- Models for surface water and sediment contamination from impacted groundwater and direct comparison with relevant national standards for these media
- The use of groundwater MCLs (maximum concentration levels) and surface water concentrations in addition to acceptable risk levels as the criteria for back-calculating clean-up targets
- The ability to calculate a site-specific target level (SSTL) for a TPH mixture using the site-specific measured concentrations of the TPH fractions detected in the soil

It is felt that Version 4.0 provides the latest and most complete package for calculating risk to human health and surface water. This version has been peer-reviewed by Arcadis, Geraghty and Miller in Cambridge, UK. Their review is included in Appendix R.

RISC DISTRIBUTION AND HELP DESK

BP is distributing the software and manual to all its U.S. and international affiliates who, in turn, are free to transfer it without charge to their regulators and risk consultants. The software is not proprietary however, and can be purchased and downloaded by third parties over the Internet at the web site, www.groundwatersoftware.com, for $450 (USD). Additional charges will apply if the recipient wants the Internet provider to supply a hard copy of the manual.

All recipients of the software should periodically check the web site, www.bprisc.com, to download upgrades related to bug fixes or minor improvements to the code. The downloads on this web site are functional only to existing software users.

Finally, any problems with the manual or software, including questionable output or data interpretation issues, should be directed to the software developer, Lynn Spence. Her details are as follows:

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Overview and Getting Started

1.1 INTRODUCTION

1.1.1 Background

BP’s Risk-Integrated Software for Cleanups (RISC) has been developed to assist in the evaluation of potential human health risks from contaminated sites. RISC is a Windows based software program that can be used to estimate the potential for adverse human health impacts (both carcinogenic and non-carcinogenic) from fourteen exposure pathways. New additions to this version allow the user to evaluate ecological risk by using surface water models and water quality and sediment criteria databases. The software contains vadose zone, saturated zone, and air fate and transport models for estimating receptor point concentrations.

The reader should note that throughout this document the term “risk” will be used to refer to the estimated potential for adverse human health impacts, for both carcinogenic and non-carcinogenic compounds. For some, this is a departure from a more narrow use of the term “risk”, where it sometimes only refers to the probability of developing cancer as a result of exposure to a chemical or group of chemicals.

1.1.2 Uses of this Software

There are at least four broad applications for the RISC software. RISC can be used to (1) estimate human health risk from exposure to contaminated media, (2) estimate risk-based clean-up levels in various media, (3) perform simple fate and transport modeling, and (4) evaluate potential ecological impacts to surface water and sediment. These four different applications are discussed in the following sections.

1.1.2.1 Human Health Risk Assessment

Human health risk assessment can be defined as the characterization of the potential adverse effects on human life or health. Calculating risk is sometimes called the “forward calculation” whereas calculating clean-up levels is called the “back calculation”.

US EPA’s Risk Assessment Guidance for Superfund, or the “RAGS” manual (US EPA, 1989), characterize the risk assessment process by dividing it into four basic steps:

1) Data Collection and Evaluation
    - Gather and analyze relevant site data
    - Identify potential chemicals of concern (CoC’s)
2) Exposure Assessment
    - Analyze contaminant releases
    - Identify exposed populations
    - Identify potential exposure pathways
    - Estimate exposure concentrations for pathways
    - Estimate contaminant intakes for pathways
3) Toxicity Assessment
    - Collect qualitative and quantitative toxicity information
    - Determine appropriate toxicity values
4) Risk Characterization
    - Characterize potential for adverse health effects to occur
    - Estimate cancer risks
    - Estimate non-cancer hazard quotients
    - Evaluate uncertainty
    - Summarize risk information

The RISC software can be used for steps 2 through 4 of the risk assessment process. It is assumed that Step 1 has already been completed, i.e. the site has been characterized as to the chemicals present, type of contaminated media, etc. Usually the user will want to pare down the total list of chemicals found by evaluating the list using a concentration-toxicity screen. This process (described in detail in RAGS) identifies the chemicals that currently pose the greatest share of the risk.

The RAGS manual states that specific objectives of the risk assessment process are to:

- provide an analysis of baseline risks and help determine the need for action at sites;
- provide a basis for determining levels of chemicals that can remain onsite and still be adequately protective of public health (section 1.1.2.4);
- provide a basis for comparing potential health impacts of various remedial alternatives; and
- provide a consistent process for evaluating and documenting public health threats at sites.

The RISC software is a powerful, flexible tool that can be used for any of the above objectives. The reader is referred to the RAGS manual (US EPA, 1989) for more detailed information on each step of the risk assessment process.

1.1.2.2 Risk-Based Clean-up Levels

Risk-Based Corrective Action (RBCA) is a decision-making process for assessment and response to subsurface contamination, and is based on protection of human health and environmental resources. One of the steps in RBCA is to calculate clean-up levels, or concentrations of contaminants that pose an acceptable risk left in place (the back-calculation). The guidelines for RBCA are published in ASTM E1739-95, Standard Guide for Risk-based Corrective Action Applied at Petroleum Release Sites.

The RBCA process was developed as a way to allocate limited resources (time, money, regulatory oversight, etc.) to multiple release sites in a way that allows innovative and cost-effective decision making while ensuring that human health and environmental resources are protected. In order to meet that goal, the process emphasizes the following:

- it integrates site assessment, remedial action selection and site monitoring so the approach is streamlined, targeted and consistent;
- site assessment activities are focused on collecting information needed to make risk-based corrective action decisions; and
- these corrective action decisions are based on site-specific factors and compliance points directed toward cost-effective alternatives that have a high probability of achieving an appropriate reduction in risk.

The RBCA process involves a tiered approach to data collection and evaluation. In general, Tier 1 of the RBCA process involves an initial site assessment and classification of the site based on conservative risk-based screening levels (RBSLs) that are not site-specific. Tiers 2 and 3 involve evaluating the site using more site-specific information (e.g., depth to groundwater, infiltration rate, etc.) and/or evaluating alternate compliance points (locations of exposure). Tier 3 is likely to involve more complex analysis such as detailed site assessment, probabilistic evaluations, and sophisticated chemical fate and transport models.

The RISC software has an Excel spreadsheet (TIER1.XLS) that can be used as a screening tool. The spreadsheet can be used "as is" for a Tier 1 look-up table or the user may enter site-specific data and for a simple Tier 2 analysis. The spreadsheet contains all of the chemicals in the RISC software and is based on the equations presented in the ASTM E1739-95 appendix. It also contains a few additional models that are not presented in the RBCA example in ASTM E1739 but which are needed for many common risk scenarios. The additional models are: Johnson and Ettinger (1991) indoor air model, Domenico (1987) model for groundwater, and Green-Ampt (1911) model for considering biodegradation of dissolved chemicals in the vadose zone. The input values in the spreadsheet are customizable so that multiple RBSL tables can be generated (e.g., different soil types) and saved under different filenames. Note that the RISC spreadsheet may not conform with the user's specific regulatory guidance but it is useful as a screen and in some cases may be updated to conform with many US state policies. The spreadsheet is not directly linked with the RISC software.

The RISC software contains fate and transport models that may be used to develop more site-specific clean-up levels. These models are normally applicable to a Tier 2 analysis under RBCA. Probabilistic exposure evaluations are possible using RISC with the Monte Carlo analysis option. This would nominally fall into a Tier 3 analysis, although a user can readily implement the Monte Carlo approach using a provided default set of distributions for the exposure parameters.

The RBCA process is not limited to a particular class of compounds, even though the ASTM E1739-95 emphasizes application of the RBCA process to sites with petroleum releases. US EPA's Soil Screening guidance (US EPA, 1996) has been developed using a risk-based approach similar to RBCA. Many U.S. states are adopting RBCA-type approaches for a wide variety of programs, not just the underground storage tank (UST) programs.

1.1.2.3 Fate and Transport Modeling

The fate and transport models in RISC are designed to be used for estimating receptor point concentrations as part of a risk assessment. The models use average annual data and are one-dimensional as far as flow regimes. The groundwater models simulate three-dimensional dispersion. These type of models are not applicable for engineering design problems, such as designing extraction wells, or for complex hydrogeological flow regimes. They can, however, be useful for evaluating several scenarios besides estimating receptor point concentrations as part of a risk assessment. Some of the questions that can be evaluated are:

- What is the maximum future concentration expected at a receptor location?
- How far downgradient will a groundwater plume stabilize (reach equilibrium in terms of its length) if degradation is at rate *x*? (The model must be run in an iterative fashion..)
- Is a more sophisticated model needed? These models can serve as a "first cut" to see whether it is necessary to go to more complex codes.
- How long will it take for the contaminants to reach groundwater? What is the estimated loading rate to groundwater?
- How long until the soil source depletes?

RISC includes the following embedded chemical fate and transport models:

- Leaching from vadose zone soil source to groundwater;

- Dispersion, advection, retardation and degradation of groundwater as it moves in an aquifer;
- Saturated soil source at the water table impacting groundwater;
- Emissions from soil to outdoor and indoor air (including models considering biodegradation);
- Emissions from groundwater to indoor air; and
- Sediment partitioning and surface water mixing models that can be linked with the groundwater model.

The models listed above may be linked together as well. For example, the saturated soil source model (at the water table) can be linked with the groundwater model and then used to estimate volatile emissions to indoor air.

1.1.2.4 Surface Water and Sediment Quality Criteria

Version 4.0 of RISC has a large surface water and sediment criteria database containing criteria several different countries. The database contains fresh water and marine surface water criteria from the following sources:

- United States Environment Protection Agency Ambient Water Quality Criteria
- United Kingdom Environmental Quality Standards (statutory and proposed)
- Australia and New Zealand Environment and Conservation Council (ANZECC) Guidelines for the Protection of Aquatic Ecosystems
- European Commission Water Quality Objective
- Canadian Council of Ministers for the Environment Freshwater Aquatic Life Guideline

The sediment criteria in the database is from the National Oceanographic and Atmospheric Administration (NOAA). The criteria listed above were chosen because they are considered “gold standards” in their respective countries. In RISC, potential surface water concentrations can be estimated using the models and then the concentrations can be compared with the criteria listed above.

In addition to the “gold standards” used within RISC, there is an Excel spreadsheet available through the “Water Quality” button in the “Supplemental Spreadsheet

Tools" area on the main screen that contains surface water and sediment criteria from many additional sources. It is anticipated that these will need to be updated periodically as the standards are revised.

1.1.3 Overview of Features

The RISC software includes many features to assist in performing and presenting risk assessments or the results of fate and transport models. Version 4.0 of RISC allows the user to:

- Follow the ASTM tiered approach by utilizing a spreadsheet based on the ASTM algorithms for Tier 1, the embedded fate and transport models in RISC for Tier 2, and the Monte Carlo option in RISC for Tier 3;
- Choose chemicals of concern from a standard library of 86 chemicals; users may also add or delete chemicals from the library and alter the physical, chemical, and toxicological properties of each;
- Perform calculations for two different exposure scenarios (with up to fourteen exposure pathways each) simultaneously (e.g. calculations for both residential and industrial scenarios can be performed at the same time);
- Determine cumulative risks from two different exposure scenarios, as might be the case when the user wants to sum the risks for the scenario where a resident is exposed during both childhood and adulthood;
- Estimate exposure point water and air (both indoor and outdoor) concentrations using predictive chemical fate and transport models;
- Allow for additivity of pathways and compounds for either a forward calculation of risk or back calculation of cleanup levels;
- Use an embedded tool to estimate average, 95th UCL, and weight-averaged concentrations for a set of parameter values; and
- Print or save tables, charts, and figures.

New features in Version 4.0 of RISC allow the user to:

- Estimate human health risk from "irrigation pathways" for groundwater used outdoors but not supplying indoor uses;
- Estimate human health risk from ingestion of vegetables grown in contaminated soil or irrigated with contaminated groundwater;
- Use surface water mixing models to estimate potential impacts to surface water and sediments from contaminated groundwater;

- Compare modeled surface water and sediment criteria with regulatory standards from around the world;
- Consider degradation in two new vapor models; and
- Calculate clean-up levels in soil and groundwater using MCLs (maximum concentration levels) or user-supplied concentrations in groundwater or surface water as targets (as opposed to risk-based calculations).

1.1.4 Organization and Scope of this Report

This User's Manual gives instructions on how to use RISC and discusses the technical details including the equations used to estimate risk, the fate and transport models included in the software, and the chemical database.

The organization of this User’s Manual mimics the organization and flow of the RISC software; specifically:

- Section 1.2 guides the user through software installation, system requirements, and general operating instructions;
- Chapter 2 describes the RBCA Tier 1 Microsoft Excel® spreadsheet;
- Chapters 3 through 8 discuss how the software can be used to perform risk assessment calculations and determine cleanup levels;
- Chapter 9 describes various output and summary options;
- Chapter 10 provides three detailed examples demonstrating how the models are used;
- Chapter 11 contains the chemical database and the surface water and sediment criteria databases; and
- The appendices provide brief descriptions of each predictive model, the accompanying RBCA Tier 1 spreadsheet, and some input considerations for Monte Carlo analyses.

1.2 GETTING STARTED

This section is divided into three sections: hardware and software requirements, installation instructions, and general instructions on using the software.

1.2.1 Hardware and Software Requirements

The computer hardware requirements for this software are:

- IBM 486 or compatible (or a PowerMac)
- 8 MB RAM
- 12 MB hard disk space

The software requirement is:

- Microsoft Windows® 95, 98, 2000, or NT

The following software is needed for accessing the optional RBCA Tier 1 spreadsheet and the complete Water Quality Database:

- Microsoft Excel® 5.0 or 7.0 (for optional spreadsheets only)

RISC can be run without Excel, however this will prevent the user from displaying the RBCA Tier 1 table or accessing the full surface water and sediment criteria databases.

1.2.2 Installation Instructions

1.2.2.1 From a Single File (from internet)

The user must save the file in a directory on their hard drive. The software can then be installed by double-clicking on the file in the Windows Explorer. At that point the user will be prompted for a directory to contain the RISC files.

1.2.2.2 From the Installation CD

To install the software from the CD to a Windows computer the user must perform the following steps:

Step 1 Insert the CD into the CD-ROM drive. If the installation package does not run automatically at this point proceed with steps 2 through 4.

Step 2 Select Run from the *Start* menu. The *Run* dialog will appear.

Step 3 In the *Open* text field, type **D:\Install** (substitute the correct letter of your CD-ROM drive if it is not D).

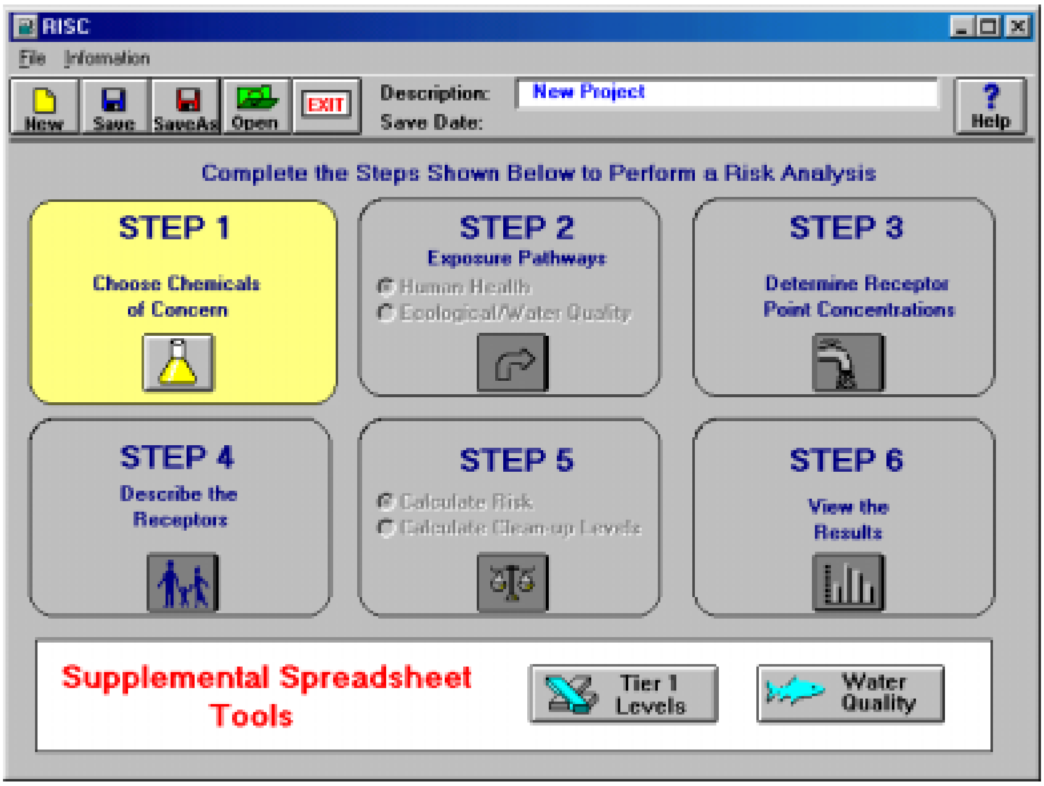
Step 4 Click on *OK*.

1.2.3 General Instructions (How to Use RISC)

To start RISC, either double-click on the “BP RISC” icon on the Windows desktop or use the “Start” button and then choose “BP RISC” and “BP RISC 4.0”. There is an option to un-install the program from this menu. The user is encouraged to start the software and use it while reading the instructions in this chapter.

1.2.3.1 Main Screen Layout

The main screen of RISC is shown in Figure 1-1. In the main part of the screen are six steps for performing a risk assessment. Chapters 3 through 8 presents detailed instructions for completing these steps. Currently only Step 1 should be available. As each step is completed, the next step will become available. The Data and Analysis Tools (at the bottom of the screen in the white box) are not required to complete a risk assessment but can be used to for supplemental information and features. These options are described in Chapter 2.



Description: New Project
Save Date:

FIGURE 1-1. The Main Screen of RISC

At the top of the main window is a series of buttons (New, Save, Open, Exit and on the far right, Help). The functions of these buttons are discussed in the next sections.

1.2.3.2 New

Selecting the "New" button will clear all user-specified data (e.g. chosen exposure routes, site-specific concentrations, etc.). Suggested default inputs and chemical database entries will be retained. This should only be used when wanting to start over. The user will be warned and given a chance to cancel before "New" clears all current information.

1.2.3.3 Saving Projects

The "Save" button on the main button bar is used to save all the information contained in the project. The user will be prompted to enter a project file name with an extension of ".prj". It is not necessary to use this extension, but it will help identify the saved project files from other files in the directory.

SaveAs

1.2.3.4 Loading Saved Projects

The "Save As" button is similar to the "Save As" function of most of the Windows programs (Excel, Word, etc.). If the project file has been saved in the current session, choosing "Save As" will update the file with any new choices without prompting the user to "OK" any overwriting of project files. If a project file has not been saved, choosing this button will prompt the user to enter a project file name (identical to the "Save" button).

Open

1.2.3.5 Opening Saved Projects

The "Open" button in the main button bar allows saved project files to be loaded into the system. The user will be prompted to choose the name of the saved file to be loaded. At this point, the user will be warned that "Open" will clear any data already entered in the system and that by continuing, this information will be lost. The user has the opportunity to "Cancel" and save current work if necessary.

EXIT

1.2.3.6 Exit

The "Exit" button in the main screen closes the RISC system. The user will be prompted to save any existing work. The user may also close the RISC software using the standard Windows options: chose **Exit** from the **File** pull-down menu, choose Close from the control menu, or click on the close window button (looks like a "X") in the top right-hand corner of the window. These options are identical to choosing the Exit button, however, these methods are available from every screen. (This means a user doesn’t have to return to the main screen in order to exit RISC.)

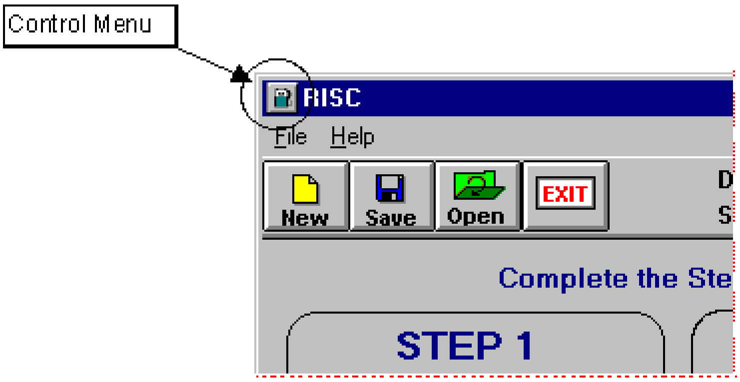


FIGURE 1-2. Exiting RISC

Help

1.2.3.7 Help System

The RISC software has on-line help that is available from every screen. This feature can be activated by choosing the HELP button. This displays the Help Window that has topic-specific information and a menu bar.

Note, some of the text displayed in the HELP window is highlighted in green. This is called HYPERTEXT and can be selected (by clicking) to view additional information on the topic.

Copy

1.2.3.8 Copying Text to the Windows Clipboard

Several windows (tables and charts) have a "Copy" button on their button bar allowing the text or graph in the window to be copied to the Windows Clipboard. The clipboard is a type of buffer that holds selected text or graphics. Once the text is in the clipboard, it can be copied to any other Windows application (such as Word or Excel). This may be useful for reformatting text or saving model output separately (from the project file).

Performing a Screen Dump

A screen dump takes a "snapshot" of what is currently on the screen and copies it to the Clipboard. To copy the current screen, push the "Print Screen" key from the keyboard. (If the keyboard does not have a "Print Screen" key, refer to the Windows manual to learn how to perform a screen dump.)

Once in the clipboard, the screen dump may be copied to other applications. With a screen dump the buffer contains a graphical image rather than text (note that "Copy" fills the buffer with a text file). This means that the image cannot be edited as a text file in a word processing program. The image may however be modified in a drawing program such as Windows Paintbrush.

This procedure will make a screen dump from any Windows application. The figures in this user's manual were generated using this procedure and then copying the image into Microsoft Excel or Word where the figure titles were added.

Print

1.2.3.9 Printing

A "Print" button appears on several screens (specifically, tables and charts). This sends the text or the figure directly to the printer. In order to use this feature, your printer must be configured in Windows and should work from other applications. The printer is configured by selecting the Windows "Control Panel" icon (usually loaded in the "Main" program group). After displaying the Control Panel, select "Printers" from the icons. The print orientation and scaling can be modified in the printer setup.

Chapter
2.0

Data And Analysis Tools

At the bottom of the Main RISC Screen, Figure 1-1, the user will find buttons leading to additional "Data and Analysis Tools". These buttons open two different spreadsheets; one is a risk-based corrective action (RBCA) Tier 1 Excel worksheet and the other presents a large surface water and sediment quality criteria table. Use of these spreadsheets are discussed in the following sections. It should be noted that using the Tier 1 spreadsheet is not required to perform calculations using the RISC software. Neither of these Excel spreadsheets are linked to the RISC software, they are additional tools for risk assessment.

Tier 1 Levels

2.1 RBCA TIER 1 SPREADSHEET

This button calls upon Excel to open a spreadsheet that calculates RBCA Tier 1 Look-Up Table values for all of the chemicals initially contained in the RISC chemical database. The values in the "RBSLs" table in this particular table are calculated using the example algorithms presented in the ASTM E1739-95 "Standard Guide to Risk-Based Corrective Action at Petroleum Release Sites" (1995) for all pathways except indoor air from soil. The volatilization to indoor air RBSL is calculated using the Johnson-Ettinger (1992) model with both the diffusive and advective terms (the RBCA algorithm only includes the diffusive term). There is an additional site-specific target level (SSTL) sheet presenting clean-up levels in soil and groundwater calculated using the Domenico groundwater model and Green-Ampt infiltration model. These clean-up levels are called SSTLs because they use models that are more complicated than the models in Tier 1 and the receptor location is assumed to be located away from the source.

The features and applications of the spreadsheet are summarized in the following section. The equations used to develop the tables are provided in Appendix H. The Johnson-Ettinger (1992) model is described in Appendix D.

2.1.1 Tier 1 Applications

In the RBCA approach, a Tier 1 Look-up Table is used to identify those chemicals and pathways that warrant further evaluation. It is generally understood that soil, groundwater, or air concentrations falling below Look-Up Table values are not of concern. It is envisioned that this RBCA Tier 1 spreadsheet could be used to identify those chemicals and pathways that warrant further evaluation through use of the RISC software. The default values in the spreadsheet have been chosen to reflect the values used by BP for their Tier 1 table.

Users should review the assumptions and inputs built into this table before using any of the values. Users should also note that there are differences between the algorithms used in this specific look-up table and those contained in the RISC software. In most cases, the algorithms used in the Tier 1 spreadsheet are simplifications (assumptions of steady-state or infinite sources) of algorithms used in the RISC software. In some cases (e.g., inhalation exposures during showering), the RISC software includes exposure pathways and algorithms not included in the sample ASTM E1739-95 (1995) “Look-Up” table.

2.1.2 Tier 2 Applications

The Tier 1 spreadsheet may also be used as the first step of a Tier 2 analysis in which site-specific input values are used in conjunction with the Tier 1 algorithms to calculate site-specific target levels (SSTLs). In this mode, site-specific inputs are substituted for the very conservative inputs assumed in Tier 1. Of course, the “Calculate Clean-up Levels” option in Step 5 of RISC may also be used to calculate SSTLs for both types of exposure points, i.e. directly at the source and at a site-specific distance from the source zone. RISC has the added capability of calculating clean-up levels that are protective of multiple routes and chemicals in an additive mode.

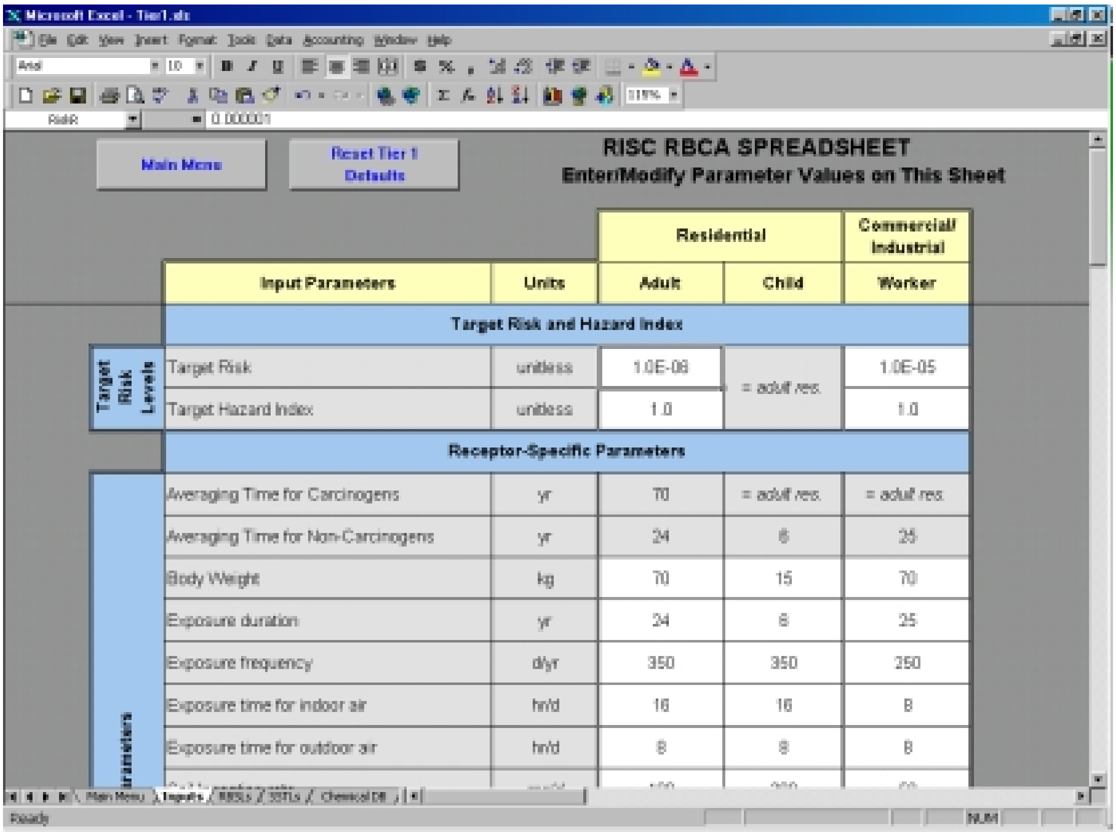
In addition to the ASTM algorithms in the Tier 1 spreadsheet there are two additional models: (1) the Domenico groundwater model, and (2) the Green-Ampt algorithm for estimating travel time through the vadose zone. These models can account for degradation in the saturated zone and vadose zone, respectively. The Domenico model can also be used for a receptor location downgradient from the source area. The Domenico and Green-Ampt models are described in more detail in Appendix H.

2.1.3 How to Use

The Tier 1 spreadsheet contains four main worksheets summarized in Table 2-1. The input parameters are entered in the "Inputs" sheet, part of which is shown in Figure 2-1. Note, there are input cells for both an adult and child residential scenario and an industrial/commercial scenario. For the residential carcinogenic risk calculation, a combination child and adult scenario is assumed. For calculating hazard indices, a child receptor is assumed for the residential scenario. The residential and industrial scenarios generate different screening levels (presented in the screening level table.) The input values may be modified by the user to reflect site-specific conditions. Changes made in the Tier 1 spreadsheet will not affect the RISC model output. The input values in the spreadsheet are only used to calculate the RBSL and SSTL tables in the spreadsheet. Appendix H discusses the Tier 1 spreadsheet in more detail.

Table 2-1. Summary of the Sheets in the Tier 1 Spreadsheet

Sheet Name	Description of Contents
Inputs	This is location to review and/or change non-chemical specific input values for the RBSL and SSTL tables.
RBSLs	Contains RBSLs calculated with the ASTM algorithms. The soil to indoor air pathway is calculated with Johnson-Ettinger model (1992). To match the ASTM algorithm for this pathway set the pressure differential between the soil and the basement equal to zero.
SSTLs	1. Contains SSTLs for the subsurface soil to protect ingestion of groundwater calculated using the following model combinations: • Green-Ampt model only. (Considers degradation in the vadose zone with a receptor point location in groundwater directly beneath source). • Domenico model only. (Considers advection/dispersion and degradation in the saturated zone with a receptor point location in groundwater downgradient of the source.) • Green-Ampt model linked with Domenico model. (Considers degradation in both the vadose and saturated zones and advection/dispersion in the saturated zone for a receptor point location in groundwater downgradient of the source.) 2. Contains SSTLs in groundwater calculated using: • Domenico model for down-gradient receptor point location in groundwater. (Considers advection/dispersion and degradation in the saturated zone.)
Chemical DB	Contains the chemical-specific toxicity and fate and transport database for the Tier 1 spreadsheet. These values may be changed/updated by the user. Note: this database is not linked to the chemical database in RISC.



RISC RBCA SPREADSHEET
Enter/Modify Parameter Values on This Sheet

	Input Parameters	Units	Residential Adult	Residential Child	Commercial/ Industrial Worker
	Target Risk and Hazard Index				
Target Risk Levels	Target Risk	unitless	1.0E-06	= adult res.	1.0E-05
	Target Hazard Index	unitless	1.0		1.0
	Receptor-Specific Parameters				
Parameters	Averaging Time for Carcinogens	yr	70	= adult res.	= adult res.
	Averaging Time for Non-Carcinogens	yr	24	6	25
	Body Weight	kg	70	15	70
	Exposure duration	yr	24	6	25
	Exposure frequency	d/yr	350	350	250
	Exposure time for indoor air	hr/d	16	16	8
	Exposure time for outdoor air	hr/d	8	8	8

Figure 2-1. Part of the "Inputs" Sheet in the Tier 1 Spreadsheet

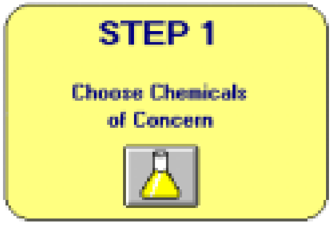
Water Quality

2.2 SURFACE WATER QUALITY CRITERIA

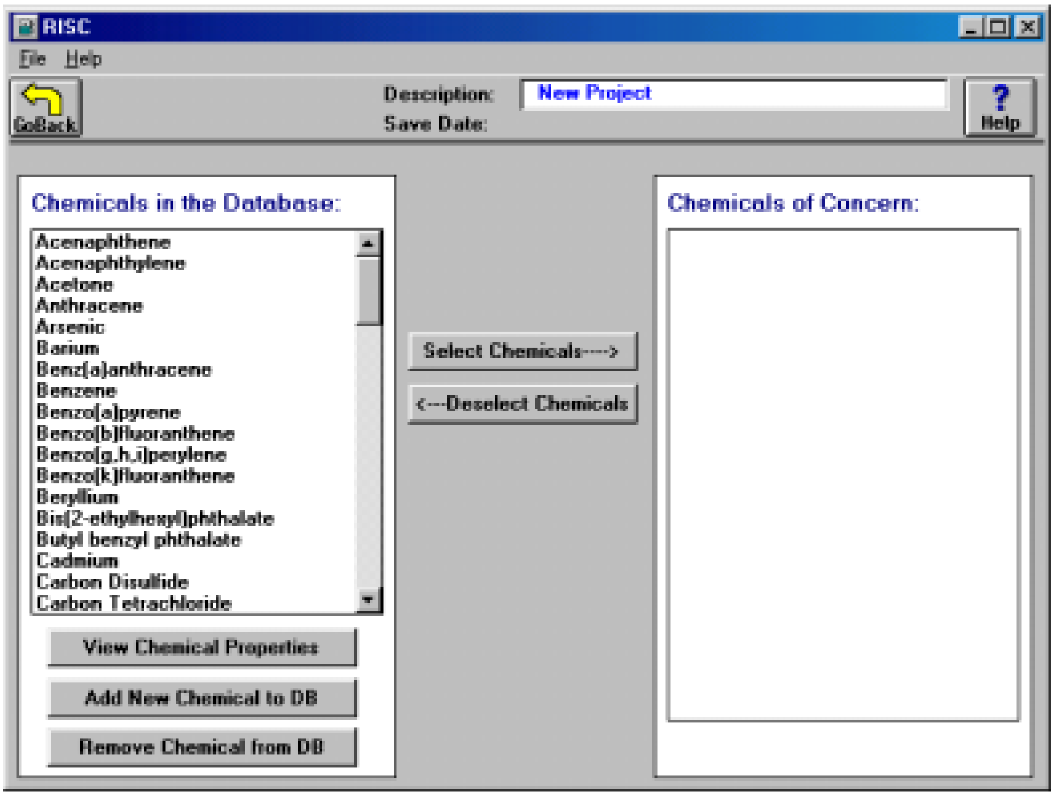
This button will use Excel to display a spreadsheet summarizing the ambient water quality criteria (acceptable surface water concentrations in fresh and marine waters) and sediment criteria contained in RISC. The spreadsheet contains many additional standards (that are not used in the RISC software itself) for water and sediment quality criteria. Changes made to this spreadsheet will not be used in the RISC software; its purpose is just to summarize existing standards (as of the release date of this version). This spreadsheet may be linked to RISC in future versions. Appendix M contains a table summarizing the data contained in this spreadsheet.

Chapter
3.0

Choose Chemicals Of Concern



In this first step users identify chemicals that are of concern for their analysis. The RISC software contains a database with 87 chemicals. The chemicals of concern may be chosen from this database or new chemicals may be added to the system database and then chosen as a chemical of concern. Figure 3-1 shows the Step 1 main screen before any chemicals have been selected.



Description: New Project
Save Date:

Chemicals in the Database:

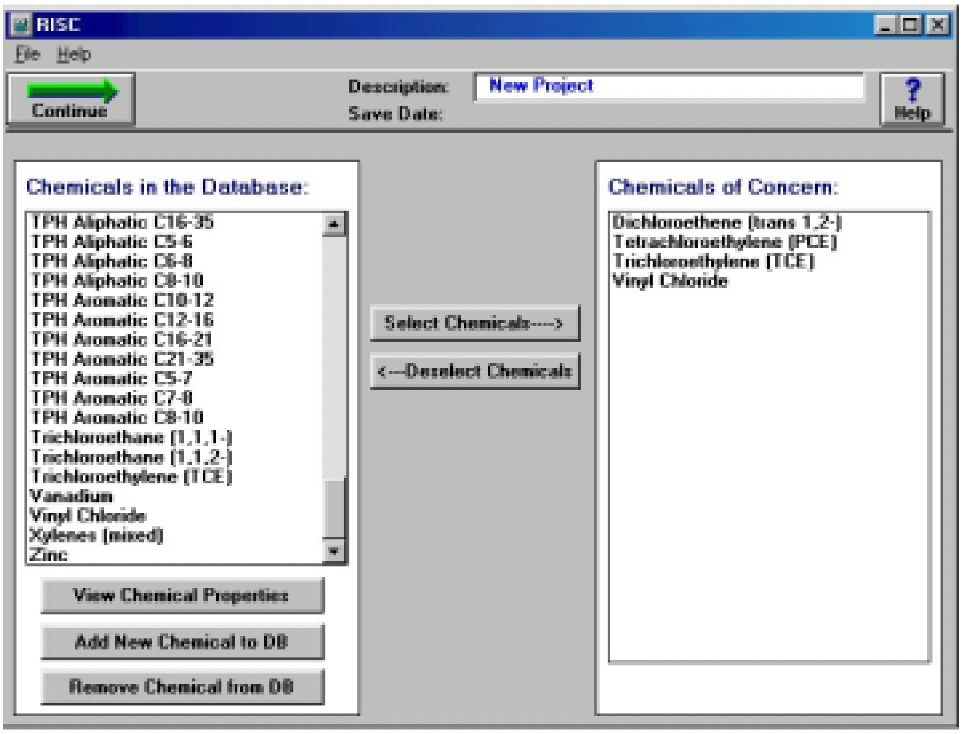
Acenaphthene
Acenaphthylene
Acetone
Anthracene
Arsenic
Barium
Benz[a]anthracene
Benzene
Benzo[a]pyrene
Benzo[b]fluoranthene
Benzo[g,h,i]perylene
Benzo[k]fluoranthene
Beryllium
Bis[2-ethylhexyl]phthalate
Butyl benzyl phthalate
Cadmium
Carbon Disulfide
Carbon Tetrachloride

Chemicals of Concern:

FIGURE 3-1. Chemical Selection Screen

3.1 CHOOSE CHEMICALS

The box on the left contains a list of all the chemicals currently in the system database. To select chemicals of concern, choose one or more chemicals from this list (by clicking on them with the mouse) and then choose the "Select Chemicals ---->" button. (Use the scroll bar to find chemicals not currently shown in the window.) The chemicals selected will be displayed in the box on the right. To "un-select" a chemical (or chemicals) of concern click on the chemical in the right box and choose the "<---Deselect Chemicals" button. Figure 3-2 shows the chemicals of concern screen with four chemicals of concern selected.



Description: New Project

Save Date:

Chemicals in the Database:

TPH Aliphatic C16-35
TPH Aliphatic C5-6
TPH Aliphatic C6-8
TPH Aliphatic C8-10
TPH Aromatic C10-12
TPH Aromatic C12-16
TPH Aromatic C16-21
TPH Aromatic C21-35
TPH Aromatic C5-7
TPH Aromatic C7-8
TPH Aromatic C8-10
Trichloroethane (1,1,1-)
Trichloroethane (1,1,2-)
Trichloroethylene (TCE)
Vanadium
Vinyl Chloride
Xylenes (mixed)
Zinc

Chemicals of Concern:

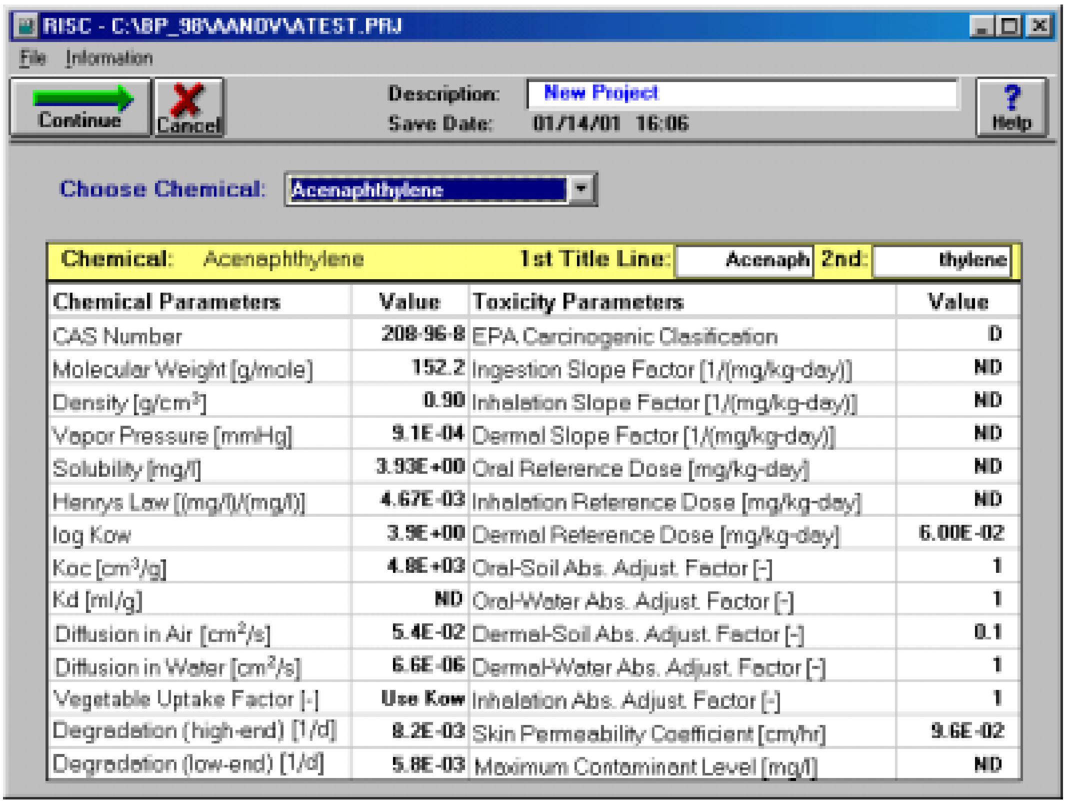
Dichloroethene (trans 1,2-)
Tetrachloroethylene (PCE)
Trichloroethylene (TCE)
Vinyl Chloride

FIGURE 3-2. Chemical Selection Screen with Four Chemicals Selected

These four chemicals will now be the only chemicals considered in the current analysis. At any point it is possible to come back to this step and add or remove chemicals from the list of chemicals selected. However, if data has been entered, fate and transport models run or a risk calculation performed with a previous suite of chemicals, information for the new chemical(s) will need to be entered and the models re-run. The number of chemicals that can be analyzed at one time is limited to 20 (due to memory limitations in the fate and transport and risk assessment computational codes).

3.2 VIEW CHEMICAL PROPERTIES

The "View Chemical Properties" allows one to view and edit the chemical properties in the system database. The physical and chemical properties were assembled from common chemical handbooks; the toxicological properties (including dose-response and absorption adjustment factors) were extracted from the an internal BP report prepared by ENSR (1995). Figure 3-3 shows the chemical properties for acenapththene. To view other chemicals, select the chemical from the list box in the top center of the screen. To edit the property values, click on the box containing the value and then enter the new value. **Any changes made to the chemical properties will be stored in the permanent system database so the user should be sure that the change is correct.**



Description: New Project
Save Date: 01/14/01 16:06

Choose Chemical: Acenaphthylene

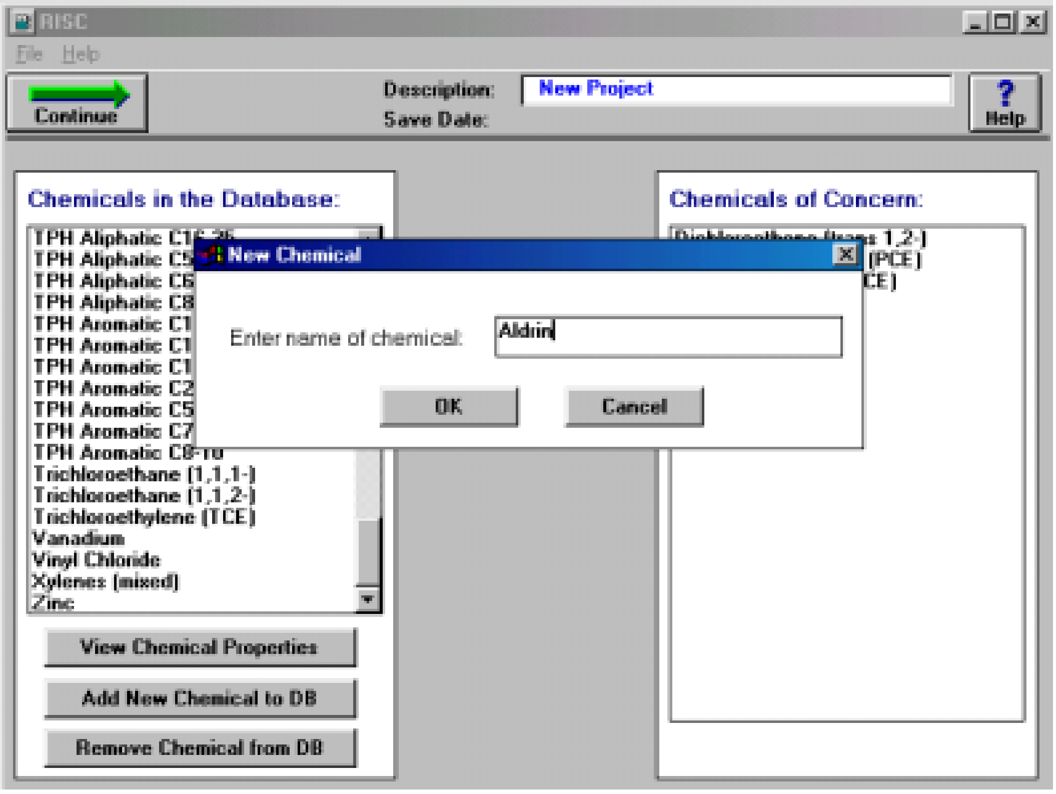
Chemical: Acenaphthylene 1st Title Line: Acenaph 2nd: thylene

Chemical Parameters	Value	Toxicity Parameters	Value
CAS Number	208-96-8	EPA Carcinogenic Clasification	D
Molecular Weight [g/mole]	152.2	Ingestion Slope Factor [1/(mg/kg-day)]	ND
Density [g/cm^3]	0.90	Inhalation Slope Factor [1/(mg/kg-day)]	ND
Vapor Pressure [mmHg]	9.1E-04	Dermal Slope Factor [1/(mg/kg-day)]	ND
Solubility [mg/l]	3.93E+00	Oral Reference Dose [mg/kg-day]	ND
Henrys Law [(mg/l)/(mg/l)]	4.67E-03	Inhalation Reference Dose [mg/kg-day]	ND
log Kow	3.9E+00	Dermal Reference Dose [mg/kg-day]	6.00E-02
Koc [cm^3/g]	4.8E+03	Oral-Soil Abs. Adjust. Factor [-]	1
Kd [ml/g]	ND	Oral-Water Abs. Adjust. Factor [-]	1
Diffusion in Air [cm^2/s]	5.4E-02	Dermal-Soil Abs. Adjust. Factor [-]	0.1
Diffusion in Water [cm^2/s]	6.6E-06	Dermal-Water Abs. Adjust. Factor [-]	1
Vegetable Uptake Factor [-]	Use Kow	Inhalation Abs. Adjust. Factor [-]	1
Degradation (high-end) [1/d]	8.2E-03	Skin Permeability Coefficient [cm/hr]	9.6E-02
Degradation (low-end) [1/d]	5.8E-03	Maximum Contaminant Level [mg/l]	ND

FIGURE 3-3: Chemical Properties Screen

3.3 ADD NEW CHEMICAL TO DATABASE

Selecting the "Add New Chemical to DB" button from the chemical selection screen (Figure 3-1) will allow one to add a chemical to the system database. The user will be prompted to enter the chemical name.



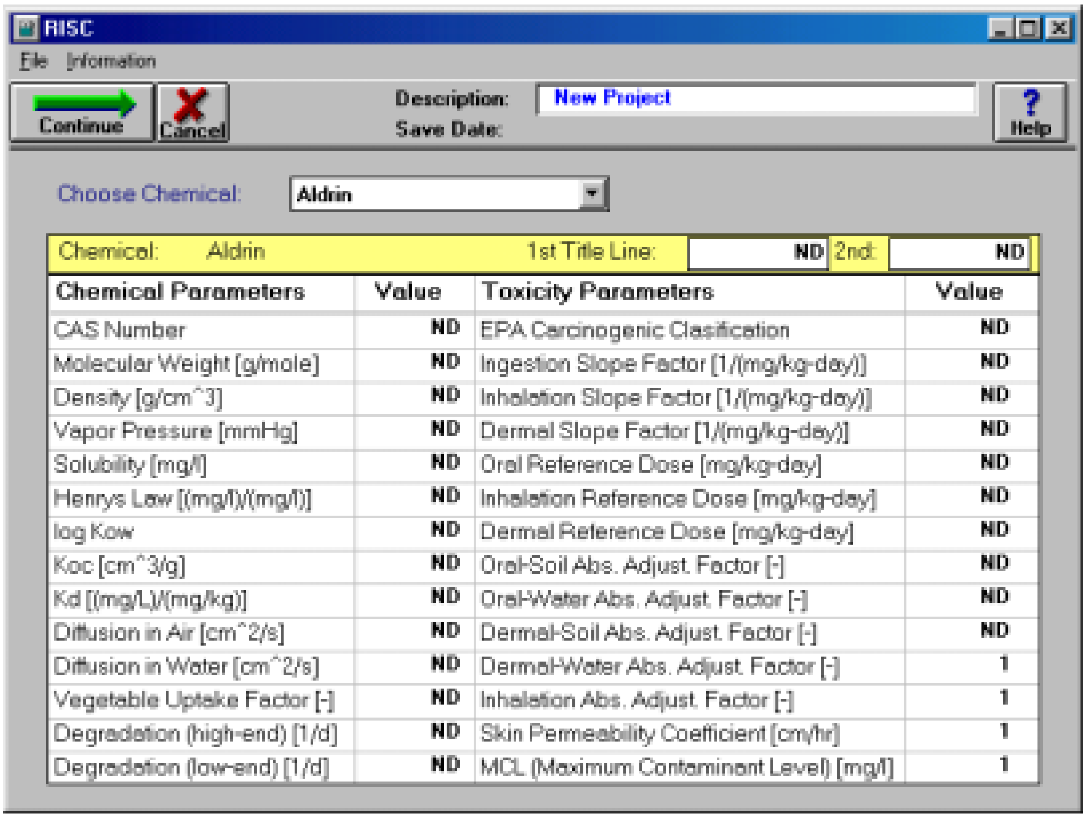
Description: New Project

Save Date:

Enter name of chemical: Aldrin

FIGURE 3-4. Adding a New Chemical

After selecting the "OK" button, the chemical properties screen for the new chemical (in this case, "aldrin") will be displayed. Most of the chemical properties are listed as "ND" for no data (or not determined) as shown in Figure 3-5. At this point the "ND"s should be replaced with the appropriate physical, chemical, and toxicological properties for the new compound.



Description: New Project
Save Date:

Choose Chemical: Aldrin

Chemical: Aldrin 1st Title Line: ND 2nd: ND

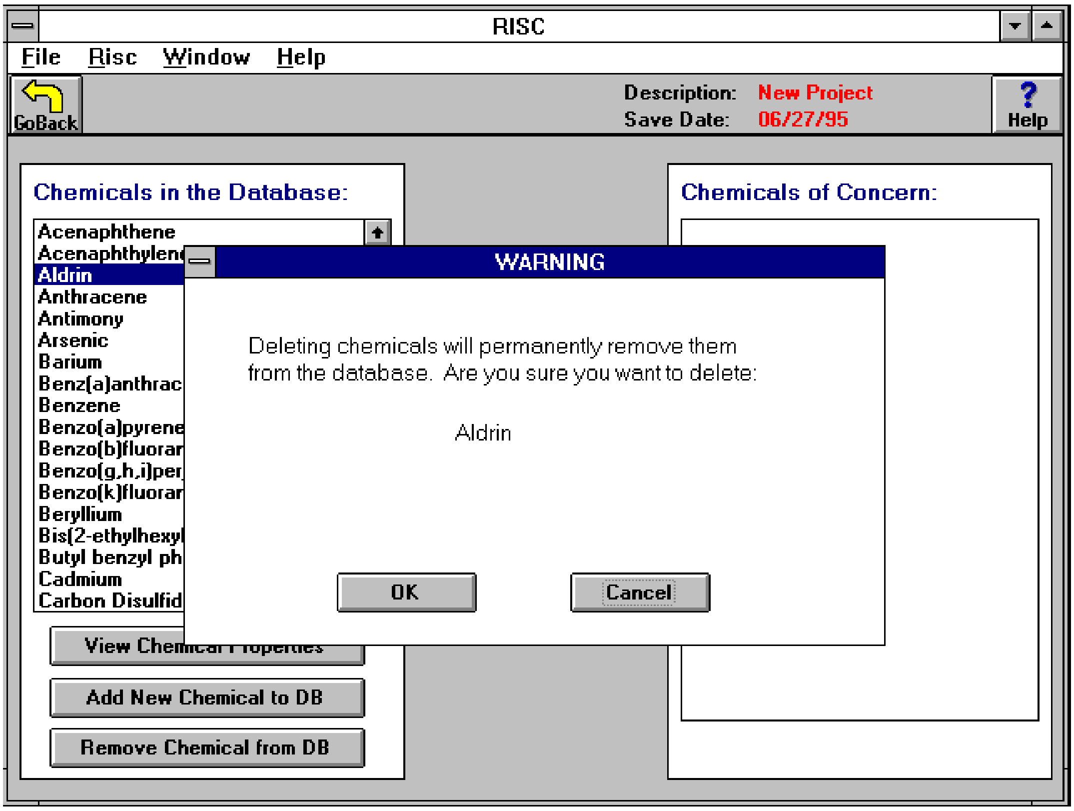
Chemical Parameters	Value	Toxicity Parameters	Value
CAS Number	ND	EPA Carcinogenic Clasification	ND
Molecular Weight [g/mole]	ND	Ingestion Slope Factor [1/(mg/kg-day)]	ND
Density [g/cm^3]	ND	Inhalation Slope Factor [1/(mg/kg-day)]	ND
Vapor Pressure [mmHg]	ND	Dermal Slope Factor [1/(mg/kg-day)]	ND
Solubility [mg/l]	ND	Oral Reference Dose [mg/kg-day]	ND
Henrys Law [(mg/l)/(mg/l)]	ND	Inhalation Reference Dose [mg/kg-day]	ND
log Kow	ND	Dermal Reference Dose [mg/kg-day]	ND
Koc [cm^3/g]	ND	Oral-Soil Abs. Adjust. Factor [-]	ND
Kd [(mg/L)/(mg/kg)]	ND	Oral-Water Abs. Adjust. Factor [-]	ND
Diffusion in Air [cm^2/s]	ND	Dermal-Soil Abs. Adjust. Factor [-]	ND
Diffusion in Water [cm^2/s]	ND	Dermal-Water Abs. Adjust. Factor [-]	1
Vegetable Uptake Factor [-]	ND	Inhalation Abs. Adjust. Factor [-]	1
Degradation (high-end) [1/d]	ND	Skin Permeability Coefficient [cm/hr]	1
Degradation (low-end) [1/d]	ND	MCL (Maximum Contaminant Level) [mg/l]	1

FIGURE 3-5. Default Chemical Properties for New Chemical

The empty boxes, "1st Title Line" and "2nd:" are used for long chemical names (more than 20 letters) when printing tables later in the software. For long chemical names that are printed in a column heading, the user has the opportunity to specify what to print on the first line and what to print on the second. The chemical name shown here (aldrin) is short, so nothing need be entered in these two edit boxes and the name will not be split into two title lines.

3.4 REMOVE CHEMICAL FROM DATABASE

After selecting a chemical (or multiple chemicals) from the chemical selection screen (Figure 3-1) they may be removed from the system database by clicking on the "Remove Chemical from DB" button. This action (if completed) will permanently remove the chemicals from the system database. It is recommended that chemicals only be removed that have been personally added in order to leave the original chemicals in the database. One reason to remove a added chemical is if it were misspelled. Figure 3-6 shows the warning window that appears when choosing to remove chemicals.



Description: New Project
Save Date: 06/27/95

WARNING

Deleting chemicals will permanently remove them from the database. Are you sure you want to delete:

Aldrin

FIGURE 3-6. The Warning Window When Removing Chemicals

3.5 RESTORING THE ORIGINAL CHEMICAL DATABASE

The chemical database is contained in a binary (non-editable) file called "chemical.cdb". A duplicate file called "chemback.cdb" has been included in the RISC system directory. If the database has been changed and at some point it would be useful to restore the original database, delete the file "chemical.cdb".

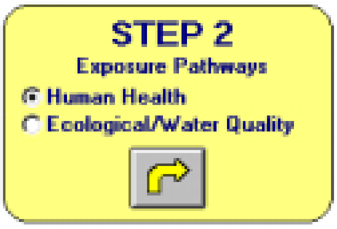
Deleting "chemical.cdb" will tell RISC to use the backup file (the original database as it was shipped with RISC). However, any changes made to the chemical database (additions, deletions and modifications of chemical properties) will be erased.

Chapter

4.0

Choose Exposure Pathways

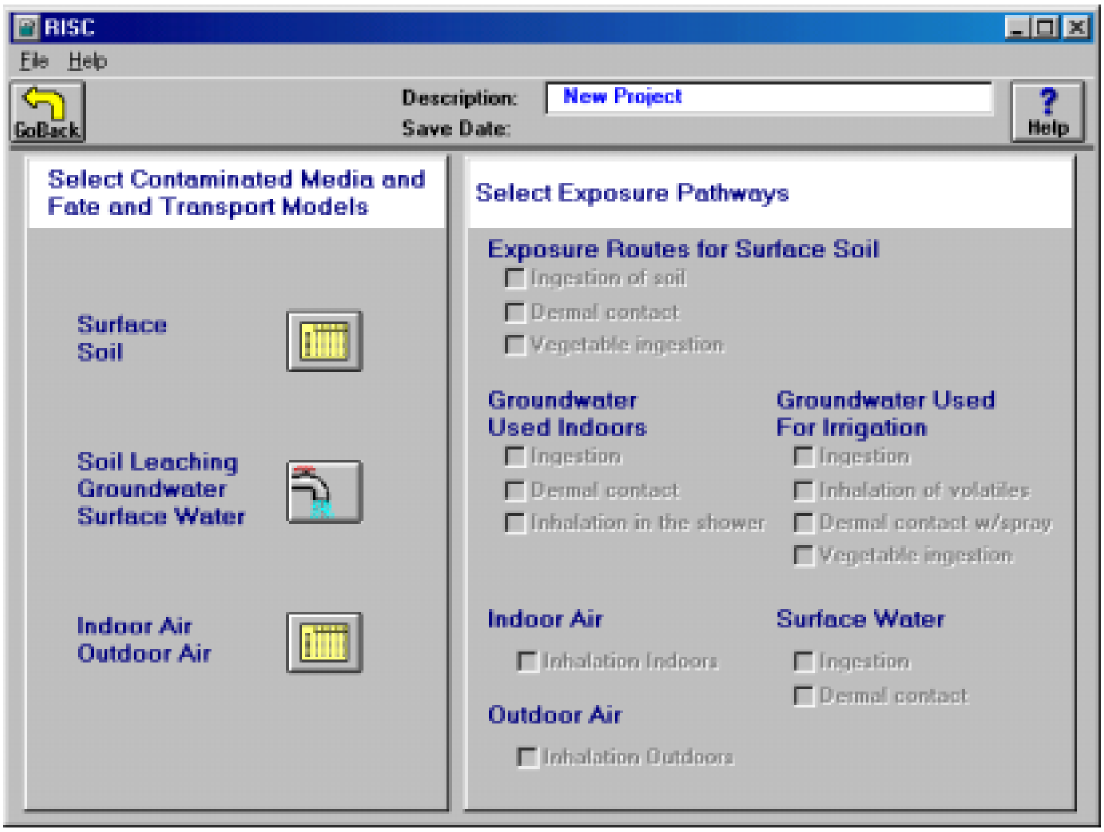
On the Step 2 button of the main menu (see chapter logo above) the user must define the exposure scenario by selecting contaminated media(s), fate and transport models (if any), and associated exposure pathways. RISC is set up so that in any single analysis, either human health exposure pathways can be evaluated or ecological/water quality concerns can be evaluated. The two main sections in this chapter will explain the choices available under each option.



4.1 HUMAN HEALTH EXPOSURE PATHWAYS

Figure 4-1 shows the screen that is displayed when the human health option is chosen. On the left of this screen the user can identify the contaminated media and/or transport models to be evaluated. The exposure pathways are listed on the right side of the screen. These exposure pathways are not available for selection until the associated media is selected from the left side.

The selection of potential transport pathways and exposure pathways is a very important step in the risk assessment process. The user needs to identify those pathways that are likely to be complete, based on knowledge of the locations of impacted soil, groundwater, air, and/or surface water relative to the location and habits of people or ecosystems that might be exposed to the chemicals of concern. The US EPA’s Risk Assessment Guidance for Superfund (1989) provides guidance for selecting appropriate exposure pathways for various human health risk assessment situations.



Description: New Project

Save Date:

FIGURE 4-1. Choose Exposure Pathways Screen

4.1.1 Select Contaminated Media and Fate and Transport Models

The three buttons shown on the left side in Figure 4-1 correspond to three separate potential source areas that can be considered in any given analysis. All the sources do not need to be selected at one time. The assumptions made by RISC for a given analysis are as follows:

- Only one receptor location is modeled in any given scenario.
- The vegetable ingestion exposure can be evaluated for surface soil or for groundwater but not from both.
- Either indoor air or outdoor air can be considered in the analysis. (Usually the indoor air pathway dominates the risk estimate if the concentrations come from the same source so adding the risk from both pathways is neither meaningful nor essential).
- Only one model (or combination of linked models) can be used to estimate concentrations in a receptor media.

- If groundwater concentrations are being modeled downgradient from the source and volatilization from groundwater to indoor air is considered, then it is assumed that the building is located downgradient. The concentrations at the receptor point in groundwater are used as the source term for the vapor model.

Figure 4-2 shows the source media options, the fate and transport mechanisms available, and the associated receptor media. The receptor media is that media which actually contacts the receptor. Concentrations must be either entered or estimated for receptor media in order to evaluate exposure routes (section 4.1.2) associated with that media.

The next subsections introduce the fate and transport model choices for each of the three source options. Use of the fate and transport models is described in more detail in Chapter 5 (Step 3: Receptor Point Concentrations) and the equations and assumptions are detailed in the Appendices.

4.1.1.1 Surface Soil

The receptor point concentrations in surface soil cannot be estimated using a fate and transport model but must be entered explicitly by the user. Surface soil is any soil that a receptor may come into contact with directly. The reason concentrations are not modeled in this media is that many models may overestimate the leaching to groundwater or other transport process away from the soil source. While this may be conservative for estimating groundwater concentrations it will tend to underestimate the time-averaged soil concentration.

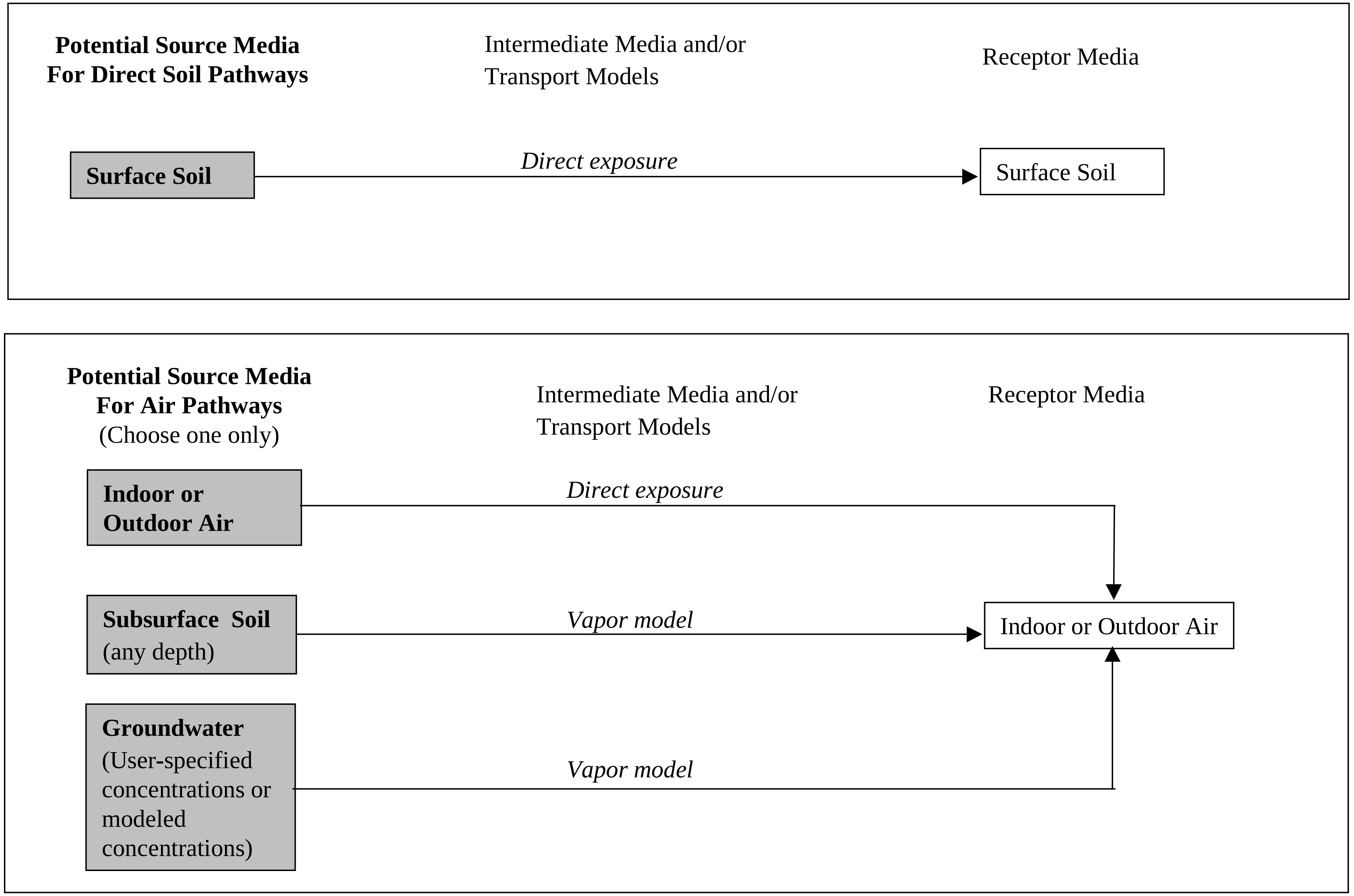


Figure 4-2a. Source and Receptor Media

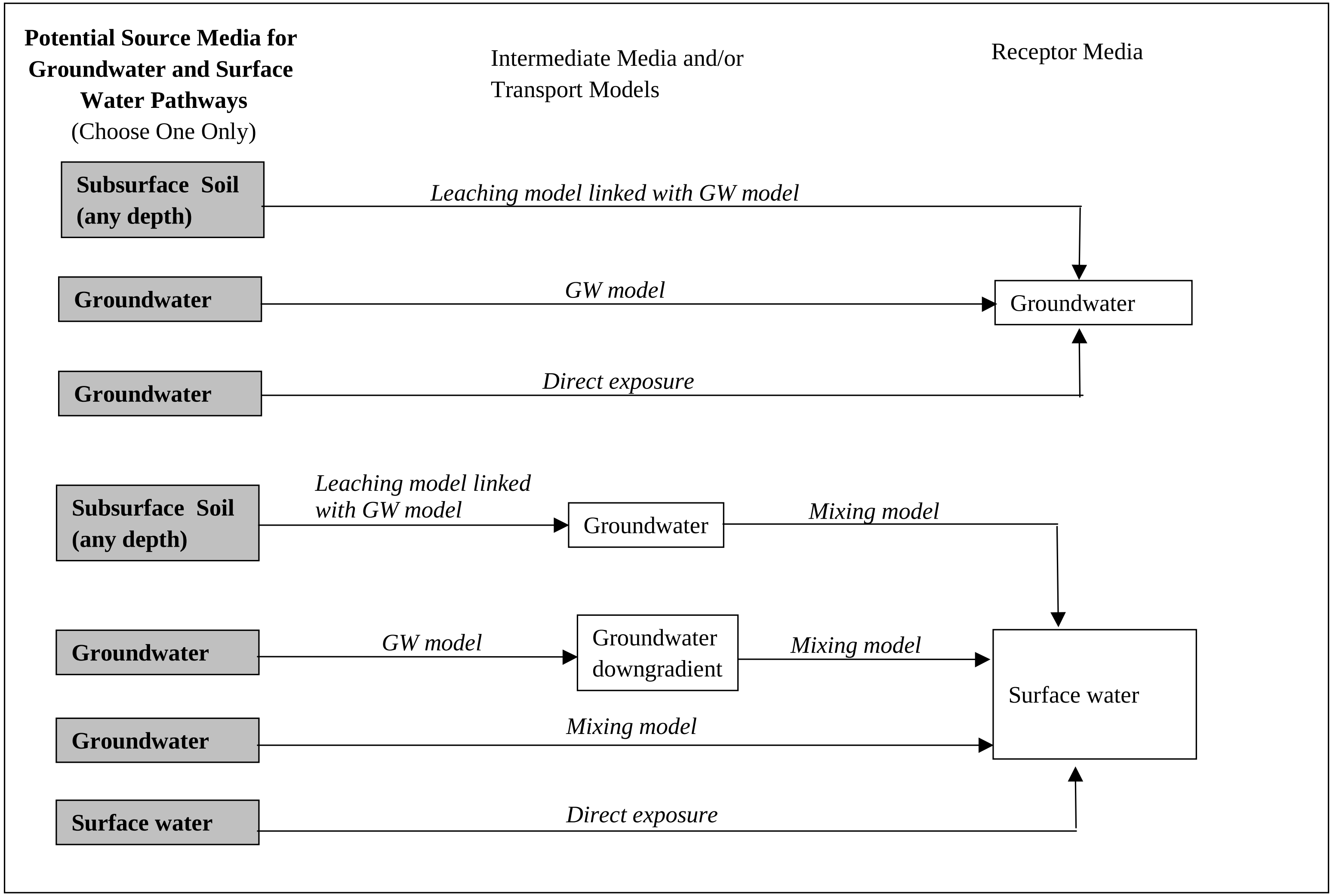
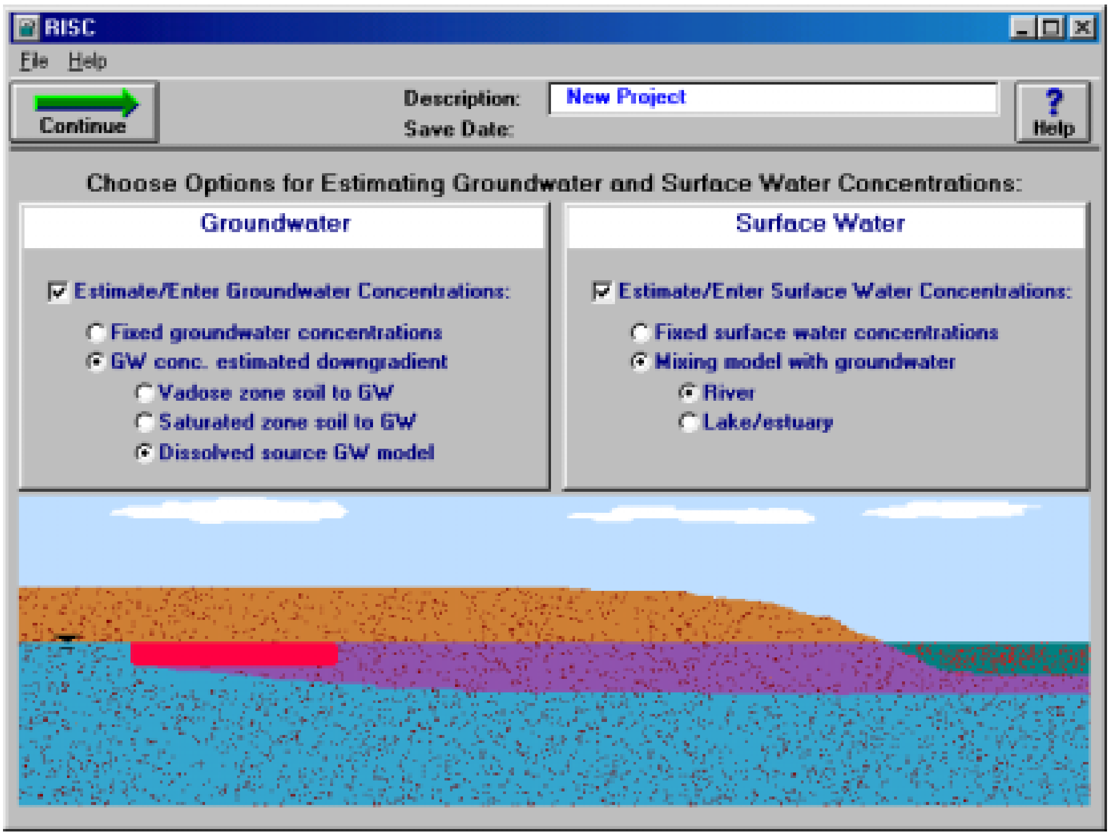


Figure 4-2b. Source and Receptor Media

4.1.1.2 Subsurface Soil, Groundwater and Surface Water

Figure 4-3 shows the screen for selecting options associated with sources in subsurface soil, groundwater, or surface water. The options on this screen define how concentrations in groundwater or surface water will be estimated. The user may select to enter concentrations for groundwater and/or surface water; the use of fate and transport models is elective and not required. In Figure 4-3, concentrations will be modeled in both media.



Description: New Project

Save Date:

Choose Options for Estimating Groundwater and Surface Water Concentrations:

Groundwater

☑ Estimate/Enter Groundwater Concentrations:

- ○ Fixed groundwater concentrations
- ● GW conc. estimated downgradient
  - ○ Vadose zone soil to GW
  - ○ Saturated zone soil to GW
  - ● Dissolved source GW model

Surface Water

☑ Estimate/Enter Surface Water Concentrations:

- ○ Fixed surface water concentrations
- ● Mixing model with groundwater
  - ● River
  - ○ Lake/estuary

Figure 4-3. Options Associated With Subsurface Soil, Groundwater, or Surface Water Sources

Groundwater

If concentrations in groundwater are to be modeled, (i.e. the “GW conc. estimated downgradient” option is chosen), the user must choose between three models: vadose zone soil to groundwater model, saturated zone soil to groundwater, or dissolved source groundwater model. Both the “saturated soil zone to groundwater model" and the “dissolved source to GW model" simulate transport of contaminants in the saturated zone only. These models differ only by the assumptions made about the source term. In the “saturated soil zone to groundwater model" the total soil concentrations in the source and the saturated depth of the source must be specified. In this option, the source is assumed to be in, or just above, the water table, enabling the effects of fluctuating water tables on groundwater loading to be modeled. The saturated zone soil to groundwater model, which allows for a depleting source, is described in Appendix C. In the "dissolved source to GW model", the dissolved phase (groundwater) concentrations in the source area must be specified. The dissolved source to groundwater model does not allow for a depleting source per se, but the source can be ‘switched off’ at a point in time (equal to the pulse length). This model is described in Appendix B. In the option, "vadose zone soil to GW model", the depleting source is assumed to be located in the vadose zone above the water table and the transport of contaminants is modeled through the vadose zone to the groundwater. Once in the groundwater, the concentrations are transported to the receptor well. This option really consists of two fate and transport models linked together: the vadose zone model and the saturated zone model (described in Appendices A and B, respectively).

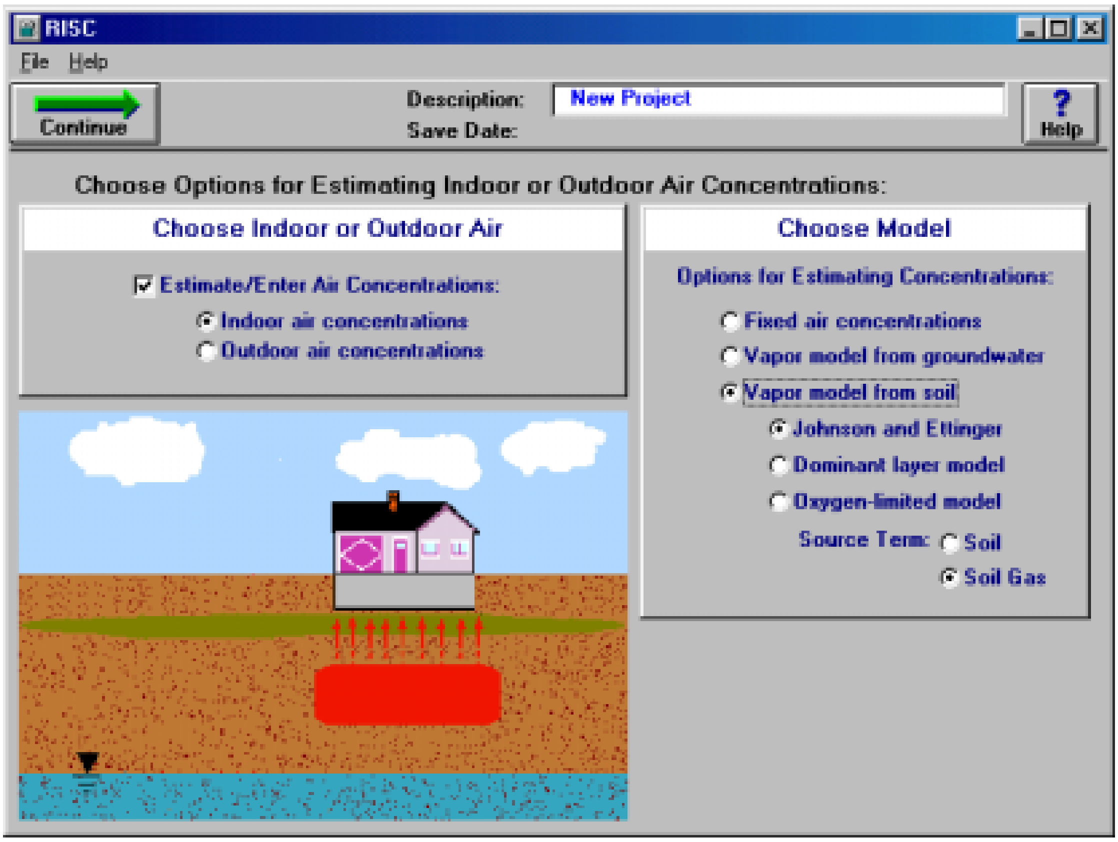
Surface Water

The concentrations in surface water can either be entered directly or estimated using a mixing model that uses groundwater concentrations as a source term. There are two surface water mixing models: river, and lake/estuary. These are essentially the same simple mixing model, they differ only in the way the input parameters are collected and the volume of the surface water body is calculated. For example, in the river mixing model one of the input parameters is cross-section of the river and the volume of water for mixing is calculated as the cross-sectional area and the impacted length of the reach. In the lake mixing model, the volume of the lake is asked for explicitly. Appendix L describes the surface water mixing model.

If a groundwater model is being used to estimate groundwater concentrations downgradient of the source area and the surface water mixing model is being used to estimate surface water concentrations from groundwater, it is assumed that these two models are linked together. In that situation, the source concentrations for the surface water mixing model are being calculated by the groundwater model and are assumed to be located at the “well” location of the groundwater model.

4.1.1.3 Indoor and Outdoor Air

Figure 4-4 shows the input screen for selecting indoor or outdoor air as a receptor media of concern. As with the other receptor media, the user can specify whether or not to model concentrations in indoor or outdoor air and which models to use if the modeling option is chosen. One of the assumptions made is that for the same source or receptor location, either indoor or outdoor air will dominate the risk estimates (usually indoor air), therefore only one of the two media can be considered in a given analysis.



Description: New Project

Save Date:

Choose Options for Estimating Indoor or Outdoor Air Concentrations:

Choose Indoor or Outdoor Air

☑ Estimate/Enter Air Concentrations:

● Indoor air concentrations

○ Outdoor air concentrations

Choose Model

Options for Estimating Concentrations:

○ Fixed air concentrations

○ Vapor model from groundwater

● Vapor model from soil

- ● Johnson and Ettinger
- ○ Dominant layer model
- ○ Oxygen-limited model

Source Term: ○ Soil ● Soil Gas

Figure 4-4. Options for Indoor and Outdoor Air

Each of the options on the right side of Figure 4-4 can be used with either indoor air or outdoor air. The models listed on the right are for vapor transport through the vadose zone. The choice of indoor or outdoor air determines the type of mixing model used once the contaminant exits the vadose zone (either into ambient air or into a building). The vapor model from groundwater uses the same approach as the ASTM (1995) RBCA model (described in Appendix E). The groundwater source concentrations may be entered by the user or they may be estimated with one of the groundwater models chosen in the "Subsurface Soil, Groundwater, and Surface Water" section (see Figure 4-3).

There are three choices for vapor transport through the vadose zone from a soil source: Johnson and Ettinger (1992), dominant layer model (Johnson and Kemblowski, 1998), and the oxygen-limited model (Johnson, to be published). All three of these three models are one-dimensional, steady-state models (infinite source terms). They differ by the processes considered and the model layering system allowed.

- Johnson and Ettinger: in RISC can simulate the presence of a "lens" of different soil material between the source and the building or ambient air. Ignores degradation. Described in Appendix D.
- Dominant Layer Model: considers three potentially different soil horizons with degradation allowed in the middle soil horizon (or layer). Described in Appendix J.
- Oxygen-Limited Model: uniform soil properties, calculates distance away from source where the oxygen concentration may be high enough to support degradation. Oxygen concentrations and transfer rates across the soil surface are input requirements. Described in Appendix K.

4.1.2 Select Exposure Pathways

After defining potential source media, transport models and receptor media, the user must select at least one human exposure route in order to continue. Routes are selected by clicking on the exposure route description or clicking on the check box (see Figure 4-1).

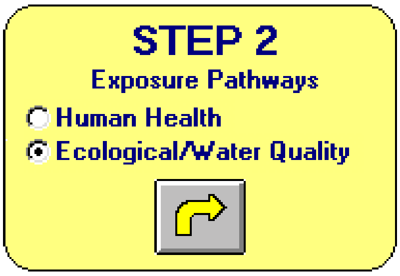
There are fourteen human exposure routes available in RISC. Table 4-1 summarizes the exposure routes available for each receptor media. Only the routes associated with receptor media chosen will become available. For example, if surficial soil is the only media selected on the left side of the Step 2 main screen (Figure 4-1), then the only exposure routes to become available for selection are: ingestion of soil, dermal contact of soil, and vegetable ingestion (from soil).

Depending on the type of appropriate receptor, it may not be appropriate to consider all of the exposure routes for a receptor media. For example, for a commercial exposure scenario for contaminated groundwater, it is not customary to consider inhalation in the shower since workers usually don't take showers at work. The default input parameter values for each exposure pathway are discussed in more detail in Chapter 6 (Step 4: Describe the Receptors). The equations used to estimate risk from each exposure pathway are presented in Chapter 7 (Step 5: Calculate Risk).

TABLE 4-1. Exposure Pathways Associated With Receptor Media

RECEPTOR MEDIA	POTENTIAL EXPOSURE PATHWAYS
Surface Soil	Ingestion Dermal contact Vegetable ingestion
Groundwater	Water used indoors: Ingestion Dermal contact Inhalation in the shower Water used outdoors: Ingestion Dermal contact Inhalation from spray (such as sprinklers) Vegetable ingestion
Outdoor Air	Inhalation
Indoor Air	Inhalation
Surface Water	Ingestion Dermal contact

4.2 ECOLOGICAL/WATER QUALITY



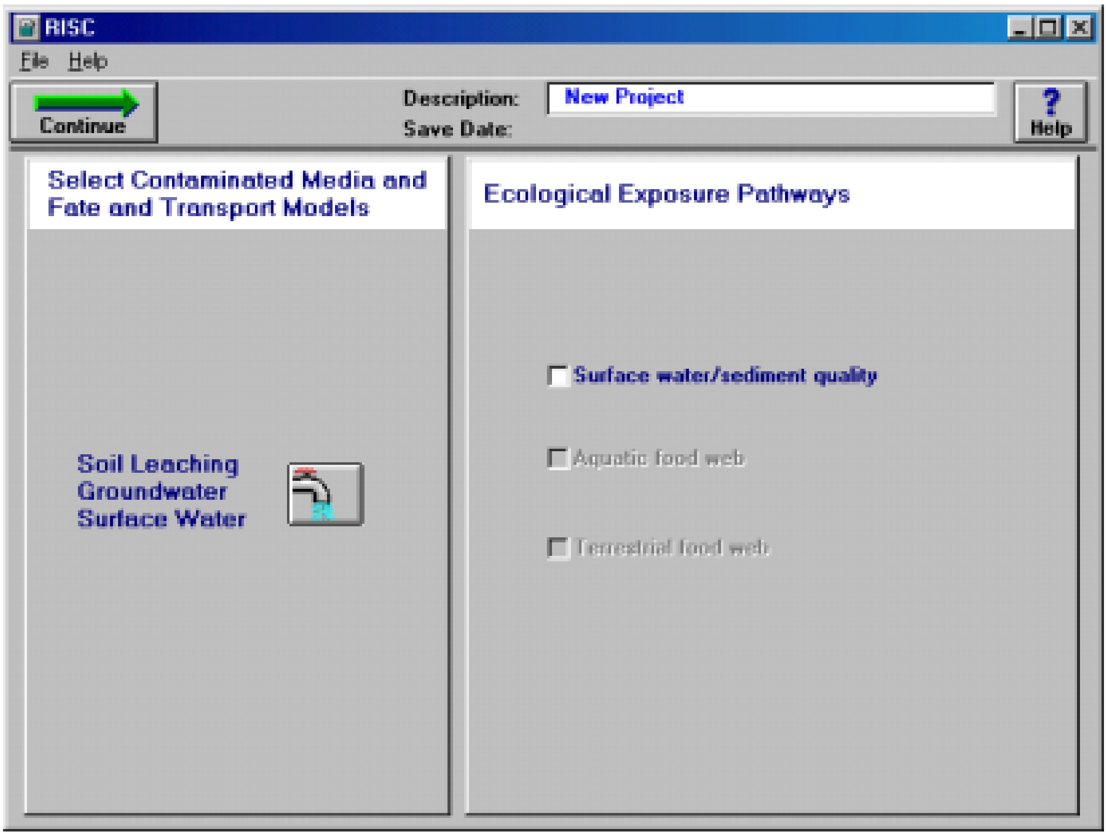
STEP 2

Exposure Pathways

○ Human Health

● Ecological/Water Quality

The ecological/water quality option is used to model concentrations in surface water and sediment for purposes of ecological concerns. The modeled concentrations are then compared with "gold standards" for surface water and sediment quality. Figure 4-5 shows the main screen in Step 2 when the "Ecological/Water Quality" option is chosen.



Description: New Project

Save Date:

Select Contaminated Media and Fate and Transport Models

Soil Leaching Groundwater Surface Water

Ecological Exposure Pathways

☐ Surface water/sediment quality

☐ Aquatic food web

☐ Terrestrial food web

Figure 4-5. Ecological/Water Quality Screen in Step 2

In future versions of RISC, food-chain modeling for aquatic and terrestrial food webs will be available when using this option. In the current version the user must specify how the surface water concentrations are to be estimated. The options are identical to the options under the human health choice for surface water discussed in section 4.1.1.2.

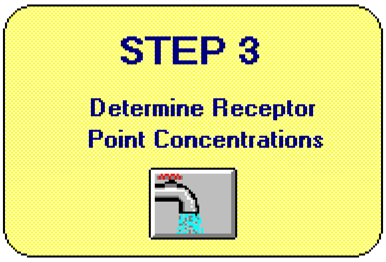
Using the ecological option, the user will run the fate and transport models in Step 3 (identical to the human health procedure) to estimate surface water and sediment concentrations. Then in Step 4, the modeled concentrations can be compared with the "gold standards" contained in the RISC database. Tables summarizing the results in Step 4 can be easily transferred to Word or other reports. The water quality and sediment criteria database in RISC contains criteria from several different countries:

- United States Environment Protection Agency Ambient Water Quality Criteria
- United Kingdom Environmental Quality Standards (statutory and proposed)
- Australia and New Zealand Environment and Conservation Council (ANZECC) Guidelines for the Protection of Aquatic Ecosystems
- European Commission Water Quality Objective
- Canadian Council of Ministers for the Environment Freshwater Aquatic Life Guideline

The sediment criteria in the database is from the National Oceanographic and Atmospheric Administration (NOAA). The criteria listed above were chosen because they are considered "gold standards" in their respective countries.

Chapter 5.0

Determine Receptor Point Concentrations

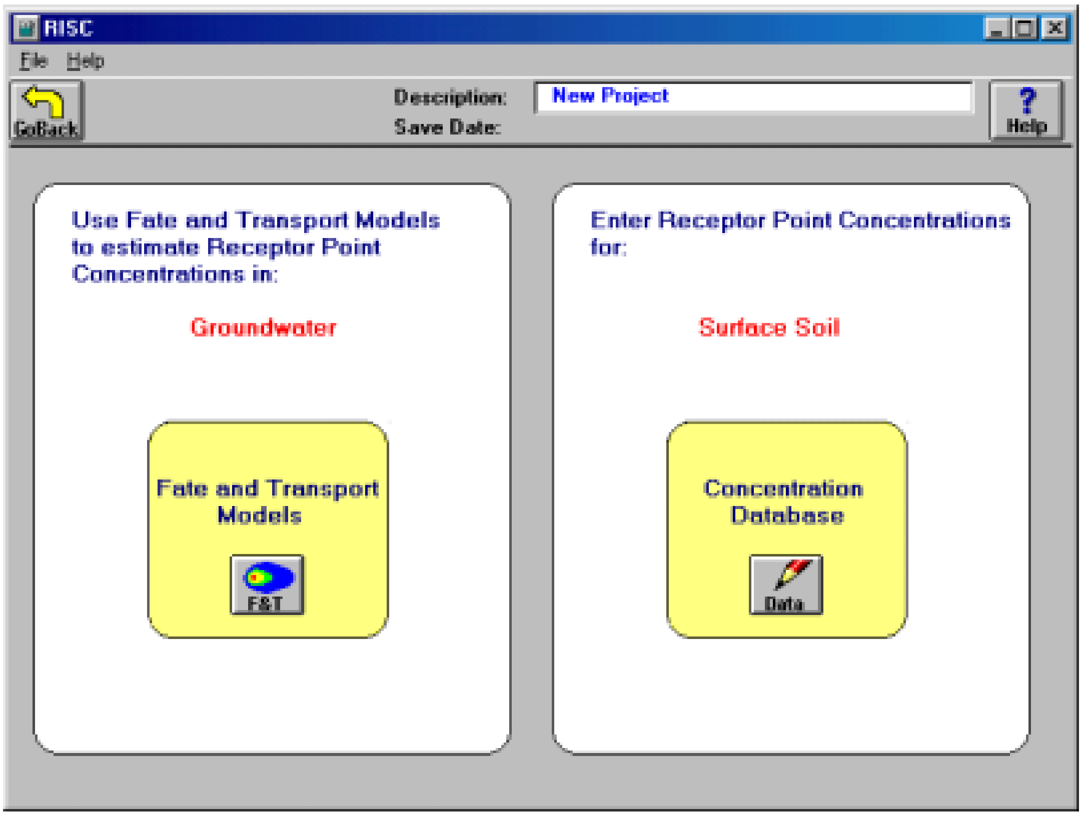


The third step in RISC is to determine receptor point concentrations for the various media of concern specified in Step 2: Choose Exposure Pathways. The Step 3 interface will appear differently depending on the choices made in Step 2. There are two methods for determining receptor point concentrations; the user can enter receptor point concentrations directly into RISC, or the user can enter source zone concentrations and then utilize chemical fate and transport models to estimate the receptor point concentrations. The method(s) to be used in Step 3 are determined by the choices made in Step 2. The Step 3 interface and options will be the same for “Human Health” and “Ecological/Water Quality” if the same models are chosen in Step 2. This chapter will describe how to use both the direct option and the modeling options for estimating receptor point concentrations.

If the concentrations in one media are to be estimated with fate and transport models, and concentrations in another media are to be entered directly, the interface will appear as in Figure 5-1. For the screen shown, a chemical fate and transport model is to be used to estimate receptor point groundwater concentrations and the receptor point concentrations in soil will be entered directly. If all the media of concern are to have concentrations entered directly, or all the media are to be modeled, the screen shown in Figure 5-1 will not appear.

5.1 USER-SPECIFIED CONCENTRATIONS

Receptor point concentrations can be specified directly by the user (as opposed to using fate and transport models) for any receptor media. There are three different ways the concentrations may be entered directly by the user: (1) as a single value, (2) as a Monte Carlo Distribution, or (3) by building a site sample database. Figure 5-2 shows the screen with the three options as they appear for an example with soil as the media of concern.


Description: New Project
Save Date:

Use Fate and Transport Models to estimate Receptor Point Concentrations in:

Groundwater

Enter Receptor Point Concentrations for:

Surface Soil

FIGURE 5-1. Main Screen for Step 3

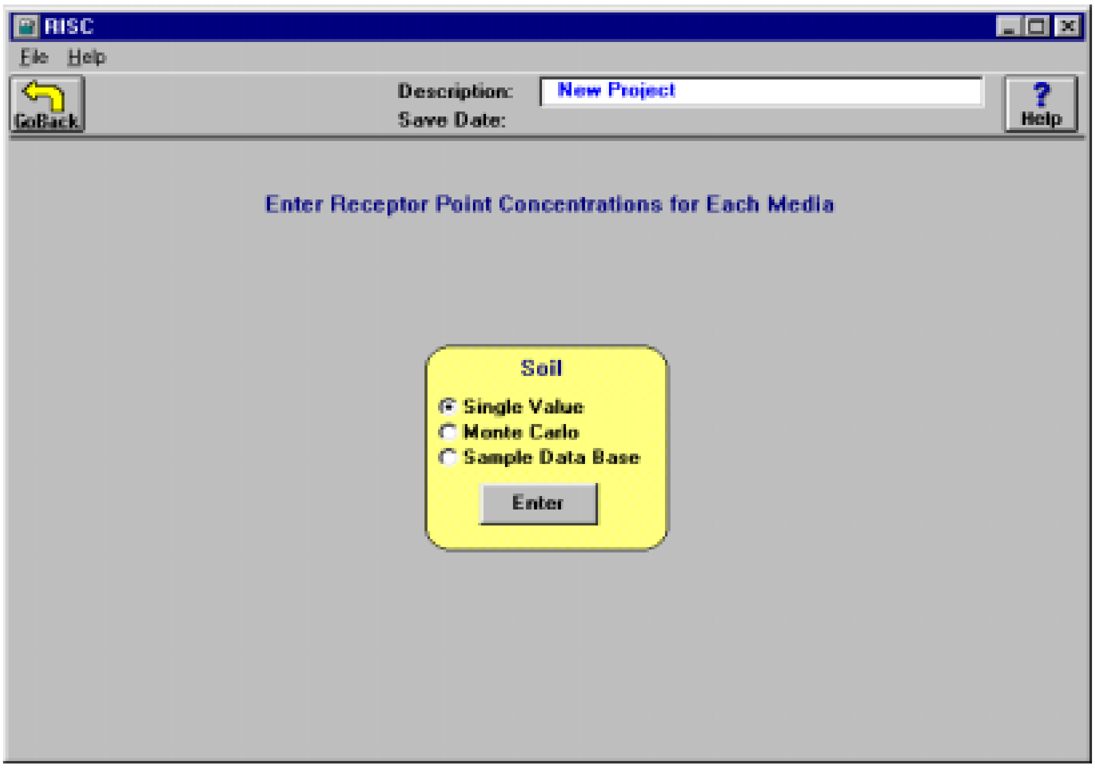
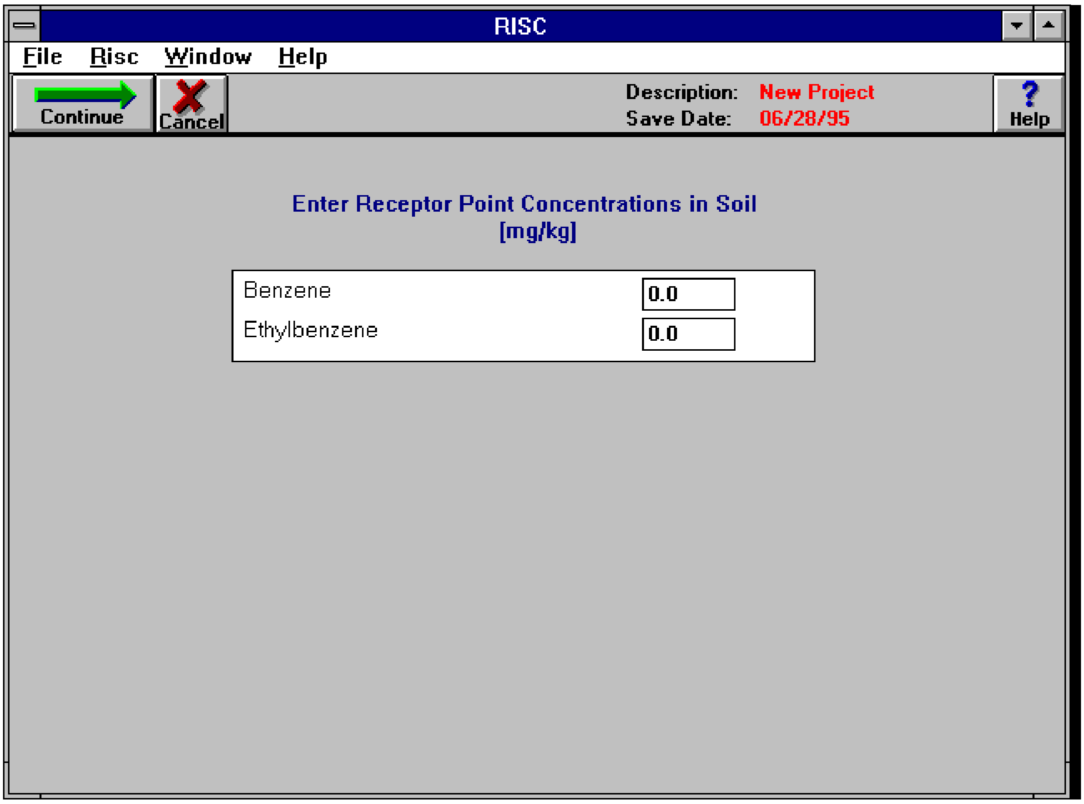


FIGURE 5-2. The Three Choices for Specifying Concentrations Directly

5.1.1 Single Value

This option is used to specify concentrations when a point value or single deterministic value is known. In this case the user will be asked to enter one concentration value for each chemical of concern. This concentration will then be used to calculate risk in Step 5. Even if a Monte Carlo analysis for the exposure parameters is chosen in Step 4 (see next chapter), the user is still free to choose to use a single media concentration, which will then be treated as constant in the Monte Carlo analysis.

Figure 5-3 shows the input screen for entering receptor point concentrations in surface soil. The values entered here will only be used for ingestion of soil, dermal contact with soil, and/or vegetable ingestion - they are not the source term for any fate and transport models. The soil concentrations entered in the screen shown in Figure 5-3 should be reflective of the concentrations that receptors are likely to come in contact with - usually the top meter of soil for residential or no deeper than typical excavation depths for a construction scenario. If the user also selects any pathways involving leaching or volatilization from subsurface soils, then a second soil concentration will be required in a later step to represent the source term for the models.



Description: New Project
Save Date: 06/28/95

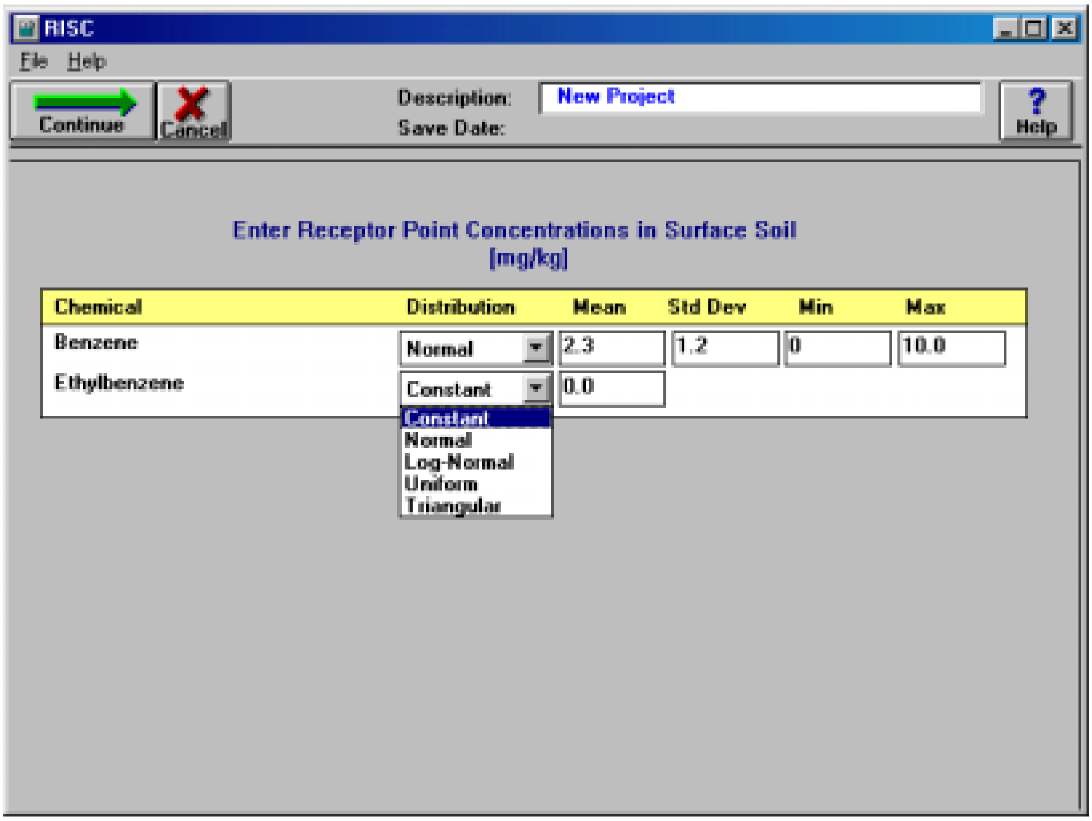
Enter Receptor Point Concentrations in Soil
[mg/kg]

Benzene	0.0
Ethylbenzene	0.0

FIGURE 5-3. Entering Single Values for Receptor Point Concentrations

5.1.2 Monte Carlo Distributions

The second option for entering receptor point concentrations is to specify a "Monte Carlo Distribution" for each concentration. These distributions are used for the "Monte Carlo" option described in the next chapter. Figure 5-4 shows the input screen for specifying Monte Carlo distributions. Note the options for the statistical distributions are chosen by clicking on the "down arrow" next to the distribution description box.



Description: New Project

Save Date:

Enter Receptor Point Concentrations in Surface Soil
[mg/kg]

Chemical	Distribution	Mean	Std Dev	Min	Max
Benzene	Normal	2.3	1.2	0	10.0
Ethylbenzene	Constant	0.0			

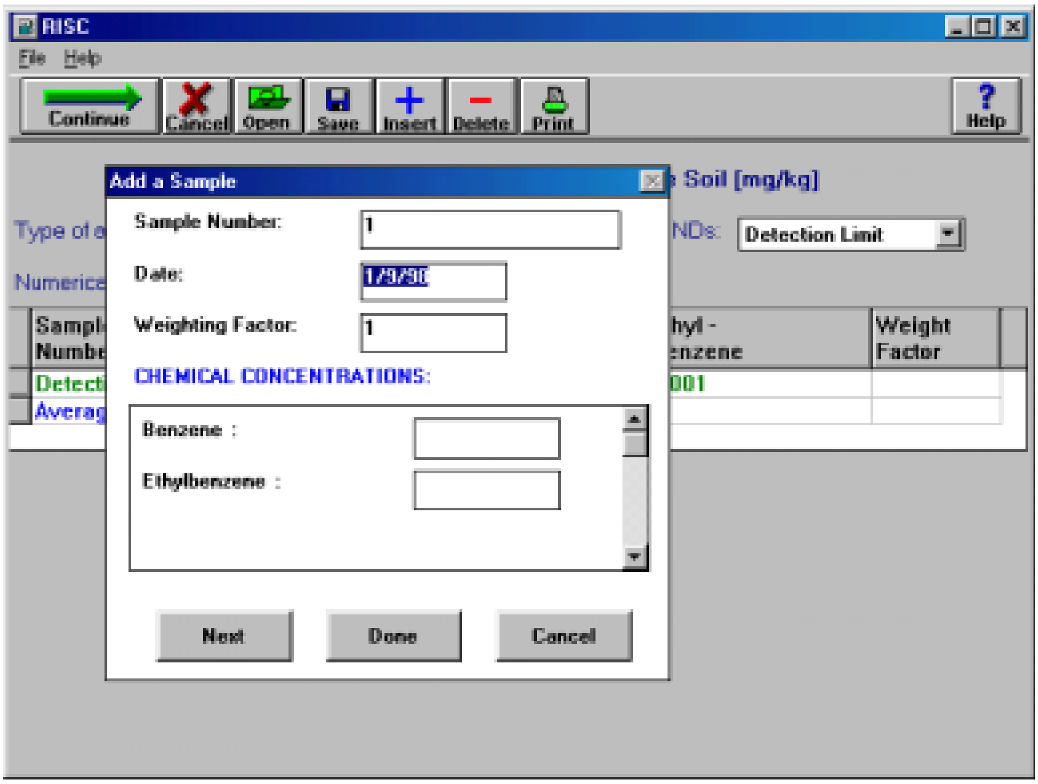
FIGURE 5-4. Entering Monte Carlo Distributions

The user may select between five distributions: Constant, Normal, Log-Normal, Uniform, or Triangular. These distributions are described in the next chapter (6.0 Describe the Receptors) under the Monte Carlo section. Note, when a distribution is chosen, the edit boxes required to describe the distribution appear. For example in Figure 5-4, benzene concentration in soil is described as having a normal distribution with the mean, standard deviation, minimum and maximum shown. If Monte Carlo distributions are specified, but a deterministic analysis is performed in Step 4, the mean value will be used in the risk calculation.

5.1.3 Sample Data Base

The RISC Sample Data Base is provided as a tool for users to summarize their site data, and if appropriate, to calculate means of the data to be used as inputs to the software. The sample data base can be used for both receptor point concentrations and for source concentrations that serve as inputs to fate and transport models.

The sample data base option is used when more than one (hopefully many more) measured concentrations exist for the chemicals of concern (i.e. multiple samples or analytical results). The data may consist of samples from different locations on the site, or it may consist of multiple samples taken at one location over time. In both cases, the sample data base is used to summarize the site data for purposes of estimating receptor point concentrations. Once all the samples are entered, the user must select a method for handling "Non-Detects" (NDs) data points and for averaging the concentration data in order to derive a value that is used to calculate risk in Step 5. When the Sample Data Base option is chosen the user will be prompted to enter concentration data for each sample (Figure 5-5).



Sample Number: 1

Date: 1/9/98

Weighting Factor: 1

NDs: Detection Limit

CHEMICAL CONCENTRATIONS:

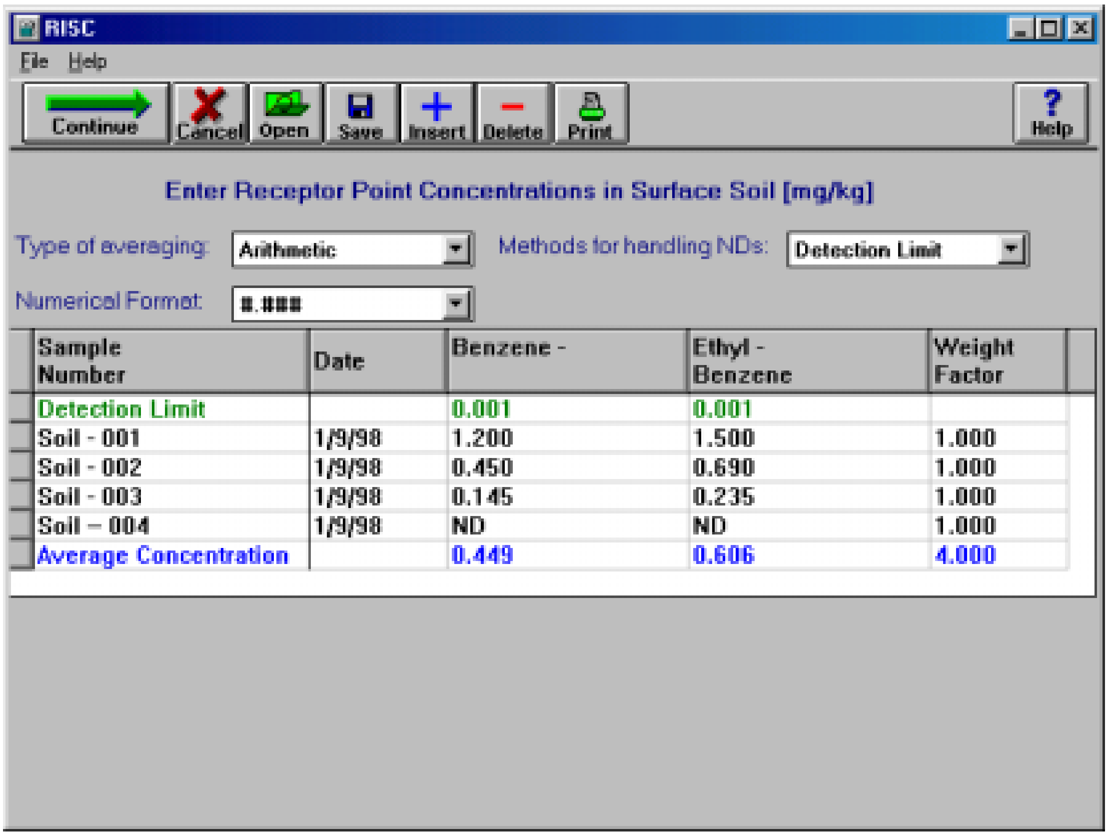
Benzene :

Ethylbenzene :

FIGURE 5-5. Entering Concentrations in the Sample Data Base

Default values have been provided for the Sample Name, Date, and Weighting Factor, however, the user is encouraged to change them to reflect the actual sample description and sampling date. The Weighting Factor is discussed below. Concentrations should be entered in the "Chemical Concentration" edit boxes, selecting "Next" to go onto the next sample. When all the samples have been entered, select "Done" to close the "Add a Sample" window and to view the data base. Figure 5-6 shows the Sample Data Base with four samples entered.

This database shows four samples, labeled Soil-001 to Soil-004, collected on 1/9/98. The concentration averaging type used in this example is "Arithmetic" so the average concentration shown in the last line corresponds to the arithmetic mean of all the concentrations for each chemical. In Figure 5-6, the method chosen to handle NDs is to use the detection limit in averaging; therefore a value of “0.001” was substituted for Soil – 004 when calculating the average. The average concentration line is not editable. The concentrations shown in the "Average Concentration" line are the values that will be used to calculated risk. To change the method of calculating average concentration, select from the "Type of Averaging" options in the drop down list at the top of the sample data base. All the rest of the lines in the data base are editable so the user can change values after the samples have been entered.



Enter Receptor Point Concentrations in Surface Soil [mg/kg]

Type of averaging: Arithmetic

Methods for handling NDs: Detection Limit

Numerical Format: #.###

Sample Number	Date	Benzene -	Ethyl - Benzene	Weight Factor
Detection Limit		0.001	0.001	
Soil - 001	1/9/98	1.200	1.500	1.000
Soil - 002	1/9/98	0.450	0.690	1.000
Soil - 003	1/9/98	0.145	0.235	1.000
Soil – 004	1/9/98	ND	ND	1.000
Average Concentration		0.449	0.606	4.000

FIGURE 5-6. The Sample Data Base with Four Samples

Method for Handling Non-Detects

For purposes of concentration averaging, the user must choose a method for handling non-detect values. There are three options. The NDs may be averaged using the detection limit, 1/2 the detection limit, or they may be considered equal to zero.

Detection Limits

The detection limit for each chemical is shown on the first line of the data base. If there are "non-detects" (NDs) entered in the data set, it is important to make sure that the detection limit is entered correctly. In this example, the soil detection limits are 0.001 mg/kg for both benzene and ethylbenzene. The detection limits may be changed by clicking on the box containing the value and typing a new value. To move to another cell (and save the change) either press the "Enter" key or the "Tab" key.

Type of Averaging

The concentrations for each chemical are averaged to get a concentration to use for calculating risk. There are five different options for averaging the concentrations: arithmetic, geometric, weighting factors, 95th Upper Confidence Level (UCL) of the Mean assuming a Normal distribution, and 95th Upper Confidence Level (UCL) of the Mean assuming a log-normal distribution.

The arithmetic mean can be used if the underlying distribution of concentrations is normal. It is calculated as follows:

$$\bar{C} = \frac{\sum_{i=1}^{n} C_i}{n} \qquad \textbf{(5-1)}$$

where

$\bar{C}$ = average concentration

n = number of samples

i = counter for sample number

C_i = concentration for sample i

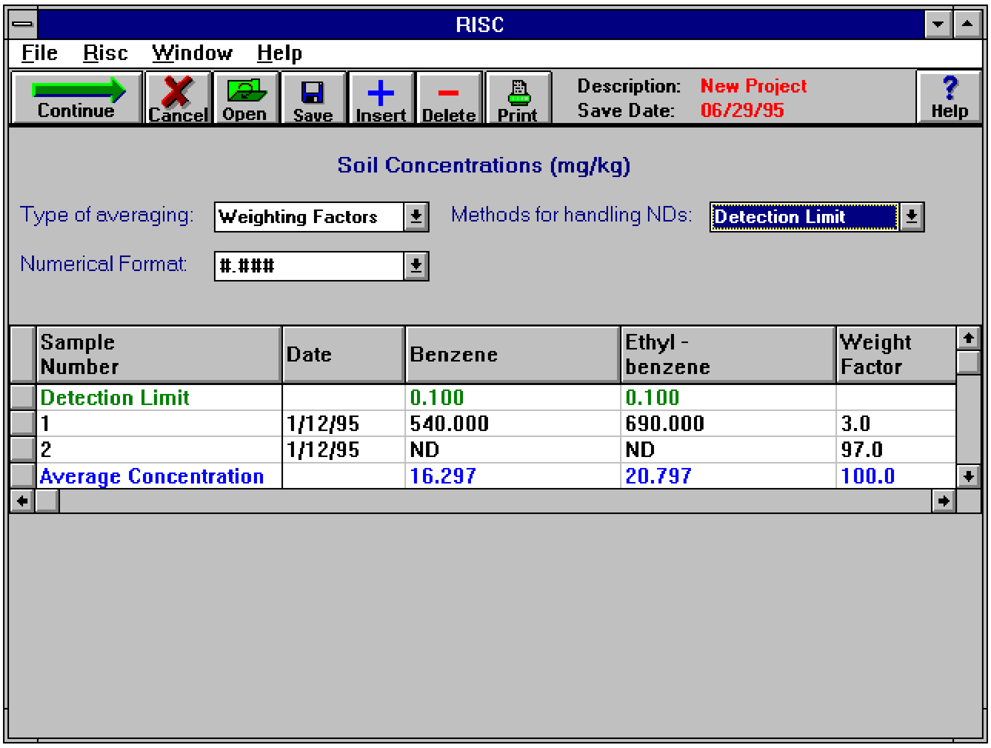
The geometric mean can be used if the underlying distribution is log-normal (usually assumed to be the case for concentration data). The geometric mean is calculated from:

$$\bar{C} = [C_1 * C_2 * C_3 * \ldots C_n]^{\frac{1}{n}} \qquad \textbf{(5-2)}$$

The geometric mean cannot be used with any zeros entered for concentrations in the data base or for the option of considering NDs as zero.

Weighting Factors

The Weighting Factor option for calculating average concentrations uses the "Weight Factor" column from the data base. This factor assigns a relative weight to each sample entered in the data base. The weight may correspond to the area of the site (or groundwater) that is assigned the given sample concentration, or, it may correspond to the number of samples at the reported concentration. Figure 5-7 shows an example where a 100 m^2 site has been sampled extensively and found to have a hot spot of 3 m^2 and the samples taken from the rest of the site were below the detection limit.



Description: New Project
Save Date: 06/29/95

Soil Concentrations (mg/kg)

Type of averaging: Weighting Factors

Methods for handling NDs: Detection Limit

Numerical Format: #.###

Sample Number	Date	Benzene	Ethyl - benzene	Weight Factor
Detection Limit		0.100	0.100	
1	1/12/95	540.000	690.000	3.0
2	1/12/95	ND	ND	97.0
Average Concentration		16.297	20.797	100.0

FIGURE 5-7. Using the Weight Factors

In this case, two samples are entered, one with a weight of "3" and one with a weight of "97". The two weights correspond to the areas of the site represented by each concentration. (The units for weighting factor could be in area or just a relative number and it is not necessary that the sum of the weighting factors equals 1, 10, or 100, etc.) It is important to remember that the total area represented in the data base should correspond to the area that a receptor may come in contact with routinely. In other words, if the site is very large and it is reasonable to expect that a receptor may only work on a small area of the site, the database should be used to estimate concentrations over that small area.

When all the weight factors are equal to one, the average concentration estimated using the weighting approach will equal the arithmetic mean.

Upper Confidence Levels of the Mean

The methods described here are based on guidance provided by EPA (May, 1992). The EPA guidance was developed for Superfund sites and should be used cautiously for sites that do not meet the assumptions outlined here.

The 95 percent Upper Confidence Level (UCL) of a mean is defined as a value that, when calculated repeatedly for randomly drawn subsets of site data, equals or exceeds the true mean 95 percent of the time. The 95% UCL provides a conservative estimate of the average concentration, however, it should not be confused with the 95th percentile on the probability density function of site concentration data. The UCL approach should only be used with a large sample data set that is based on random sampling. If the sampling is performed at targeted "hot spots" or contains few data points, this method may generate UCL means that are higher than the maximum concentration detected. EPA recommends that the data sets consist of 20 to 30 samples in order to provide fairly consistent estimates of the UCL mean. Of course, a higher number of samples is even better. Data sets containing less than 10 samples provide poor estimates of the UCL mean concentration (i.e., there is a large difference between the sample mean and the 95% UCL).

Method for Calculating the 95% UCL of the Mean Assuming a Normal Distribution

In this approach the underlying data is assumed to be normally distributed. The 95% UCL is calculated as follows:

$$UCL = \overline{C} + t\left(\frac{s}{\sqrt{n}}\right) \qquad \textbf{(5-3)}$$

where

UCL = upper confidence limit (in units of concentration)

$\overline{C}$ = arithmetic mean of the concentrations

s = standard deviation of the data

t = Student-t statistic (for 95% UCL)

n = number of samples

The Student-t statistic has been programmed in RISC to calculate the 95% UCL.

Method for Calculating the 95% UCL of the Mean Assuming a Log-Normal Distribution

In this approach the underlying data is assumed to be log-normally distributed (usually the case for random concentration data). This is the method recommended by EPA (May, 1992) for randomly sampled Superfund sites. In this approach, the concentrations are transformed by taking the log of each. Then the mean and standard deviation is calculated for the transformed data. The 95% UCL is calculated as follows:

$$UCL = e^{\left(\overline{C} + 0.5s^2 + \frac{sH}{\sqrt{n-1}}\right)} \qquad \textbf{(5-4)}$$

where

UCL = upper confidence limit (in units of concentration)

$\overline{C}$ = arithmetic mean of the transformed concentrations

s = standard deviation of the transformed data

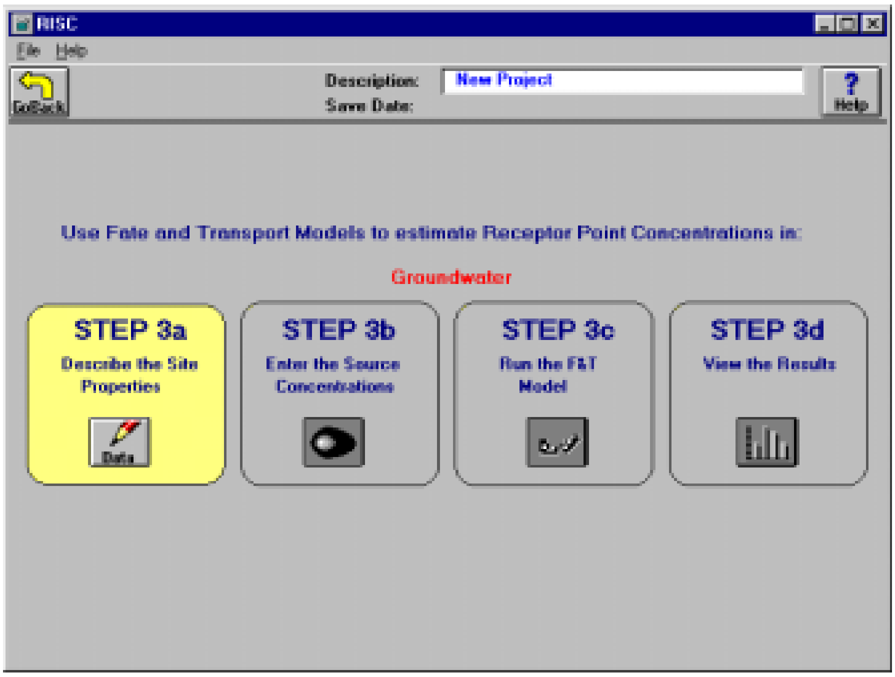
H = H-statistic (for 95% UCL)

n = number of samples

Tables of the H-statistic can be found in Gilbert (1987). The H-statistic has been programmed in RISC to calculate the UCL. The 95% UCL cannot be calculated for a log-normal distribution when any individual data point is zero or NDs are considered to be zero. The user must choose the NDs to be equal to the detection limit or 1/2 the detection limit.

5.2 FATE AND TRANSPORT MODELS

As an alternative to entering concentrations directly, fate and transport models can be used to estimate receptor point concentrations in groundwater, surface water, outdoor air, or indoor air. The models to be used in this step are determined by the choices made in Step 2. Figure 5-8 shows the four basic steps in using the fate and transport models.



Description: New Project
Save Date:

Use Fate and Transport Models to estimate Receptor Point Concentrations in:

Groundwater

STEP 3a
Describe the Site Properties

STEP 3b
Enter the Source Concentrations

STEP 3c
Run the F&T Model

STEP 3d
View the Results

FIGURE 5-8. The Four Steps of the Fate and Transport Screen

Step 3a: Describe the Site Properties

In this step, the user is asked to enter site-specific data needed to run the model(s) chosen. Figure 5-9 shows the input screen that appears when a "Dissolved Source GW model" is chosen to estimate receptor point concentrations in groundwater.

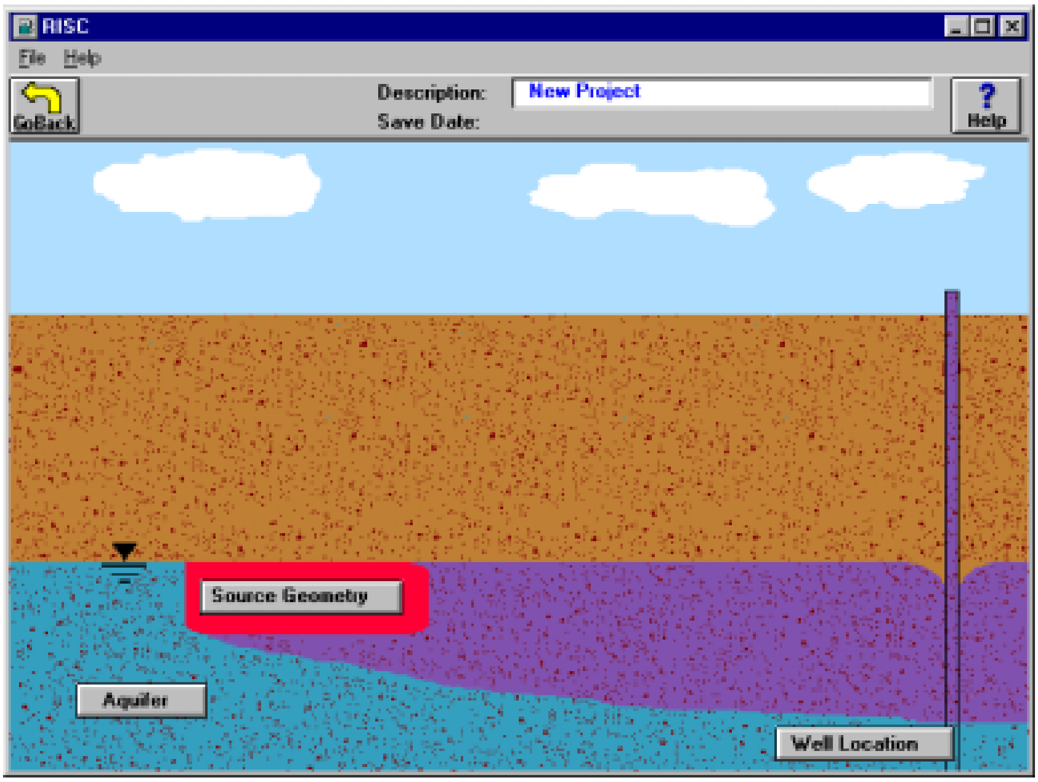
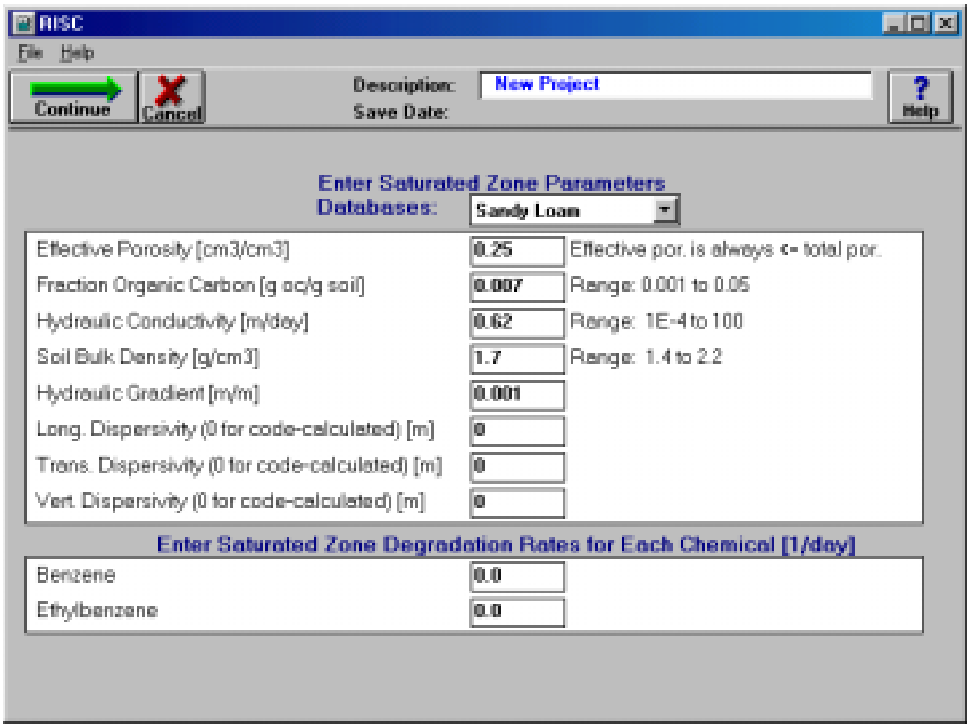


FIGURE 5-9. Describing the Site for the Dissolved Concentrations Model

In this example there are only three groups of data that need be entered: Source Geometry, Aquifer properties, and the Well Location. Depending on the model(s) chosen, the screen in Figure 5-9 will look different and there will be additional groups of data required. Note that when asked to specify aquifer or soil properties, the user is provided with suggested default values and parameter ranges for up to 9 soil types, ranging from gravel to clay. An example of the parameter input screens is shown in Figure 5-10. This screen shows the input parameters needed to specify aquifer properties in the saturated zone. The drop-down list (with "Sandy Loam" shown) allows the user to select a different default soil type. When the down arrow on the drop-down list is selected the vertical scroll bar (shown in Figure 5-11) can be used to view all the soil data types.



Description: New Project
Save Date:

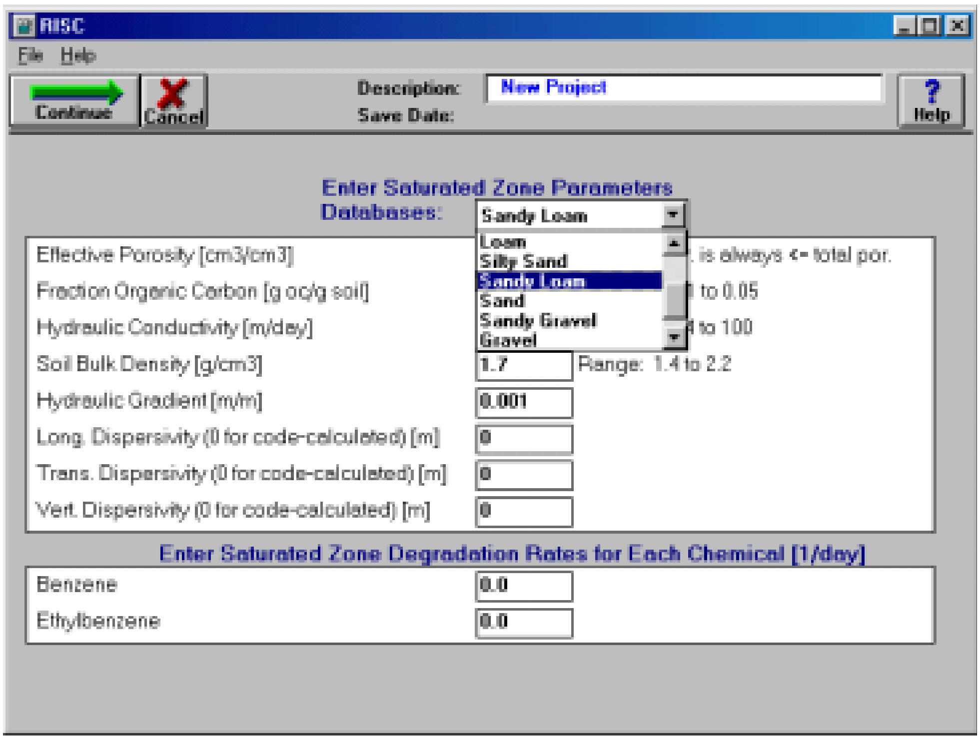
Enter Saturated Zone Parameters
Databases: Sandy Loam

Effective Porosity [cm3/cm3]	0.25	Effective por. is always <= total por.
Fraction Organic Carbon [g oc/g soil]	0.007	Range: 0.001 to 0.05
Hydraulic Conductivity [m/day]	0.62	Range: 1E-4 to 100
Soil Bulk Density [g/cm3]	1.7	Range: 1.4 to 2.2
Hydraulic Gradient [m/m]	0.001	
Long. Dispersivity (0 for code-calculated) [m]	0	
Trans. Dispersivity (0 for code-calculated) [m]	0	
Vert. Dispersivity (0 for code-calculated) [m]	0	

Enter Saturated Zone Degradation Rates for Each Chemical [1/day]

Benzene	0.0
Ethylbenzene	0.0

FIGURE 5-10. Input Parameter Screen for Aquifer



Description: New Project
Save Date:

Enter Saturated Zone Parameters
Databases: Sandy Loam

Effective Porosity [cm3/cm3]		. is always <= total por.
Fraction Organic Carbon [g oc/g soil]		l to 0.05
Hydraulic Conductivity [m/day]		4 to 100
Soil Bulk Density [g/cm3]	1.7	Range: 1.4 to 2.2
Hydraulic Gradient [m/m]	0.001	
Long. Dispersivity (0 for code-calculated) [m]	0	
Trans. Dispersivity (0 for code-calculated) [m]	0	
Vert. Dispersivity (0 for code-calculated) [m]	0	

Enter Saturated Zone Degradation Rates for Each Chemical [1/day]

Benzene	0.0
Ethylbenzene	0.0

FIGURE 5-11. Input Parameter Screen Showing Soil Property Database Selection

Table 5-1 shows the default values contained in the soil properties database. The soil bulk density for all soil types has been set to 1.7 g/cm^3. Since this parameter is almost always measured during field work, it is suggested that the user update it with the site specific value.

These soil properties are based on best professional judgment and they are not necessarily conservative. They are discussed in detail in the appendices containing the model descriptions (Appendices A through E). The van Genuchten's n parameter is used to calculate water content in the unsaturated zone and is described in both Appendix A and Appendix C.

Step 3b: Enter the Source Concentrations

The source concentrations required to run the fate and transport models are entered in this step. Depending on the model(s) selected, the source may be a dissolved phase concentration in groundwater, a soil concentration in the vadose zone, or a soil concentration in/at the water table. Table 5-2 lists the models available and the type of source term required.

Table 5-1. Soil Properties Database

SOIL TYPE	Total Porosity* cm^3/cm^3	Effective Porosity** cm^3/cm^3	Irreducible Water Content cm^3/cm^3	Fraction Organic Carbon g oc/g soil	Saturated Hydraulic Conductivity m/d	van Genuchten's n Parameter -	Height Capillary Fringe cm	Air Content Capillary Fringe cm^3/cm^3	Water Content in Soil Below Building cm^3/cm^3	Intrinsic Permeability (for advection of vapors) cm^2
Clay	0.45	0.20	0.17	0.02	0.015	1.09	152	0.005	0.40	1E-13
Silty Clay	0.40	0.25	0.21	0.015	0.022	1.09	152	0.005	0.32	1E-11
Silt	0.35	0.25	0.21	0.005	0.25	1.37	152	0.005	0.25	1E-11
Silty Loam	0.35	0.30	0.17	0.008	0.16	1.41	50	0.005	0.22	1E-9
Loam	0.30	0.25	0.15	0.008	0.32	1.56	50	0.005	0.18	1E-8
Sandy Loam	0.25	0.25	0.1	0.007	0.62	1.89	10	0.01	0.15	1E-8
Silty Sand	0.25	0.20	0.12	0.005	0.86	1.5	50	0.005	0.15	1E-10
Sand	0.30	0.30	0.05	0.002	5	2.68	10	0.01	0.12	1E-7
Sandy Gravel	0.25	0.25	0.04	0.002	10	2.7	5	0.03	0.10	1E-6
Gravel	0.30	0.30	0.03	0.002	20	2.7	5	0.03	0.10	1E-5

*Total porosity (i.e., all the void space) is used in the vadose zone and vapor models.
**Effective porosity (i.e., the 'connected' void space) is used in the saturated zone model.

Table 5-2. List of Fate and Transport Models and Source Terms Required for Each Model

Fate and Transport Model	**Source Term Required for Model**	**Receptor Point Concentration Estimated by Model**
Vadose Zone Model *Linked With Groundwater Model*	Soil Concentrations in the Vadose Zone	Groundwater
Dissolved Phase Source *Groundwater Model*	Groundwater Concentrations	
Saturated Soil *Groundwater Model*	Soil Concentrations in Saturated Zone	
Johnson and Ettinger Model *Vapor Transport Model Without Degradation*	Soil or Soil Gas Concentrations in the Vadose Zone	Indoor or Outdoor Air
Dominant Layer Model *Vapor Transport Model considering Degradation*		
Oxygen-Limited Model *Vapor Transport Model Considering Degradation*		
Vapor Emissions from Groundwater	Groundwater Concentrations or Use Linked With One of the Groundwater Models	

Step 3c: Run the F&T Model

In this step, the simulation time and source pulse length are entered. The source pulse length, which is used for the dissolved concentrations groundwater model only, is the time the source is active, i.e. before it is either physically removed or assumed to be depleted (either intrinsically or by active remediation). The fate and transport models are run once (automatically) for each chemical of concern. When the simulations have finished the user is notified to continue.

Step 3d: View the Results

In this step, the user can view tables and charts of the model results. The options for the types of tables and charts will vary depending on the model(s) run. There is always an “Model Input Summary” listing all of the input parameter values. The other tables summarize concentrations in one media (per table) or model calculations and are designed for quick review or for inclusion in the modeling write-up.

Both the tables and charts can be transferred to another software application (such as a word processor) by clicking on the 'Copy' button. Then the user can minimize or close the RISC main screen, open the new destination software, and choose "Paste" (or the Shift and Insert keys). The tables and charts can also be printed directly from the model results screens. Note: these tables are not tab-delimited so they look best in Word when displayed with a courier (or other fixed point size) font.

Chapter

6.0

Describe The Receptors

STEP 4

Describe the Receptors

The screens in this step appear differently depending on the type of analysis chosen in Step 2 (human health or ecological). These two options are described in the following sections.

6.1 HUMAN HEALTH

In Step 4, the receptor(s) of concern are chosen and the receptor-specific intake parameters are entered. The RISC software contains both deterministic and stochastic (Monte Carlo input) default data on exposure for many different types of receptors. The user is free to use the default data provided or to change the intake parameters to reflect actual site-specific values. Figure 6-1 shows the main screen for Step 4.

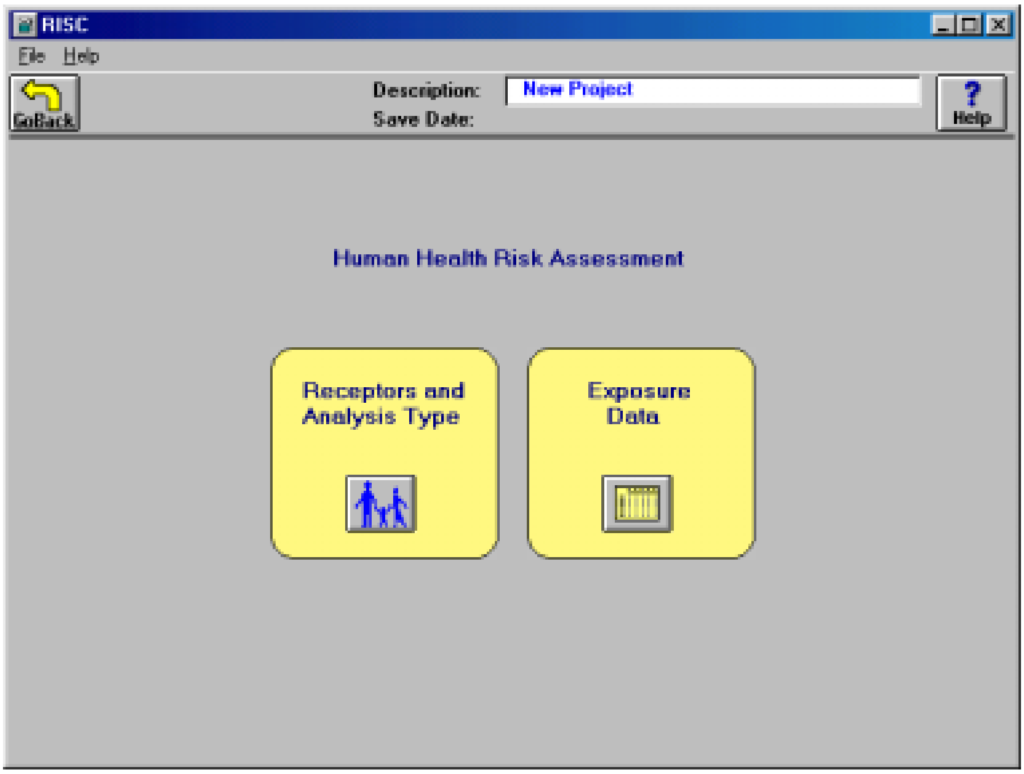


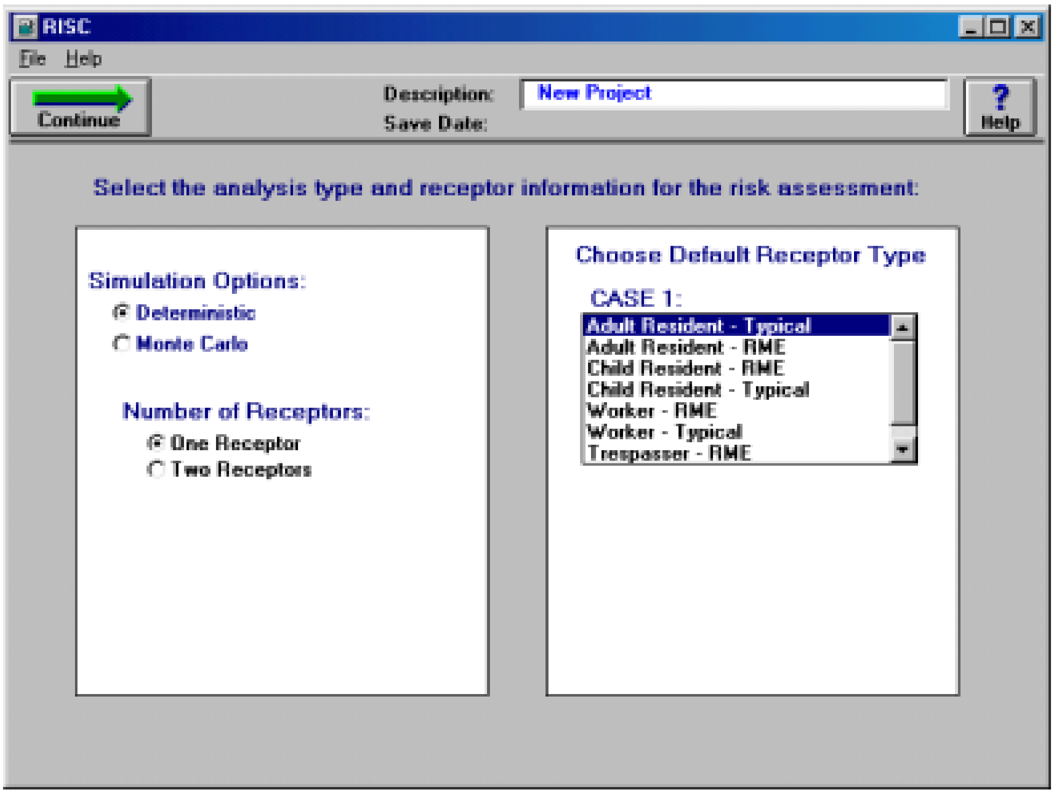
FIGURE 6-1. The Two Steps Required to Describe the Receptor(s)

6.1.1 STEP 4a: CHOOSE RECEPTORS AND ANALYSIS TYPE

The decisions that must be made in this step are:

- Will the analysis be deterministic or Monte Carlo?
- If deterministic, will one or two receptors of concern be considered?
- If two receptors are being considered, are the exposures to be summed (e.g. a receptor is considered as both a child and an adult)?
- Are default, or user-specified, site-specific exposure parameters and/or Monte Carlo distributions to be used?

Figure 6-2 shows the input screen for Step 4a.



Description: New Project
Save Date:

Select the analysis type and receptor information for the risk assessment:

Simulation Options:
● Deterministic
○ Monte Carlo

Number of Receptors:
● One Receptor
○ Two Receptors

Choose Default Receptor Type
CASE 1:
Adult Resident - Typical
Adult Resident - RME
Child Resident - RME
Child Resident - Typical
Worker - RME
Worker - Typical
Trespasser - RME

FIGURE 6-2. Input Screen for Step 4a

One the left side of the input screen the user must choose between: (1) performing a deterministic or Monte Carlo analysis, (2) if deterministic, to evaluate one or two receptors, and (3) if two receptors, whether or not to calculate the additive case. These options are described in the following sections.

On the right side of the input screen the default receptor types are listed. If only one receptor is to be analyzed, then a lower box ("Case 2:") will not be shown. There are eight receptors types to choose from for the deterministic case and four for the "Monte Carlo" case. The default receptor types and the potential exposure routes considered for each are shown in Table 6-1 (all tables appear at the end in this chapter). The choices made here will affect how the exposure data input screen appears.

6.1.1.1 Deterministic and Monte Carlo Analyses

The risk calculations may be performed in either a deterministic mode or using Monte Carlo sampling. The deterministic mode means that a single value (point estimate) will be used for each intake parameter and therefore a single value of risk will be calculated for the analysis.

In a Monte Carlo analysis, on the other hand, probability distributions are specified for each of the input parameters and values are randomly drawn from these input distributions. The model is run many times (recommended 1000 to 10,000 iterations) and the resultant risks are evaluated statistically. The Monte Carlo analysis is a powerful tool for estimating exposures when population distribution data exists. The results indicate the wide range of exposures that might occur as well as the probability of each exposure happening. The results from a Monte Carlo analysis can be presented by summarizing the output statistics in tabular form or by generating probability density functions or cumulative probability density functions of the output. These output options are described in Sections 8.1 and 8.2.

6.1.1.2 One or Two Receptors

The risk analysis may be performed for one or two receptors simultaneously. When two receptors are chosen, the results between the two may be compared in the same table or chart. For example, one might examine the effect of changing exposure assumptions by comparing very conservative exposure parameter estimates with that calculated for a more representative “average” member of the population. The default “typical” exposure inputs correspond to this latter case, while the default “RME” (reasonable maximum exposure) inputs correspond to the conservative parameter estimates.

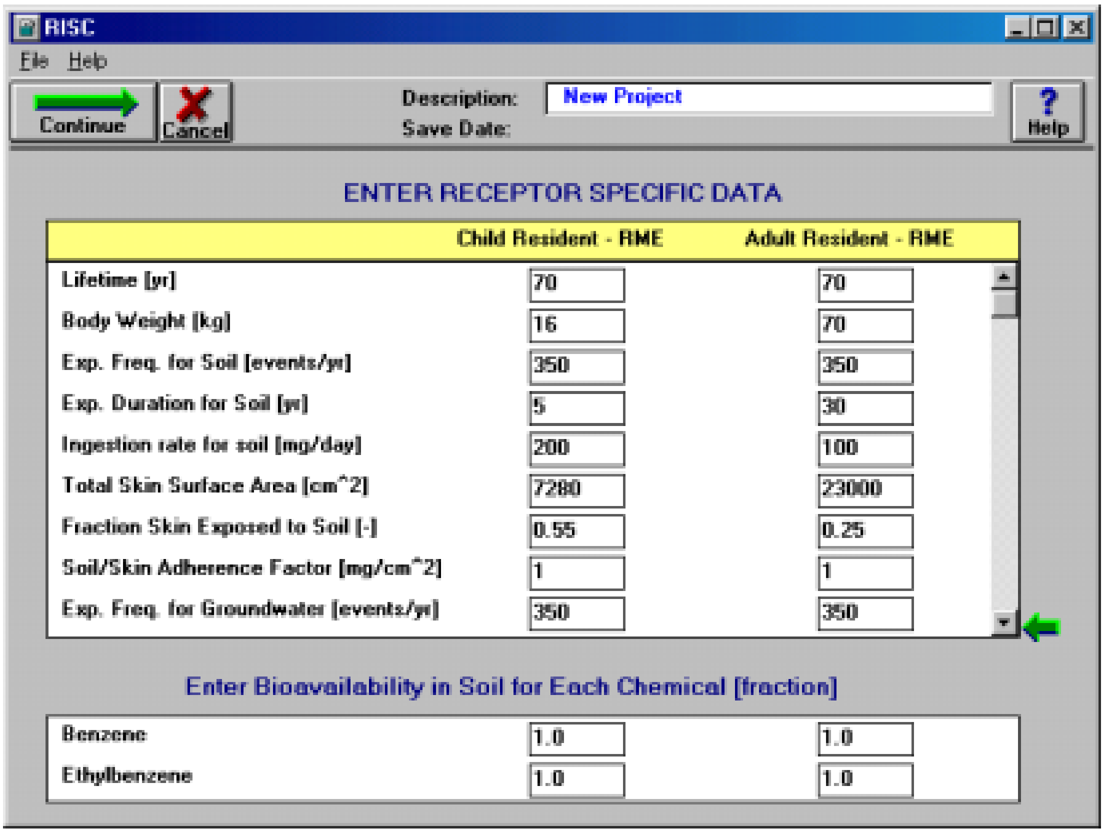
6.1.1.3 Additive Case

In the additive case the exposures for two receptors are evaluated and then summed. This option can be used for the situation where the user wants to consider a residential receptor that is assumed to be a child for a certain number of years (with appropriate child intake values) and an adult for a certain number of years.

6.1.2 STEP4b: ENTER EXPOSURE DATA

For deterministic analysis, default sets of intake parameters have been developed for a “Reasonable Maximum Exposure” (RME) and a “Typical Exposure” for adults, children, workers, and trespassers for a total of eight data sets. The “Reasonable Maximum Exposure” is a term originally used by USEPA to refer to an 85-95 percentile exposure when given a cumulative probability distribution of exposure values. It has since also been used to refer to an exposure risk from a pathway (e.g. vapor inhalation in a shower) in which individual exposure parameters that define the pathway (e.g. time in the shower, flow and temperature of the water, etc) are conservatively selected from the 85-95 percentile of their individual distributions. In this latter case, the overall pathway risk often exceeds the 95 percentile of the cumulative probability distribution of exposure values. Thus, the RME exposure scenario is typically regarded as a very conservative exposure scenario, but is often used as a base case for calculations (e.g. in the development of a RBCA Tier 1 Look-Up Table). Because the RME exposure is generally considered to be overly conservative, a “Typical” default set of exposure inputs is also included in RISC. These are more representative of the characteristics of an “average” member of the general population, rather than a “maximum exposed individual” (MEI).

Tables 6-2 through 6-5 show the deterministic default values for the receptors. There are many parameters that are highly site-specific such as exposure duration and frequency. The database has default values for these parameters, however, it is important to use site-specific data where available. Figure 6-3 shows the input screen for a deterministic case with two receptors. Because ingestion of soil was chosen in Step 2, the user is asked to enter soil bioavailability values for each chemical. (Bioavailability reflects the fact that not all the contaminant that is present in the soil - and extractable with a solvent - is actually toxic to a human because it is not available for uptake or capable of being metabolized.) If no soil routes had been chosen, this second lower window would not appear. Note the arrows indicate that additional exposure parameters must be accessed by using the scroll bar.



Description: New Project
Save Date:

ENTER RECEPTOR SPECIFIC DATA

	Child Resident - RME	Adult Resident - RME
Lifetime [yr]	70	70
Body Weight [kg]	16	70
Exp. Freq. for Soil [events/yr]	350	350
Exp. Duration for Soil [yr]	5	30
Ingestion rate for soil [mg/day]	200	100
Total Skin Surface Area [cm^2]	7280	23000
Fraction Skin Exposed to Soil [-]	0.55	0.25
Soil/Skin Adherence Factor [mg/cm^2]	1	1
Exp. Freq. for Groundwater [events/yr]	350	350

Enter Bioavailability in Soil for Each Chemical [fraction]

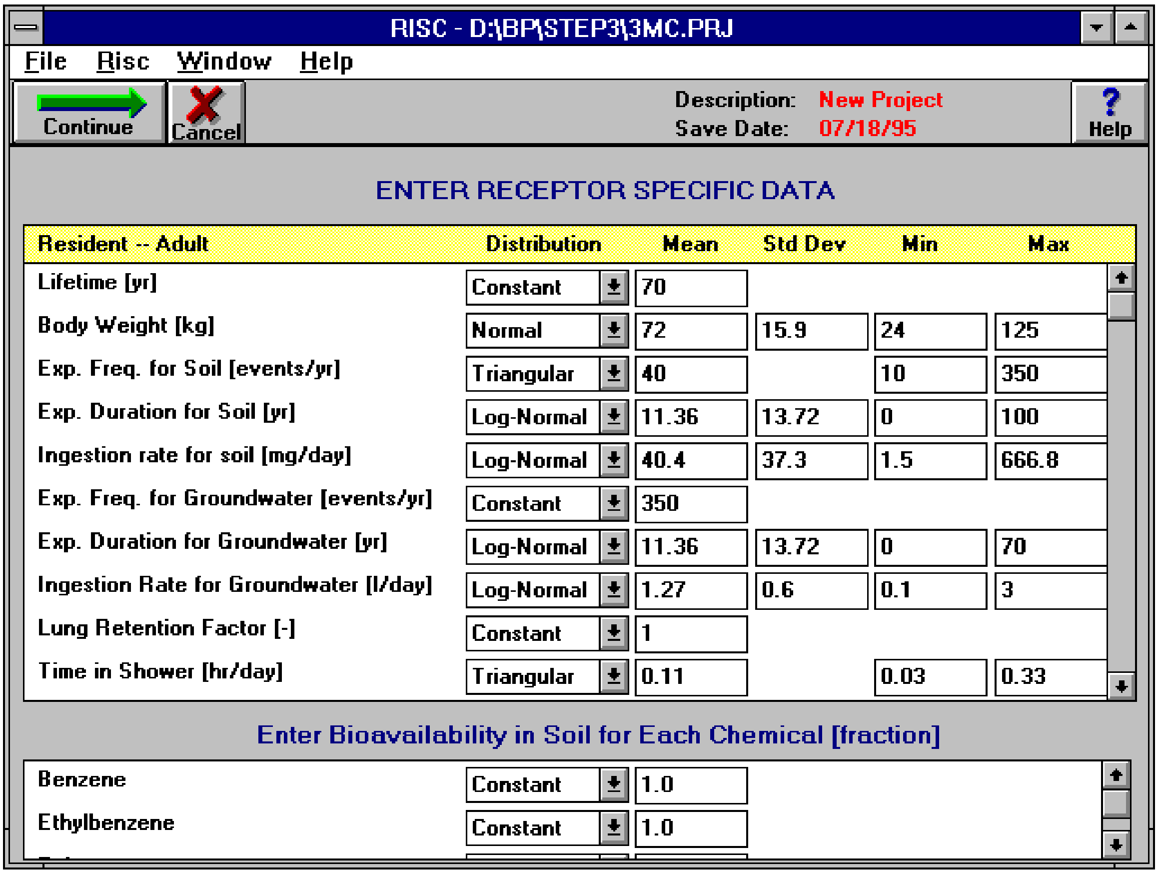
Benzene	1.0	1.0
Ethylbenzene	1.0	1.0

Figure 6-3. Input Screen for Step 4b for a Deterministic Analysis

Table 6-6 shows the default distributions for the Monte Carlo case. The majority of these distributions were extracted from the guidance document from the American Institute of Health Council (AIHC), entitled "Exposure Factors Sourcebook" (1994). Appendix H describes the methodology behind the development of these distributions.

Figure 6-4 shows the input screen for a Monte Carlo analysis. The distribution types are selected from the drop-down lists shown. When a distribution type is changed (e.g. from "Constant" to "Log-Normal") the boxes to the right change to reflect the required inputs for the selected distribution.

The constant distribution is defined with a single value in the "Mean" column. The normal and log-normal distributions must be defined with four statistics: mean, standard deviation, minimum and maximum. The triangular distribution is defined by the expected value (the peak of the triangle) entered in the "mean" box and by a minimum and a maximum (the x-axis parameter values where the two lines on the probability density function cross this axis).



Description: New Project
Save Date: 07/18/95

ENTER RECEPTOR SPECIFIC DATA

Resident -- Adult	Distribution	Mean	Std Dev	Min	Max
Lifetime [yr]	Constant	70			
Body Weight [kg]	Normal	72	15.9	24	125
Exp. Freq. for Soil [events/yr]	Triangular	40		10	350
Exp. Duration for Soil [yr]	Log-Normal	11.36	13.72	0	100
Ingestion rate for soil [mg/day]	Log-Normal	40.4	37.3	1.5	666.8
Exp. Freq. for Groundwater [events/yr]	Constant	350			
Exp. Duration for Groundwater [yr]	Log-Normal	11.36	13.72	0	70
Ingestion Rate for Groundwater [l/day]	Log-Normal	1.27	0.6	0.1	3
Lung Retention Factor [-]	Constant	1			
Time in Shower [hr/day]	Triangular	0.11		0.03	0.33

Enter Bioavailability in Soil for Each Chemical [fraction]

Benzene	Constant	1.0
Ethylbenzene	Constant	1.0

Figure 6-4. Input Screen for Step 4b for a Monte Carlo Analysis

Table 6-1. Default Receptor Types and Exposure Routes

Default Receptors Types for the Deterministic Case	Default Receptors Types for the Monte Carlo Case	Potential Exposure Routes Considered
Adult Resident – Typical Adult Resident – RME*	Adult Resident	Ingestion of Soil Dermal Contact with Soil Vegetable Ingestion from Soil Media Ingestion of Groundwater Dermal Contact with Groundwater Vegetable Ingestion from GW Media Inhalation in the Shower Inhalation of Outdoor Air Inhalation of Indoor Air Ingestion of Surface Water (Swimming) Dermal Contact with Surface Water Dermal Contact with Irrigation Water Ingestion of Irrigation Water Inhalation of Irrigation Water Spray
Child Resident - Typical Child Resident – RME*	Child Resident	Ingestion of Soil Dermal Contact with Soil Vegetable Ingestion from Soil Media Ingestion of Groundwater Dermal Contact with Groundwater Vegetable Ingestion from GW Media Inhalation in the Shower Inhalation of Outdoor Air Inhalation of Indoor Air Ingestion of Surface Water (Swimming) Dermal Contact with Surface Water Dermal Contact with Irrigation Water Ingestion of Irrigation Water Inhalation of Irrigation Water Spray
Trespasser - Typical Trespasser – RME*	Trespasser	Ingestion of Soil Dermal Contact with Soil Inhalation of Outdoor Air Ingestion of Surface Water (Swimming) Dermal Contact with Surface Water
Worker – Typical Worker – RME*	Worker	Ingestion of Soil Dermal Contact with Soil Ingestion of Groundwater Inhalation of Outdoor Air Inhalation of Indoor Air

*RME = Reasonable Maximum Exposure

Table 6-2. Intake Parameters for Adult Residents (page 1 of 2)

Parameter	Units	Reasonable Maximum Exposure	Typical Exposure
Common to All Routes			
Body Weight	kg	70	70
Lifetime	years	70	70
Exposure Duration	years	30	9
Exposure Frequency (unless specified under route-specific parameters)	days/year	350	350
Ingestion of Drinking Water			
Ingestion Rate	l/day	2	1.1
Dermal Contact While Showering			
Exposure Time	hours/day	0.2	0.12
Skin Surface Area	cm^2	23,000	18,400
Inhalation During Shower			
Exposure Time in Shower per day	hours/day	0.2	0.12
Inhalation Rate in Shower	m^3/hr	0.6	0.6
Volume of Bathroom	m^3	3	5.2
Flowrate of Shower Water	l/min	10	8
Temperature of Shower	^oC	48	45
Inhalation of Outdoor Air			
Exposure Time Outdoors	hours/day	2.5	1.1
Inhalation Rate Outdoors	m^3/hr	0.83	0.625
Inhalation of Indoor Air			
Exposure Time Indoors	hours/day	24	18.3
Inhalation Rate Indoors	m^3/hr	0.83	0.625
Dermal Contact with Soil			
Exposure Frequency	days/year	350	40
Total Skin Surface Area	cm^2	23,000	18,400
Fraction of Total Skin Surface Area Exposed to Soil	cm^2/cm^2	0.56	0.11
Soil to Skin Adherence Factor	mg/cm^2	0.2	0.2
Ingestion of Soil			
Exposure Frequency	days/year	350	40
Ingestion Rate	mg/day	100	40
Bioavailability in Soil	fraction	Chemical-Specific	Chemical-Specific

Table 6-2. Intake Parameters for Adult Residents (page 2 of 2)

Parameter	Units	Reasonable Maximum Exposure	Typical Exposure
Dermal Contact with Surface Water			
Exposure Frequency	days/year	36	5
Exposure Time	hours/day	2.6	2.6
Total Skin Surface Area	cm^2	23,000	18,400
Incidental Ingestion of Water While Swimming			
Exposure Frequency	days/year	36	5
Exposure Time	hours/day	2.6	2.6
Ingestion Rate	ml/hr	50	10
Dermal Contact with Irrigation Water			
Exposure Frequency	days/year	150	20
Exposure Time	hours/day	2	0.5
Total Skin Surface Area	cm^2	23,000	18,400
Fraction of Skin Surface Area for Dermal Contact with Water	fraction	0.5	0.1
Ingestion of Irrigation Water			
Exposure Frequency	days/year	150	20
Exposure Time	hours/day	2.6	0.5
Ingestion Rate	ml/hr	50	10
Inhalation of Irrigation Water Spray			
Exposure Frequency	days/year	150	20
Exposure Time	hours/day	2	0.5
Width of Sprinkler Spray	m	9	25
Temperature of Irrigation Water	^oC	25	20
Flowrate of Sprinkler	l/min	50	30
Diameter of Sprinkler Droplet	cm	0.2	0.2
Droplet Droptime	sec	5	5
Height of Breathing Zone	m	2	2
Average Wind Speed	m/sec	2.25	3.5
Ingestion of Vegetables			
Ingestion Rate for Above Ground Vegetables	g/day	127	127
Ingestion Rate for Root Vegetables	g/day	87.5	87.5
Fraction of Vegetables Grown in Contaminated Soil or Water	g/g	0.25	0.1
Fraction Organic Carbon in Garden Soil	g oc/g soil	0.05	0.05

Table 6-3. Intake Parameters for Child Residents (page 1 of 2)

Parameter	Units	Reasonable Maximum Exposure	Typical Exposure
Common to All Routes			
Body Weight	kg	15	15
Lifetime	years	70	70
Exposure Duration	years	6	6
Exposure Frequency (unless specified under route-specific parameters)	days/year	350	350
Ingestion of Drinking Water			
Ingestion Rate	l/day	1	0.5
Dermal Contact While Showering			
Exposure Time	hours/day	0.2	0.12
Skin Surface Area	cm^2	7280	6800
Inhalation During Shower			
Exposure Time in Shower per day	hours/day	0.2	0.12
Inhalation Rate in Shower	m^3/hr	0.6	0.6
Volume of Bathroom	m^3	3	5.2
Flowrate of Shower Water	l/min	10	8
Temperature of Shower	^oC	48	45
Inhalation of Outdoor Air			
Exposure Time Outdoors	hours/day	24	2.2
Inhalation Rate Outdoors	m^3/hour	0.83	0.83
Inhalation of Indoor Air			
Exposure Time Indoors	hours/day	24	19.6
Inhalation Rate Indoors	m^3/hour	0.83	0.625
Dermal Contact with Soil			
Exposure Frequency	days/year	350	130
Fraction of Total Skin Surface Area Exposed to Soil	cm^2/cm^2	0.55	0.13
Soil to Skin Adherence Factor	mg/cm^2	0.2	0.2
Ingestion of Soil			
Exposure Frequency	days/year	350	130
Ingestion Rate	mg/day	200	90
Bioavailability in Soil	fraction	Chemical-Specific	Chemical-Specific

Table 6-3. Intake Parameters for Child Residents (page 2 of 2)

Parameter	Units	Reasonable Maximum Exposure	Typical Exposure
Dermal Contact with Surface Water			
Exposure Frequency	days/year	36	5
Exposure Time	hours/day	2.6	2.6
Skin Surface Area	cm^2	7280	6800
Incidental Ingestion of Water While Swimming			
Exposure Frequency	days/year	36	5
Exposure Time	hours/day	2.6	2.6
Ingestion Rate	ml/hour	50	10
Dermal Contact with Irrigation Water			
Exposure Frequency	days/year	150	20
Exposure Time	hours/day	2	0.5
Total Skin Surface Area	cm^2	7280	6800
Fraction of Skin Surface Area for Dermal Contact with Water	fraction	0.5	0.1
Ingestion of Irrigation Water			
Exposure Frequency	days/year	150	20
Exposure Time	hours/day	2.6	0.5
Ingestion Rate	ml/hour	50	10
Inhalation of Irrigation Water Spray			
Exposure Frequency	days/year	150	20
Exposure Time	hours/day	2	0.5
Width of Sprinkler Spray	m	9	25
Temperature of Irrigation Water	^oC	25	20
Flowrate of Sprinkler	l/min	50	30
Diameter of Sprinkler Droplet	cm	0.2	0.2
Droplet Droptime	sec	5	5
Height of Breathing Zone	m	2	2
Average Wind Speed	m/sec	2.25	3.5
Ingestion of Vegetables			
Ingestion Rate for Above Ground Vegetables	g/day	55.8	55.8
Ingestion Rate for Root Vegetables	g/day	48.5	48.5
Fraction of Vegetables Grown in Contaminated Soil or Water	g/g	0.25	0.1
Fraction Organic Carbon in Garden Soil	g oc/g soil	0.05	0.05

Table 6-4. Intake Parameters for Workers

Parameter	Units	Reasonable Maximum Exposure	Typical Exposure
Common to All Routes			
Body Weight	kg	70	70
Lifetime	years	70	70
Exposure Duration	years	25	8
Exposure Frequency (unless specified under route-specific parameters)	days/year	250	250
Ingestion of Drinking Water			
Ingestion Rate	l/day	1	0.5
Inhalation of Volatile Soil Emissions			
Time Outdoors	hours/day	8	4
Inhalation Rate	m^3/hour	2.5	0.83
Dermal Contact with Soil			
Exposure Frequency	days/year	250	125
Fraction of Total Skin Surface Area Exposed to Soil	cm^2/ cm^2	0.57	0.11
Adherence Factor	mg/cm^2	0.2	0.2
Ingestion of Soil			
Exposure Frequency	days/year	250	125
Ingestion Rate	mg/day	100	40
Inhalation of Indoor Air			
Exposure Frequency	days/year	250	125
Exposure Time Indoors	hours/day	8	4
Inhalation Rate Indoors	m^3/hour	0.83	0.625

Table 6-5. Intake Parameters for Trespassers

Parameter	Units	Reasonable Maximum Exposure	Typical Exposure
Common to All Routes			
Body Weight	kg	42	42
Lifetime	years	70	70
Exposure Duration	years	12	9
Exposure Frequency (unless specified under route-specific parameters)	days/year	52	26
Inhalation of Volatile Soil Emissions			
Exposure Time	hours/day	3	1.5
Inhalation Rate	m^3/hr	2.3	1.68
Dermal Contact with Soil			
Fraction of Skin Surface Area Exposed to Soil	fraction	0.57	0.11
Adherence Factor	mg/cm^2	1	0.2
Ingestion of Soil			
Ingestion Rate	mg/day	100	40
Dermal Contact with Surface Water			
Exposure Frequency	days/year	36	5
Exposure Time	hours/day	2.6	2.6
Skin Surface Area	cm^2	16550	14000
Incidental Ingestion of Water While Swimming			
Exposure Frequency	days/year	36	5
Exposure Time	hours/day	2.6	2.6
Ingestion Rate	ml/hr	50	10

Table 6-6. Monte Carlo Default Distributions

Parameter	Units	Distribution Type	Expected Value	Standard Deviation	Min.	Max.	Point Estimate		Reference for Monte Carlo Distributions
							Typical	RME	
Body Weight	kg								
Adult Resident		Normal	72	15.9	24	125	70	70	AIHC (1994)
Child Resident (Age 1-6)		Normal	15.6	3.7	6	30	15	15	Anderson et al. (1985)
Trespasser		Normal	47	8.3	20	120	42	42	Anderson et al. (1985)
Worker		Normal	72	15.9	24	125	70	70	AIHC (1994)
Lifetime	yr								
Adult Resident		Constant	70	NA	NA	NA	70	70	EPA (1989)
Child Resident (1-6)		Constant	70	NA	NA	NA	70	70	EPA
Trespasser		Constant	70	NA	NA	NA	70	70	EPA
Worker		Constant	70	NA	NA	NA	70	70	EPA
Exposure Duration (All Exposure Routes)	yr								
Adult Resident		Lognormal	11.36	13.72	0	70	9	30	Israeli and Nelson (1992); data for owners
Child Resident (1-6)		Uniform	NA	NA	1	5	5	5	Best Profession Judgement (BPJ)
Trespasser		Lognormal	11.36	13.72	0	70	9	12	Israeli and Nelson (1992); data for owners
Worker		Lognormal	8.3	8.7	0	50	8	25	Bureau of Labor Statistics (1992)

Table 6-6. Monte Carlo Default Distributions

Parameter	Units	Distribution Type	Expected Value	Standard Deviation	Min.	Max.	Point Estimate		Reference for Monte Carlo Distributions
							Typical	RME	
Exposure Frequency (Indoor Air and Groundwater)	d/yr								
Adult Resident		Constant	350	NA	NA	NA	350	350	
Child Resident (1-6)		Constant	350	NA	NA	NA	350	350	Defaults to be modified based upon site-specific observations and information.
Trespasser		NA	NA	NA	NA	NA	NA	NA	
Worker		Constant	250	NA	NA	NA	250	250	
Exposure Frequency (Soil Routes)	d/yr								
Adult Resident		Triangular	40	NA	10	350	40	350	
Child Resident (1-6)		Triangular	130	NA	10	350	130	350	Defaults to be modified based upon Site-specific observations and information.
Trespasser		Triangular	26	NA	0	52	26	52	
Worker		Triangular	125	NA	10	250	125	250	
Exposure Frequency (Swimming)	d/yr								
Adult Resident		Triangular	7	NA	0	60	5	36	Expected: EPA (1988); Remainder: BJP
Child Resident (1-6)		Triangular	7	NA	0	60	5	36	Same as above
Trespasser		Triangular	7	NA	0	60	5	36	Same as above
Worker		NA	NA	NA	NA	NA	NA	NA	

Table 6-6. Monte Carlo Default Distributions

Parameter	Units	Distribution Type	Expected Value	Standard Deviation	Min.	Max.	Point Estimate		Reference for Monte Carlo Distributions
							Typical	RME	
Total Skin Surface Area (Showering/Swimming)	cm^2								
Adult Resident		Normal	18400	2300	8000	30000	18400	23000	AIHC
Child Resident (1-6)		Normal	6800	600	5000	11000	6800	7280	Anderson et al.
Trespasser		Normal	14000	1700	7000	20000	14000	16550	AIHC
Worker		NA	NA	NA	NA	NA	NA	NA	
Fraction of Total Skin Surface Area Exposed to Soil (Soil Contact/Wading)	cm^2								
Adult Resident		Triangular	0.11	NA	0	0.56	0.11	0.56	Anderson et al. (1985)
Child Resident (1-6)		Triangular	0.13	NA	0	0.55	0.13	0.55	Anderson et al. (1985)
Trespasser		Triangular	0.11	NA	0	0.57	0.11	0.57	Anderson et al. (1985)
Worker		Triangular	0.11	NA	0	0.19	0.11	0.19	Anderson et al. (1985)
Soil Ingestion	mg/d								
Adult Resident		Lognormal	40.4	37.3	1.5	666.8	40	100	Assumed to be one-half child soil ingestion rate
Child Resident (1-6)		Lognormal	86	84	3	1854	90	200	Thompson and Burmaster (1991)
Trespasser		Lognormal	41	36.9	1.4	518.9	40	100	Assumed to be one-half child soil ingestion rate
Worker		Lognormal	40	37.3	1.8	437.1	40	100	Assumed to be one-half child soil ingestion rate

Table 6-6. Monte Carlo Default Distributions

Parameter	Units	Distribution Type	Expected Value	Standard Deviation	Min.	Max.	Point Estimate		Reference for Monte Carlo Distributions
							Typical	RME	
Soil-On-Skin Adherence Factor	mg/cm^2								
Adult Resident		Triangular	0.2	NA	0.0	1	0.2	0.2	Expected value from EPA (1998)
Child Resident (1-6)		Triangular	0.2	NA	0.0	1	0.2	0.2	Expected value from EPA (1998)
Trespasser		Triangular	0.2	NA	0.0	1	0.2	0.2	Expected value from EPA (1998)
Worker		Triangular	0.2	NA	0.0	1	0.2	0.2	Expected value from EPA (1998)
Drinking Water Ingestion	l/d								
Adult Resident		Lognormal	1.27	0.6	0.1	3	1.1	2	Roseberry and Burmaster (1992): age group 20-65
Child Resident (1-6)		Lognormal	0.7	0.35	0.1	2	0.5	1	Roseberry and Burmaster (1992): age group 1-11
Trespasser		NA	NA	NA	NA	NA	NA	NA	
Worker		Lognormal	0.63	0.3	0.1	2	0.5	1	Assumed to be one-half adult resident watering rate
Swimming Ingestion Rate	l/d								
Adult Resident		Uniform	NA	NA	0	50	10	50	EPA (1988)
Child Resident (1-6)		Uniform	NA	NA	0	50	10	50	EPA (1988)
Trespasser		Uniform	NA	NA	0	50	10	50	EPA (1988)
Worker		NA	NA	NA	NA	NA	NA	NA	

Table 6-6. Monte Carlo Default Distributions

Parameter	Units	Distribution Type	Expected Value	Standard Deviation	Min.	Max.	Point Estimate		Reference for Monte Carlo Distributions
							Typical	RME	
Swimming Exposure Time	hr/d								
Adult Resident		Triangular	2.6	NA	0.5	6	2.6	2.6	Expected: EPA (1988); Remainder: BPJ
Child Resident (1-6)		Triangular	2.6	NA	0.5	6	2.6	2.6	Same as above
Trespasser		Triangular	2.6	NA	0.5	6	2.6	2.6	Same as above
Worker		NA	NA	NA	NA	NA	NA	NA	
Time Spent Outdoors	hr/d								
Adult Resident		Triangular	1.1	NA	0.25	2.5	1.1	2.5	Expected: AIHC (1994); Remainder: BPJ
Child Resident (1-6)		Triangular	2.2	NA	0.5	5	2.2	5	Same as Adult
Trespasser		Triangular	1.5	NA	0.25	3	1.5	3	BPJ
Worker		Triangular	4	NA	2	6	4	6	BPJ
Time Spent Indoors	hr/d								
Adult Resident		Triangular	18.3	NA	8	24	18.3	24	Expected: EPA (1988); Remainder: BPJ
Child Resident (1-6)		Triangular	19.6	NA	10	24	19.6	24	Same as above
Trespasser		NA	NA	NA	NA	NA	NA	NA	
Worker		Triangular	4	NA	2	6	4	6	Same as above

Table 6-6. Monte Carlo Default Distributions

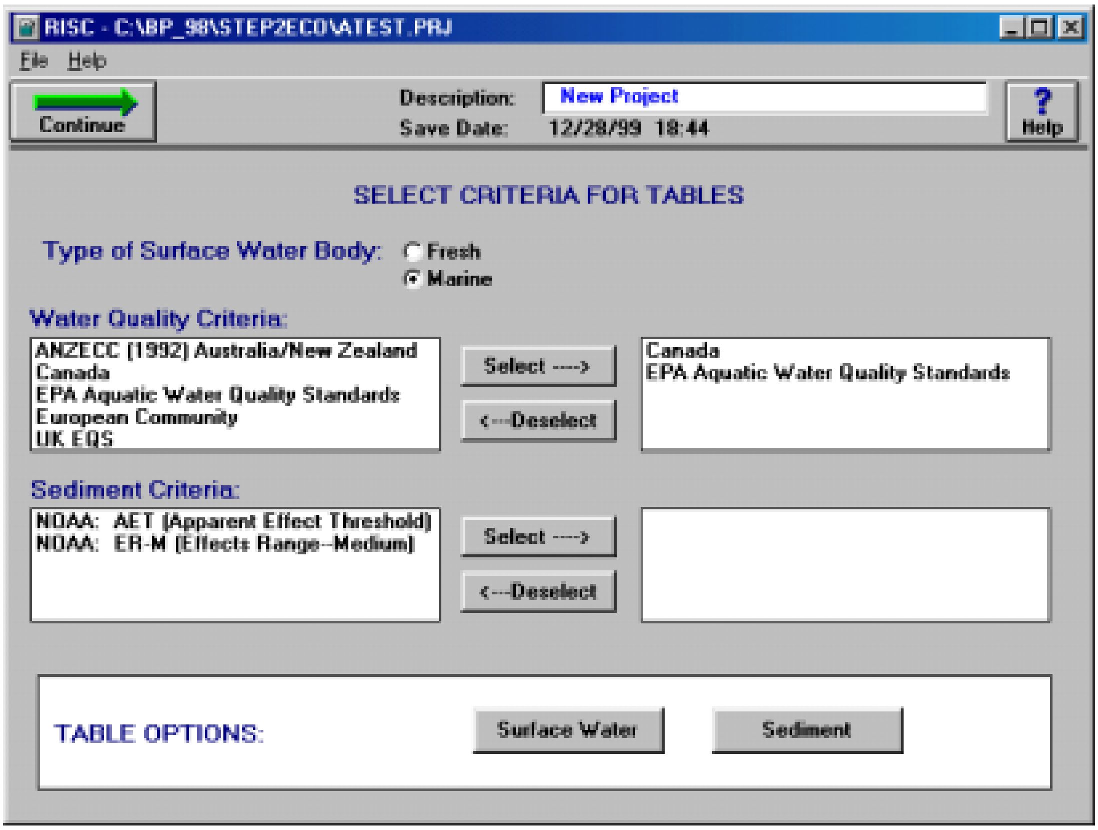
Parameter	Units	Distribution Type	Expected Value	Standard Deviation	Min.	Max.	Point Estimate		Reference for Monte Carlo Distributions
							Typical	RME	
Inhalation Rate (Indoor and Outdoor Air)	m^3/hr								
Adult Resident		Triangular	0.79	NA	0.25	1.33	0.83	0.83	AIHC (1994)
Child Resident (1-6)		Triangular	0.72	NA	0.35	1.18	0.83	0.83	AIHC (1994)
Trespasser		Triangular	1.68	NA	1.06	2.3	1.68	2.3	Anderson et al. (1985)
Worker		Triangular	0.8	NA	0.7	2.5	0.8	2.5	Anderson et al. (1985)
Inhalation Rate (In the Shower)	m^3/hr								
Adult Resident		Constant	0.6	NA	NA	NA	0.6	0.6	EPA (1989)
Child Resident (1-6)		Constant	0.6	NA	NA	NA	0.6	0.6	EPA (1989)
Trespasser		NA	NA	NA	NA	NA	NA	NA	
Worker		NA	NA	NA	NA	NA	NA	NA	
Flowrate of Shower	l/min								
Adult Resident		Lognormal	8	2.7	0	30	8	10	Finley and Paustenbach (1994)
Child Resident (1-6)		Lognormal	8	2.7	0	30	8	10	Finley and Paustenbach (1994)
Trespasser		NA	NA	NA	NA	NA	NA	NA	
Worker		NA	NA	NA	NA	NA	NA	NA	

Table 6-6. Monte Carlo Default Distributions

Parameter	Units	Distribution Type	Expected Value	Standard Deviation	Min.	Max.	Point Estimate		Reference for Monte Carlo Distributions
							Typical	RME	
Water Temperature (Showering)	C								
Adult Resident		Triangular	45	NA	35	50	45	48	Smith (1994)
Child Resident (1-6)		Triangular	45	NA	35	50	45	48	Smith (1994)
Trespasser		NA	NA	NA	NA	NA	NA	NA	
Worker		NA	NA	NA	NA	NA	NA	NA	
Volume of Bathroom (Showering)	m^3								
Adult Resident		Triangular	2.9	NA	2	6	5.2	3	Smith (1994)
Child Resident (1-6)		Triangular	2.9	NA	2	6	5.2	3	Smith (1994)
Trespasser		NA	NA	NA	NA	NA	NA	NA	
Worker		NA	NA	NA	NA	NA	NA	NA	
Exposure Time (Showering)	hr/d								
Adult Resident		Triangular	0.11	NA	0.03	0.33	0.12	0.2	AIHC (1994)
Child Resident (1-6)		Triangular	0.11	NA	0.03	0.33	0.12	0.2	AIHC (1994)
Trespasser		NA	NA	NA	NA	NA	NA	NA	
Worker		NA	NA	NA	NA	NA	NA	NA	

6.2 ECOLOGICAL/WATER QUALITY

Figure 6-5 shows the input screen for selecting water quality criteria (with some marine surface water criteria selected).



Description: New Project
Save Date: 12/28/99 18:44

Type of Surface Water Body: ○ Fresh ● Marine

Water Quality Criteria:

ANZECC (1992) Australia/New Zealand
Canada
EPA Aquatic Water Quality Standards
European Community
UK EQS

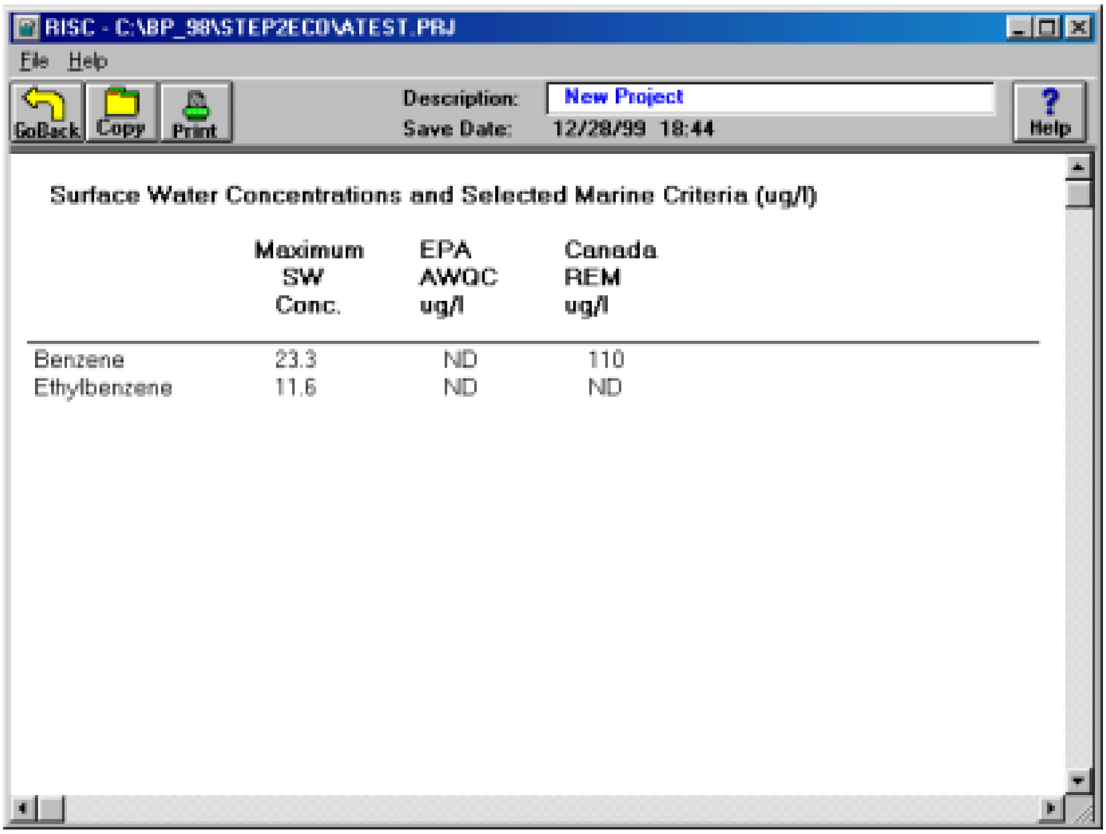
Selected:
Canada
EPA Aquatic Water Quality Standards

Sediment Criteria:

NOAA: AET (Apparent Effect Threshold)
NOAA: ER-M (Effects Range--Medium)

Figure 6-5. Step 4 Screen for Selecting Water Quality and Sediment Criteria

The procedure for creating a summary table in this step is to select the criteria desired and then select the appropriate button from the “Table Options” group. Figure 6-6 shows an example of the surface water criteria table.



Description: New Project

Save Date: 12/28/99 18:44

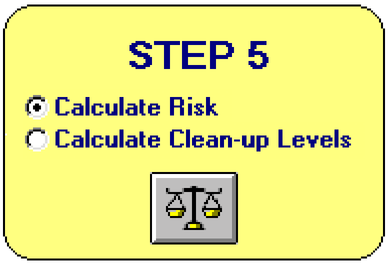
Surface Water Concentrations and Selected Marine Criteria (ug/l)

	Maximum SW Conc.	EPA AWQC ug/l	Canada REM ug/l
Benzene	23.3	ND	110
Ethylbenzene	11.6	ND	ND

Figure 6-6. Example of the Surface Water Criteria Table

Chapter 7.0

Calculate Risk



STEP 5

● Calculate Risk

○ Calculate Clean-up Levels

The potential carcinogenic risk and non-carcinogenic hazard are calculated using equations presented in EPA's Risk Assessment Guidance for Superfund (EPA, 1989a). The following exposure routes are considered in the software:

1. Dermal contact with contaminated soil.
2. Ingestion of contaminated soil.
3. Ingestion of contaminated groundwater.
4. Dermal contact with contaminated groundwater (while showering).
5. Inhalation while showering.
6. Inhalation of outdoor air (either from soil or groundwater emissions).
7. Inhalation of indoor air (either from soil or groundwater emissions).
8. Ingestion of surface water (e.g. while swimming).
9. Dermal contact with surface water.
10. Ingestion of home-grown vegetables grown in contaminated soil.
11. Ingestion of home-grown vegetables irrigated with contaminated groundwater.
12. Ingestion of irrigation water (groundwater used outdoors).
13. Dermal contact with irrigation water.
14. Inhalation of irrigation water spray (from sprinklers etc.).

Pathways 1-3 and 6-7 represent some of the more common exposure pathways for many petroleum contaminated sites (e.g. former gas stations). If surface water bodies are present on the site, exposure pathways eight and nine may be important. Pathways 11 – 14 represent the potential pathways associated with irrigation water and will usually only be of concern if the house has its own well while drinking water used in the house is provided by a municipality.

As mentioned previously, the reader should note that throughout this document the term “risk” will be used to refer to the estimated potential for adverse human health impacts, for both carcinogenic and non-carcinogenic compounds. For some, this is a departure from the more rigorous use of the term “risk”, where it is sometimes only used to refer to the probability of developing cancer as a result of exposure to a chemical or group of chemicals.

7.1 DESCRIPTION OF EACH INTAKE ROUTE

The first step in the risk calculation is to estimate the intake rate for each chemical of concern from each exposure route. This intake rate, or dose, is expressed in milligrams per day of chemical taken into the body per unit body weight [mg/kg-d). EPA's Risk Assessment Guidance for Superfund (RAGS) manual (EPA, 1989a) recommends that when evaluating longer-term exposure to non-carcinogenic toxicants, the intake is to be calculated by averaging the intake over the period of exposure (or averaging time). The resulting term is called the chronic average daily dose (CADD) and is used to estimate the hazard quotient from each route by comparison with a safe "reference dose". Because this dose is derived for exposure periods greater than seven years, the *maximum 7-year average* concentration of the compound is used in the CADD calculations (rather than the average of the exposure duration). If the exposure duration is specified to be less than 7 years, the average concentration over the exposure duration is used.

For carcinogens, the intake rate is calculated by time-averaging the cumulative dose over a 70-year lifetime. In this case, the averaging time is considered to be the receptors lifetime, while the exposure duration may be considerably shorter. The Lifetime Averaged Daily Dose (LADD) is used to estimate the incremental excess lifetime cancer risk (IELCR) by multiplying the LADD by a toxicity factor (known as the slope factor). In cases where time-varying concentrations are considered, algorithms in the RISC software compute the maximum average receptor point concentration over the exposure duration.

Sections 7.1.1 through 7.1.14 present the equations used to estimate CADD and LADD for each exposure pathway. Section 7.2 discusses the calculation of carcinogenic risk and section 7.3 discusses calculation of the hazard quotients and resulting hazard index for non-carcinogens.

For reference, there is a detailed description of the absorption adjustment factors and their derivation in Appendix I. The numerical values are listed in Table 9-1. For a description of the skin permeability coefficients the reader is referred to the EPA EPA's Dermal Exposure Assessment: Principles and Applications (1992).

7.1.1 Ingestion of Soil

Adults working outdoors may ingest soil through incidental contact of the mouth with hands and clothing. Soil ingestion by children is often the primary exposure route of concern for contaminated soils (Paustenbach, 1989a,b). Intake of contaminants in soil by ingestion is estimated as follows:

$$CADD = \frac{C_{\max} \times IR \times AAF \times EF \times BIO}{BW \times 365 \frac{d}{yr}} \times 10^{-6} \frac{kg}{mg} \qquad \textbf{(7-1a)}$$

$$LADD = \frac{C_{ave} \times IR \times AAF \times EF \times ED \times BIO}{LT \times BW \times 365 \frac{d}{yr}} \times 10^{-6} \frac{kg}{mg} \qquad \textbf{(7-1b)}$$

where

CADD = chronic average daily dose [mg/kg-day]

LADD = lifetime average daily dose [mg/kg-day]

C_{max} = maximum 7-year average concentration of chemical in soil [mg/kg]

C_{ave} = time-averaged concentration of chemical in soil over the exposure duration [mg/kg]

IR = soil ingestion rate [mg/day]

AAF = chemical-specific oral-soil absorption adjustment factor [mg/mg]

BIO = bioavailability of chemical in soil [mg/mg]

EF = exposure frequency [events/year]

ED = exposure duration [years]

LT = lifetime = 70 years [by definition]

BW = body weight [kg]

Note, in RISC, the soil concentration is assumed to be constant with time.

7.1.2 Dermal Contact with Soil

Some soil contaminants may be absorbed across the skin into the bloodstream. Absorption will depend upon the amount of soil in contact with the skin, the concentration of chemicals in soil, the skin surface area exposed, and the potential for the chemical to be absorbed across skin. The intake is computed as follows:

$$CADD = \frac{C_{\max} \times SA \times AAF \times AF \times EF \times BIO}{BW \times 365 \frac{d}{yr}} \times 10^{-6} \frac{kg}{mg} \tag{7-2a}$$

$$LADD = \frac{C_{ave} \times SA \times AAF \times AF \times EF \times ED \times BIO}{LT \times BW \times 365 \frac{d}{yr}} \times 10^{-6} \frac{kg}{mg} \tag{7-2b}$$

where

C_{max} = maximum 7-year average concentration of chemical in soil [mg/kg]

C_{ave} = time-averaged concentration of chemical in soil over the exposure duration [mg/kg]

SA = skin surface area exposed to soil [cm^2]

AAF = dermal-soil chemical specific absorption adjustment factor [mg/mg]

BIO = bioavailability of chemical in soil [mg/mg]

AF = soil-to-skin adherence factor [mg/cm^2/event]

and the rest of the variables are as defined previously.

The skin surface area available for soil exposure will vary seasonally and between receptors. For example workers would most likely have less skin exposed than children playing in the summer. Note, in RISC, the soil concentration is assumed to be constant with time.

7.1.3 Ingestion of Groundwater

Intake from ingestion of contaminated water is estimated using the following equations:

$$CADD = \frac{C_{\max} \times IR \times AAF \times EF}{BW \times 365 \frac{d}{yr}} \qquad \textbf{(7-3a)}$$

$$LADD = \frac{C_{ave} \times IR \times AAF \times EF \times ED}{LT \times BW \times 365 \frac{d}{yr}} \qquad \textbf{(7-3b)}$$

where

$C_{\max}$ = maximum 7-year average concentration of chemical in drinking water [mg/l]

C_{ave} = time-averaged concentration of chemical in drinking water over the exposure duration [mg/l]

IR = water ingestion rate [l/day]

AAF = chemical-specific oral-water absorption adjustment factor [mg/mg]

and the rest of the variables are as defined previously.

Note that in the above equations, *IR* is the rate of ingestion from the contaminated water source only, and is not necessarily equal to the total daily fluid intake.

7.1.4 Dermal Intake in the Shower

During showers and baths receptors may absorb dissolved contaminants across the skin into the bloodstream. The dose depends upon the absorption characteristics of the chemical (permeability coefficient), the surface area of skin in contact with the water, and the duration of the bath or shower:

$$CADD = \frac{C_{\max} \times SA \times AAF \times ET \times PC \times EF}{BW \times 365 \dfrac{d}{yr}} \times 10^{-3} \frac{l}{cm^3} \quad \textbf{(7-4a)}$$

$$LADD = \frac{C_{\max} \times SA \times AAF \times ET \times PC \times EF \times ED}{LT \times BW \times 365 \dfrac{d}{yr}} \times 10^{-3} \frac{l}{cm^3} \quad \textbf{(7-4b)}$$

where

C_{max} = maximum 7-year average concentration of chemical in drinking water [mg/l]

C_{ave} = time-averaged concentration of chemical in drinking water over the exposure duration [mg/l]

SA = total skin surface area [cm^2]

AAF = dermal-water chemical specific absorption adjustment factor [mg/mg]

PC = chemical-specific skin permeability constant [cm/hr]

ET = bath or shower duration [hr/day]

and the rest of the variables are as defined previously.

The permeability constant, *PC*, quantifies the diffusion properties of the skin and the chemical; values of PC are tabulated in EPA's Dermal Exposure Assessment: Principles and Applications (1992). This document also describes methods for estimating values of PC from other chemical parameters, such as the octanol water partition coefficient, K_{ow}.

7.1.5 Inhalation in the Shower

While showering, chemicals in the shower water can volatilize into the air not only within the shower stall but into the bathroom and potentially the remainder of the house. Studies have shown that risks from inhalation while bathing can be comparable to, or greater than, risks from drinking contaminated water (McKone, 1987). Inhalation intake during showering is computed as a function of the concentration of volatiles in the shower air, the inhalation rate, and the duration of the shower:

$$CADD = \frac{C_{\max} \times InhR \times AAF \times ET \times LRF \times EF}{BW \times 365 \frac{d}{yr}} \qquad \textbf{(7-5a)}$$

$$LADD = \frac{C_{ave} \times InhR \times AAF \times ET \times LRF \times EF \times ED}{LT \times BW \times 365 \frac{d}{yr}} \qquad \textbf{(7-5b)}$$

where

C_{max} = maximum concentration of chemical in bathroom air [mg/m^3] (calculated from the *maximum 7-year average groundwater* concentration)

C_{ave} = time-averaged concentration of chemical in bathroom air [mg/m^3] (calculated from the *maximum average groundwater* concentration over the exposure duration)

$InhR$ = inhalation rate while showering [m^3/hr]

ET = shower duration [hr/day]

AAF = chemical-specific inhalation absorption adjustment factor [mg/mg]

LRF = lung retention factor [dimensionless]

and the rest of the variables are as defined previously.

These equations assume that the concentration in the bathroom air is known. RISC calculates this concentration using a shower volatilization model developed by Foster and Chrostowski (1986). The equations used in this model are described in Appendix F.

7.1.6 Inhalation of Outdoor Air

In this exposure pathway the inhalation of chemicals in outdoor air due to volatile chemical emissions is considered. The intake is computed as follows:

$$CADD = \frac{C_{\max} \times InhR \times ET \times AAF \times LRF \times EF}{BW \times 365 \frac{d}{yr}} \qquad \textbf{(7-6a)}$$

$$LADD = \frac{C_{ave} \times InhR \times ET \times AAF \times LRF \times EF \times ED}{LT \times BW \times 365 \frac{d}{yr}} \qquad \textbf{(7-6b)}$$

where

C_{max} = maximum 7-year concentration of chemical in outdoor air [mg/m^3)

C_{ave} = time-averaged concentration of chemical in outdoor air over the exposure duration [mg/m^3)

$InhR$ = inhalation rate outdoors [m^3/hr]

ET = exposure time outdoors [hr/day]

AAF = chemical-specific inhalation absorption adjustment factor [mg/mg]

LRF = lung retention factor [mg/mg]

and the rest of the variables are as defined previously.

For sites where hydrocarbon-contaminated soil is the primary media of concern, the chemicals in the air are assumed to have volatilized from the soil.

7.1.7 Inhalation of Indoor Air

In this exposure pathway the inhalation of chemicals in buildings is considered. Chemicals may volatilize from contaminated soil or groundwater and migrate through the vadose zone and into a building. The intake is computed using the same equations as for outdoor air:

$$CADD = \frac{C_{\max} \times InhR \times ET \times AAF \times LRF \times EF}{BW \times 365 \frac{d}{yr}} \quad \textbf{(7-7a)}$$

$$LADD = \frac{C_{ave} \times InhR \times ET \times AAF \times LRF \times EF \times ED}{LT \times BW \times 365 \frac{d}{yr}} \quad \textbf{(7-7b)}$$

where

$C_{\max}$ = maximum 7-year averaged concentration of chemical in indoor air [mg/m^3]

C_{ave} = time-averaged concentration of chemical in indoor air over the exposure duration [mg/m^3]

$InhR$ = inhalation rate indoors [m^3/hr]

ET = exposure time indoors [hr/day]

AAF = chemical-specific inhalation absorption adjustment factor [mg/mg]

LRF = lung retention factor [mg/mg]

7.1.8 Ingestion of Surface Water

Water may be incidentally ingested while swimming or playing in surface water. Exposure duration and frequency will be less for recreational users than for residents living nearby. Intake is calculated similar to that for ingestion of drinking water (Equation 7-3):

$$CADD = \frac{C_{\max} \times IR_{sw} \times ET \times AAF \times EF}{BW \times 365 \frac{d}{yr}} \times 10^{-3} \frac{l}{ml} \quad \textbf{(7-8a)}$$

$$LADD = \frac{C_{ave} \times IR_{sw} \times ET \times AAF \times EF \times ED}{LT \times BW \times 365 \frac{d}{yr}} \times 10^{-3} \frac{l}{ml} \quad \textbf{(7-8b)}$$

where

C_{max} = maximum 7-year average contaminant concentration in surface water [mg/l]

C_{ave} = time-averaged contaminant concentration in surface water over the exposure duration [mg/l]

IR = water ingestion rate [ml/hr]

ET = exposure time for surface water [hr/day]

AAF = chemical-specific oral-water absorption adjustment factor [mg/mg]

Workers are not expected to be exposed via this pathway.

7.1.9 Dermal Contact With Surface Water

If a site contains surface water that is contaminated or has the potential of becoming contaminated, the risk to swimmers (or waders) should be evaluated. The intake from this exposure pathway is calculated similarly to that of dermal intake while showering (Section 7.1.5):

$$CADD = \frac{C_{\max} \times SA \times AAF \times PC \times ET \times EF}{BW \times 365 \frac{d}{yr}} \times 10^{-3} \frac{l}{cm^3} \qquad \textbf{(7-9a)}$$

$$LADD = \frac{C_{ave} \times SA \times AAF \times ET \times PC \times EF \times ED}{LT \times BW \times 365 \frac{d}{yr}} \times 10^{-3} \frac{l}{cm^3} \qquad \textbf{(7-9b)}$$

where

C_{max} = maximum 7-year average contaminant concentration in surface water [mg/l]

C_{ave} = time-averaged contaminant concentration in surface water over the exposure duration [mg/l]

SA = total skin surface area exposed to surface water [cm^2]

PC = chemical-specific skin permeability constant [cm/hr]

ET = exposure time for surface water [hr/day]

AAF = dermal-water chemical-specific absorption adjustment factor [mg/mg]

The parameter values used in this calculation should reflect the a plausible situation. For example, if the surface water is a stream and swimming is impossible, intake values should reflect a more realistic case such as wading or playing in the water. In this situation the skin surface area exposed would be less than for a swimming scenario.

7.1.10 Ingestion of Home-Grown Vegetables Grown in Contaminated Soil

This exposure route is identical to 7.1.11 (vegetables watered with contaminated groundwater) except in the way that the concentration of chemical in the vegetable is calculated. For purposes of estimating concentrations and uptakes, the vegetables are divided into root vegetables and above-ground (or leafy) vegetables. The total dose is the sum of the root vegetables and the above-ground consumed. Concentrations in the root and above-ground vegetables are calculated by multiplying the concentration in soil by an appropriate vegetable uptake factor from soil, B_{vr} or B_{va}, respectively. The calculation of the vegetable uptake factors is presented in Appendix O (Section O.8, specifically for a summary).

$$CADD = \left[\frac{\left(B_{vr} \times IR_{vr} + B_{va} \times IR_{va}\right) \times FI \times EF}{BW \times 365 \dfrac{d}{yr}} \right] \times C_{\max} \times 10^{-3} \frac{kg}{g} \qquad \textbf{(7-10a)}$$

$$LADD = \left[\frac{\left(B_{vr} \times IR_{vr} + B_{va} \times IR_{va}\right) \times FI \times EF \times ED}{LT \times BW \times 365 \dfrac{d}{yr}} \right] \times C_{ave} \times 10^{-3} \frac{kg}{g} \qquad \textbf{(7-10b)}$$

where

B_{vr} = soil-to-root uptake factor [mg chemical/kg root per mg chemical/kg soil]

B_{va} = above ground soil-to-root uptake factor [mg chemical/kg root per mg chemical/kg soil]
C_{max} = maximum 7-year average contaminant concentration in soil [mg/kg]
C_{ave} = time-averaged contaminant concentration in soil over the exposure duration [mg/kg]
IR_{vr} = ingestion rate of root vegetables [g/day]
IR_{va} = ingestion rate of above-ground vegetables [g/day]
FI = fraction of the ingested vegetables grown in contaminated soil [-]

Note, in RISC, the soil concentration is assumed to be constant with time. Workers and trespassers are not expected to be exposed via this pathway.

7.1.11 Ingestion of Home-Grown Vegetables Irrigated With Groundwater

This exposure route is identical to 7.1.10 (vegetables grown in contaminated soil) except in the way that the concentration of chemical in the vegetable is calculated. For purposes of estimating concentrations and uptakes, the vegetables are divided into root vegetables and above-ground (or leafy) vegetables. The total dose is the sum of the root vegetables and the above-ground vegetables consumed. Concentrations in the root and above-ground vegetables are calculated by multiplying the concentration in groundwater by the root concentration factor, *RCF*, or the above-ground vegetable concentration factor, *ABCF*. The calculation of the uptake factors is presented in Appendix O (Section O.8, specifically, for a summary) .

$$CADD = \left[\frac{\left(RCF \times IR_{vr} + ABCF \times IR_{va}\right) \times FI \times EF}{BW \times 365 \frac{d}{yr}} \right] \times C_{\max} \times 10^{-3} \frac{kg}{g} \qquad \textbf{(7-11a)}$$

$$LADD = \left[\frac{\left(RCF \times IR_{vr} + ABCF \times IR_{va}\right) \times IR_{r} \times FI \times EF \times ED}{LT \times BW \times 365 \frac{d}{yr}} \right] \times C_{ave} \times 10^{-3} \frac{kg}{g} \qquad \textbf{(7-11b)}$$

where

RCF = root concentration factor [(mg chem/kg veg)/(mg chem/l water)]

$ABCF$ = above-ground vegetable concentration factor [(mg chem/kg veg)/(mg chem/l water)]

C_{max} = maximum 7-year average contaminant concentration in irrigation water [mg/l]

C_{ave} = time-averaged contaminant concentration in irrigation water over the exposure duration [mg/l]

IR_{vr} = ingestion rate of root vegetables [g/day]

IR_{va} = ingestion rate of above-ground vegetables [g/day]

FI = fraction of the ingested vegetables grown with contaminated irrigation water [-]

In RISC, the concentration in irrigation water may be estimated using the groundwater models. Workers and trespassers are not expected to be exposed via this pathway.

7.1.12 Ingestion of Irrigation Water

Ingestion of irrigation water may occur if children are playing in sprinklers or if the irrigation water is used to fill a swimming pool. Similar to 7.1.3, Ingestion of Groundwater, intake from ingestion of contaminated irrigation water is estimated using the following equations:

$$CADD = \frac{C_{\max} \times IR_{iw} \times ET_{iw} \times AAF \times EF}{BW \times 365\frac{d}{yr}} \times 10^{-3}\frac{l}{ml} \tag{7-12a}$$

$$LADD = \frac{C_{ave} \times IR_{iw} \times ET_{iw} \times AAF \times EF \times ED}{LT \times BW \times 365\frac{d}{yr}} \times 10^{-3}\frac{l}{ml} \tag{7-12b}$$

where

C_{max} = maximum 7-year average concentration of chemical in drinking water [mg/l]

C_{ave} = time-averaged concentration of chemical in drinking water over the exposure duration [mg/l]

IR_{iw} = water ingestion rate [ml/hr]

ET_{iw} = exposure time for irrigation water [hr/day]

AAF = chemical-specific oral-water absorption adjustment factor [mg/mg]

and the rest of the variables are as defined previously.

Note that in the above equations, IR is the rate of ingestion from the contaminated water source only, and is not necessarily equal to the total daily fluid intake.

7.1.13 Dermal Intake with Irrigation Water

This pathway estimates the intakes for dermal contact with irrigation water. Exposure to irrigation water may occur while playing in the sprinkler or watering a garden. Similar to 7.1.4, Dermal Contact in the Shower, the dose depends upon the absorption characteristics of the chemical, the permeability coefficient, the surface area of skin in contact with the water, and the duration of the sprinkler operation:

$$CADD = \frac{C_{\max} \times SA \times FS \times AAF \times ET \times PC \times EF}{BW \times 365 \frac{d}{yr}} \times 10^{-3} \frac{l}{cm^3} \qquad \textbf{(7-13a)}$$

$$LADD = \frac{C_{ave} \times SA \times FS \times AAF \times ET_{iw} \times PC \times EF \times ED}{LT \times BW \times 365 \frac{d}{yr}} \times 10^{-3} \frac{l}{cm^3} \qquad \textbf{(7-13b)}$$

where

C_{max} = maximum 7-year average concentration of chemical in irrigation water [mg/l]

C_{ave} = time-averaged concentration of chemical in irrigation water over the exposure duration [mg/l]

SA = total skin surface area [cm^2]

FS = fraction of total skin surface area exposed to irrigation water [cm^2/cm^2]

AAF = dermal-water chemical specific absorption adjustment factor [mg/mg]

PC = chemical-specific skin permeability constant [cm/hr]

ET_{iw} = exposure time for irrigation water [hr/day]

and the rest of the variables are as defined previously.

The permeability constant, *PC*, quantifies the diffusion properties of the skin and the chemical; values of *PC* are tabulated in EPA's Dermal Exposure Assessment: Principles and Applications (1992). This document also describes methods for estimating values of *PC* from other chemical parameters, such as the octanol water partition coefficient, K_{ow}.

7.1.14 Inhalation of Irrigation Water Spray

Volatilization from water used for irrigation may occur while sprinkling or watering a garden. This exposure route assumes a width of sprinkler spray, droplet size, and time for the water to infiltrate or leave the area. The method used to estimate the concentration in the air uses the shower model (Appendix G) with exposure parameters chosen to reflect an outdoor exposure. The application of the shower model for outdoor exposures is also discussed in Appendix G. Inhalation intake from irrigation spray is computed as a function of the concentration of volatiles in the air, the inhalation rate, and the length of time spent in or around irrigation spray:

$$CADD = \frac{C_{\max} \times InhR \times AAF \times ET_{iw} \times LRF \times EF}{BW \times 365 \dfrac{d}{yr}} \qquad \textbf{(7-14a)}$$

$$LADD = \frac{C_{ave} \times InhR \times AAF \times ET_{iw} \times LRF \times EF \times ED}{LT \times BW \times 365 \dfrac{d}{yr}} \qquad \textbf{(7-14b)}$$

where

C_{max} = maximum concentration of chemical in outdoor air [mg/m^3] (calculated from the *maximum 7-year average groundwater* concentration)

C_{ave} = time-averaged concentration of chemical in outdoor air [mg/m^3] (calculated from the *maximum average groundwater* concentration over the exposure duration)

$InhR$ = inhalation rate outdoors [m^3/hr]

ET_{iw} = exposure time for irrigation water [hr/day]

AAF = chemical-specific inhalation absorption adjustment factor [mg/mg]

LRF = lung retention factor [dimensionless]

and the rest of the variables are as defined previously.

7.2 CALCULATION OF CARCINOGENIC RISK

For carcinogens, risks are estimated as the incremental probability of an individual developing cancer over a lifetime as a result of exposure to the potential carcinogen. This risk is referred to as the individual excess lifetime cancer risk, *IELCR*, or just carcinogenic risk. Published values of chemical carcinogenic toxicity (slope factor) are used to calculate risk from the *LADD*:

$$IELCR_{ij} = SF_{ij}\, LADD_{ij} \qquad \textbf{(7-15)}$$

where

$IELCR_{ij}$ = individual excess lifetime cancer risk for chemical *i*, exposure route i [dimensionless]

SF_{ij} = slope factor for chemical *i*, exposure route *j* [mg/kg-d]$^{-1}$

$LADD_{ij}$ = lifetime average daily dose for chemical *i*, exposure route *j* [mg/kg-d]

This approach to estimating risk is based on the linear low-dose cancer risk model described by the EPA (1989a), and is considered valid for risks below 0.01. The model assumes that exposure to any amount of a carcinogen will increase the risk of cancer, i.e. there is no safe or threshold dosage. This assumption is fundamentally different from that assumed for non-carcinogens, where a safe "reference dose" exists.

Ideally the slope factor used in Equation 7-15 should reflect the route of intake (e.g., ingestion, inhalation, or dermal absorption). Unfortunately, toxicological data is not always available for each route (e.g., inhalation data only might be available), and so route-to-route extrapolations must be made. In such cases one sometimes assumes that the slope factor for one unknown intake route is equal to the slope factor for some known route. (It is quite common to use the oral slope factor for dermal exposures.) Risks are assumed to be additive from multiple chemicals and routes, therefore the total risk is estimated by:

$$IELCR_t = \sum IELCR_{ij} \qquad \textbf{(7-16)}$$

where

$IELCR_t$ = total individual excess lifetime cancer risk (or, incremental cancer occurrences/individuals exposed)

7.3 CALCULATION OF HAZARD INDEX

The potential for non-carcinogenic effects is evaluated by comparing an exposure level over the exposure duration (maximum of 7 years) with a reference dose derived for a similar exposure period. This ratio of exposure to toxicity for an individual pathway and chemical is called a hazard quotient. The hazard quotients are usually added across all chemicals and routes to estimate the hazard index. Some, however, will argue that it is more appropriate to only sum the hazard quotients for chemicals that affect the same target organ (e.g. liver or blood).

The noncancer hazard quotient assumes that there is a level of exposure below which it is unlikely that even sensitive populations would experience adverse health effects (EPA 1989a). This reference dose, or *RfD*, is a toxicity value for evaluating non-carcinogenic effects. It has the same units as intake and it is assumed that if the intake is below the *RfD* (hazard quotient < 1) no adverse health affects occur, even if the receptor is exposed to this dose continuously over a lifetime. Two types of *RfDs* are generally used: a subchronic *RfD* for short-term exposures and a chronic *RfD* for long-term exposure. The chemical database in RISC contains the values for chronic *RfDs*. If a subchronic case is being evaluated, it is important to modify the *RfD*.

The hazard quotient for an individual chemical and individual route is calculated by:

$$HQ_{ij} = CADD_{ij} / RfD_{ij} \qquad \textbf{(7-17)}$$

where

HQ_{ij} = hazard quotient for chemical *i*, exposure route *j* [dimensionless]

$CADD_{ij}$ = chronic daily intake for chemical *i*, exposure route *j* [mg/kg-d]

$\mathrm{RfD}_{\mathrm{ij}}$ = reference dose for chemical *i*, exposure route *j* [mg/kg-d]

The hazard quotients from each chemical and route are then added to obtain the hazard index:

$$\mathrm{HI} = \sum \sum \mathrm{HQ}_{\mathrm{ij}} \qquad \textbf{(7-18)}$$

where

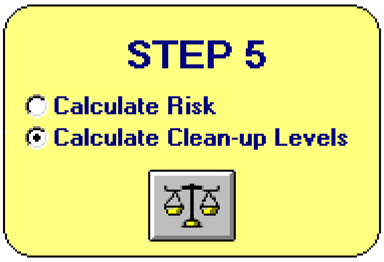
HI = hazard index [dimensionless]

HQ_{ij} = hazard quotient for chemical i, exposure route j [dimensionless]

As discussed previously, the hazard index is an indication of the potential for adverse noncarcinogenic effects, and is not a probabilistic risk. As a rule, the greater the value of the hazard index, the greater the level of concern. Hazard indices above one generally indicate the potential for adverse health effects and suggest the need to undertake a further level of investigation or possibly remedial action.

Chapter
8.0

Calculate Clean-Up Levels


STEP 5

○ Calculate Risk

● Calculate Clean-up Levels

When the “Calculate Clean-up Levels” option is chosen from Step 5, RISC can be used to “back-calculate” clean-up levels using the models and assumptions selected in the current analysis. In the “forward risk” assessment, risk is calculated from input or estimated receptor point concentrations and receptor input parameters. In the back-calculation, the user specifies target risks or concentrations (e.g. MCLs) and then the software calculates “allowable” source concentrations (clean-up levels). The clean-up levels represent source and/or receptor point concentrations for the chemicals of concern such that the risk levels are not exceeded for the scenario outlined.

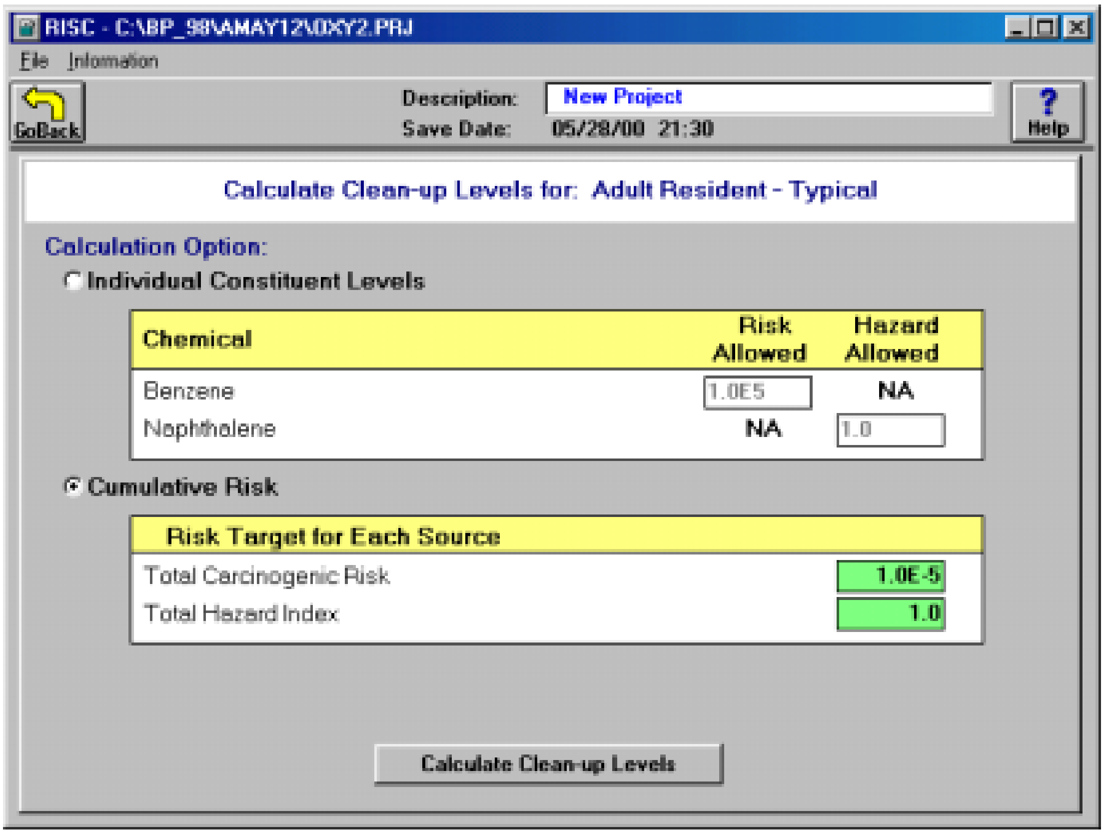
There are several options for selecting targets in Step 5. The user may specify a target risk or hazard index either for individual chemicals or for a cumulative scenario where the risks are summed across all chemicals of concern. If groundwater or surface water is a receptor media the user may enter target concentrations (e.g. MCLs in groundwater) for these media. Note, since the surface water is linked to the groundwater models, if surface water is being modeled then only target concentrations in surface water may be entered. The groundwater concentrations will be dependent on the surface water target concentrations.

8.1 SET-UP THE SIMULATION

The first four steps involved in calculating clean-up levels are the same first four steps used in making a “forward” calculation of risk. First, the user describes the scenario by choosing chemicals of concern (Step 1, main menu). In Step 2, the user chooses pathways and fate and transport models to be used, if any. Next, the receptor point concentrations are specified, and/or fate and transport models are run (Step 3). In Step 4, “Define the Receptors”, one receptor is selected and the intake parameters describing the scenario are defined.

For scenarios involving transport models, clean-up levels can only be calculated for one receptor at a time. Note that this receptor may be defined as the "additive" child + adult case. However, multiple chemicals and exposure pathways may be considered simultaneously for the single receptor. Clean-up levels may only be calculated using the deterministic scenario. The reader is reminded that the ASTM Tier 1 spreadsheet distributed with RISC may be used to establish initial, relatively conservative, clean-up levels (without pathway or chemical additivity, however).

Figure 8-1 shows a sample input screen for specifying the target risk and hazard index without any groundwater pathways.



Description: New Project
Save Date: 05/28/00 21:30

Calculate Clean-up Levels for: Adult Resident - Typical

Calculation Option:

○ Individual Constituent Levels

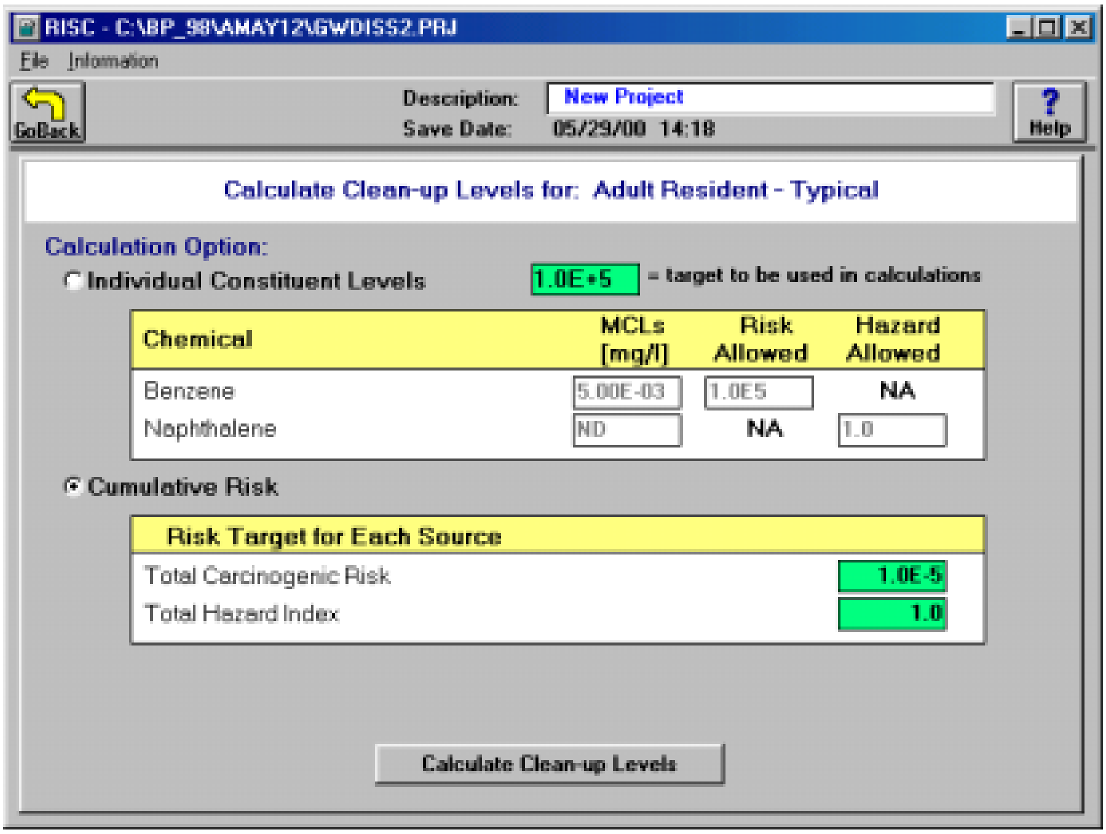
Chemical	Risk Allowed	Hazard Allowed
Benzene	1.0E5	NA
Naphthalene	NA	1.0

● Cumulative Risk

Risk Target for Each Source	
Total Carcinogenic Risk	1.0E-5
Total Hazard Index	1.0

Figure 8-1. Target Risk Input Screen

Figure 8-2 shows how the input screen would look like if groundwater pathways are being considered (e.g. a groundwater model is used to estimate groundwater concentrations downgradient of a soil source). In Figure 8-2, the user has the option of specifying MCLs in groundwater (or target concentrations in surface water if this media were selected in Step 2) under the "Individual Constituent Levels" option.



RISC - C:\BP_98\AMAY12\GWDISS2.PRJ

Description: New Project
Save Date: 05/29/00 14:18

Calculate Clean-up Levels for: Adult Resident - Typical

Calculation Option:

○ Individual Constituent Levels 🟩 1.0E+5 = target to be used in calculations

Chemical	MCLs [mg/l]	Risk Allowed	Hazard Allowed
Benzene	5.00E-03	1.0E5	NA
Naphthalene	ND	NA	1.0

● Cumulative Risk

Risk Target for Each Source	
Total Carcinogenic Risk	1.0E-5
Total Hazard Index	1.0

Figure 8-2. Target Risk Input Screen for a Scenario With Groundwater Pathways

If the "Individual Constituent Levels" option is chosen and the MCL or target surface water concentration displayed in the MCL column is not equal to "ND" (no data), then this concentration will be used in the back-calculation rather than the target risk or hazard level. To use risk or hazard targets for the individual chemicals the values in the target concentration column (either MCLs or surface water targets) must be changed to "ND".

During the back-calculation, each individual chemical source concentration used in the model is reduced or increased to achieve the selected target levels. If the "Cumulative Risk" option is chosen and the scenario includes fate and transport models, the concentrations of each chemical are increased or reduced proportionately to each other in order until the target is reached. In this case, the same relative concentrations as were originally specified in the source term (Step 3b) will be used.

After the targets and method used to adjust the source are specified, the back-calculation code is run by clicking on the “Start Simulation” button. If no fate and transport models are used, the code should run quickly. If fate and transport models are used, however, they must be run iteratively until the source concentrations converge to meet the target. This may require the models to be run up to 7 times, so the simulation time may be up to 7 times longer than running the fate and transport models in Step 3. The actual methods used to estimate the clean-up levels for the “direct pathways” and the “fate and transport pathways” are described in the following sections.

8.2 "RULES" USED IN THE BACK-CALCULATION

This section provides a brief summary of the rules used by the code to calculate clean-up levels. If the "Individual Constituent Levels" option is chosen the following rules will apply:

- If groundwater or surface water concentrations are being modeled, then the user will have the option of entering target concentrations for each chemical of concern. Since the calculated surface water concentration is dependent on the groundwater concentration, if both surface water and groundwater are media of concern, the user will only have the opportunity to enter surface water concentrations.
- If there is a concentration entered in the MCL or Target Surface Water Concentration box for the chemical, this value will be used as the target for the chemical rather than the target risk and hazard indices. This option does not consider risk in the calculations, therefore additivity across chemicals or pathways does not apply.

- If the value entered in the MCL or surface water target concentration box equals "ND" then the risk and hazard targets will be used for that chemical.
- If multiple pathways that emanate from a single source media have been chosen, RISC will add each pathway contribution to risk and hazard for each source media. For example, if a soil to groundwater model is chosen to estimate groundwater concentrations for both drinking water and volatilization from groundwater to indoor air, the clean-up level calculated for the soil source will be protective of both of these pathways added together.
- If individual compounds have a TPH concentration (to identify them as part of a mixture) in a fate and transport model source term, the original mole fraction of each chemical will be maintained. This will mean that the TPH concentrations may be adjusted up or down accordingly (and they may differ for each chemical modeled).

If the "Cumulative Risk" option is chosen the following rules will apply:

- The targets for this scenario cannot be specified as concentrations.
- The clean-up levels calculated for each source area will reflect the additive effects from each chemical and each pathway associated with the source media.
- The risk from multiple source media is not summed for purposes of calculating the clean-up levels. If multiple sources are being considered, the user may want to adjust the targets so that the total risk across all sources, all chemicals, and all pathways doesn't exceed the desired overall target.
- The concentrations of each chemical in a given source are increased or reduced proportionately to each other in order to reach the target. For example, if the original concentrations of two chemicals are such that one chemical is twice the concentration of the other chemical, the concentrations at the final solution will also have this ratio.
- If individual compounds have a TPH concentration (to identify them as part of a mixture) in a fate and transport model source term, the original mole fraction of the limiting chemical will be maintained. The limiting chemical is the chemical that is driving the risk..

8.3 DESCRIPTION OF METHOD USED TO CALCULATE CLEAN-UP LEVELS

The approach used to calculate clean-up levels differs slightly between (1) direct pathways and (2) pathways involving fate and transport models. The next two sections will describe the two approaches.

8.3.1 Direct Pathways

This section describes the approach used for direct pathways, i.e. for the cases where no fate and transport models are used in Step 3. Target groundwater or surface water concentrations are not specified for direct pathways since the target concentrations are the solution already. The steps used to calculate clean-up levels for direct scenarios are:

1) Determine how many separate source areas there are and the pathways associated with each source. Perform steps 2 through 4 for each source area.
2) Calculate target concentrations in the receptor media that meet the target risk. If the "Individual Constituent Levels" option is chosen, this is the only step in the back-calculation process.
3) If the chemical is both a carcinogen and a non-carcinogen (that is, it has both a slope factor and a reference dose), the receptor concentrations are calculated to meet the targets for both cases and the lowest concentration of the two solutions becomes the clean-up level.
4) If the "Cumulative Risk" option is chosen with a direct pathway, the fraction of contribution to the overall risk is calculated for each chemical. The clean-up levels are adjusted so the original ratios between the chemical concentrations are maintained.

8.3.2 Pathways Using Fate and Transport Models

For pathways that use receptor point concentrations calculated using fate and transport models, the clean-up levels are calculated in the source area such that the risk from the modeled receptor point concentrations meets the specified target. The approach used to calculate clean-up levels using models differs slightly from the steps described in 8.3.1. The reason for this difference is that the fate and transport models use chemical-specific data and many of the models are non-linear, that is, the receptor concentration is not linearly correlated with the source concentration. In other words, for one chemical a source reduction of one-half may result in a 50% reduction of the receptor concentration but for another chemical the same source reduction could cause the chemical not to reach the downgradient receptor media at all. (This can especially be true for cases with degradation.)

For the cumulative target risk option using models, the source concentrations are adjusted so that the original concentration ratios (entered by the user) are maintained. The receptor point concentrations calculated using these source concentrations may not maintain the same ratios. The following steps then are used for the cumulative modeled scenarios:

1) Determine how many separate source areas use fate and transport models. Perform the following steps for each source area.
2) Segregate the chemicals of concern into carcinogens and non-carcinogens. Some chemicals may be in both groups.
3) For the cumulative risk option, the fractional contribution towards the total risk or total hazard is calculated for each chemical in the two groups.
4) The "limiting" chemical and limiting risk type is determined. The limiting or driving chemical is the chemical that generates the most risk among the chemicals of concern. The limiting risk type is determined by comparing the current estimated risk with the target risk for the carcinogenic and non-carcinogenic chemical groups. The group with the higher initial percentage of risk is the limiting risk type.
5) The fate and transport models are run for the limiting chemical so that the overall risk for that single chemical equals the same initial proportion of total

risk allocated to the chemical in Step 2. This involves:

   a) The clean-up level (solution) for the limiting chemical is "bound". That means that two source concentrations are determined, one that generates a risk above the target risk fraction and one that generates a risk lower than the target fraction.

   b) After the solution is bound, a numerical solver (the secant method) is used to calculate the source concentration that meets the initial target. The secant method (a standard non-linear solver described in many numerical method texts) allows the solution to be found in fewer iterations than many other numerical methods (such as bisection). Most problems in RISC can be solved in less than 6 iterations.

6) The source concentrations for the other chemicals are adjusted according to their initial concentration ratios. The fate and transport model is run for all chemicals and the resultant risk calculated.

7) The total risk is compared against the target risk specified. If the target is not met (within a certain tolerance of 0.1%), the source concentrations are adjusted slightly and the models re-run.

8.3.3 Equations Used to Calculate Target Receptor Point Concentrations

The equations used to calculate receptor point concentrations that meet the specified risk target for direct pathways are simply the equations from in Chapter 7 (Calculate Risk) rearranged to solve for the media concentration. All of the pathways associated with each source are added together when calculating the clean-up level for that source. If the "Cumulative Risk" option is chosen, the risk from all pathways and from all chemicals are added together for each source.

For carcinogens, equation 7-15 can be rearranged to solve for the Lifetime Average Daily Dose (LADD). For non-carcinogens, equation 7-17 is rearranged to solve for the chronic daily intake (CADD):

$$\mathrm{LADDij} = \mathrm{IELCRij} / \mathrm{SFij} \qquad \textbf{(8-1a)}$$

$$CADD_{ij} = RfD_{ij}\, HQ_{ij} \qquad \textbf{(8-1b)}$$

where

$IELCR_{ij}$ = the individual excess lifetime cancer risk for chemical i, exposure route j (dimensionless)

SF_{ij} = the slope factor for chemical i, exposure route j (mg/kg-d)-1

$LADD_{ij}$ = the lifetime average daily dose for chemical i, exposure route j (mg/kg-d)

HQ_{ij} = the hazard quotient for chemical i, exposure route j (dimensionless)

$CADD_{ij}$ = the chronic daily intake for chemical i, exposure route j (mg/kg-d)

RfD_{ij} = the reference dose for chemical i, exposure route j (mg/kg-d)

The LADD and CADD are functions of the media concentration.

$$LADD_{ij} = CONCcarc_i\, FACTORcarc_j \qquad \textbf{(8-2a)}$$

$$CADD_{ij} = CONCnon_i\, FACTORnon_j \qquad \textbf{(8-2b)}$$

where

$CONCcarc_i$ = the concentration of chemical i averaged over the exposure duration (for carcinogens)

$CONCnon_i$ = the concentration of chemical i averaged over 7 years (for non-carcinogens)

$FACTORcarc_j$ = the carcinogenic route-specific exposure factor defined in equations 7-1 through 7-14.

$FACTORnon_j$ = the non-carcinogenic route-specific exposure factor defined in equations 7-1 through 7-14.

The total daily doses (LADDs and CADDs) are summed for all of the exposure routes associated with one source media:

$$LADD_i = CONCcarc_i \sum_j FACTORcarc_j \qquad \textbf{(8-3a)}$$

$$CADD_i = CONCnon_i \sum_j FACTORnon_j \qquad \textbf{(8-3b)}$$

Equations 8-1a and 8-1b can now be solved for media concentration; the user-specified target risk and target hazard are substituted for the IELCR and HQ, respectively:

$$CONCcarc_i = TR_i / \sum_j (SF_{ij} * FACTOR_j) \qquad \textbf{(8-3a)}$$

$$CONCnon_i = THQ_i / \sum_j (RfD_{ij} * FACTOR_j) \qquad \textbf{(8-3a)}$$

where

TR_i = the target excess cancer risk for chemical i (user-specified) (-)

THQ_i = the target hazard quotient for chemical i (user-specified) (-)

For direct pathways, the concentrations calculated in Equations 8-3 are the clean-up levels. If there are multiple source media with direct exposure pathways, equation 8-3 is calculated for each media. If a chemical is both a carcinogen and a non-carcinogen, the lowest concentration is assumed to be the clean-up level.

8.4 RESULTS OF THE CLEAN-UP LEVEL CALCULATION

For direct pathways (i.e., no fate and transport models), the back-calculation code will calculate receptor point concentrations for each media so that the target risk and hazard index will not be exceeded *for that media.* If there are exposure pathways emanating from one source that use different receptor point media, the target risk will be met for each source media. Therefore, if there are more than one source media, the total risk will equal the product of the specified target risk and the total number of source media. For example, if a groundwater model is used and the following pathways are chosen:

- Ingestion of groundwater
- Dermal contact with groundwater
- Inhalation in the shower
- Inhalation of indoor air with emissions from groundwater

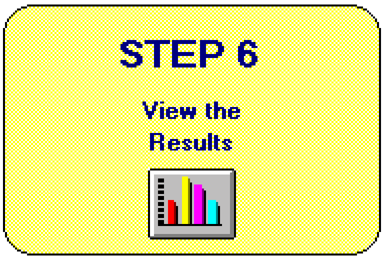
the clean-up level in the source region will be calculated so that the sum of the risks from all four of these exposure routes equals the target risk. If ingestion of soil and dermal contact with soil were also considered in this scenario there would be two source media (soil and groundwater). The clean-up levels for each media would equal the target and if a receptor was actually was exposed to both soil and groundwater at the clean-up levels calculated, the total risk would be equal to twice the target risk specified.

For direct pathways, if both carcinogens and non-carcinogenic chemicals are present, both the target risk and the target hazard will be met. Within each group of chemicals (carcinogenic or non-carcinogenic) the concentration ratios relative to each other (entered in Step 3) will be maintained. However, the concentration ratio between carcinogens and non-carcinogens will not be maintained.

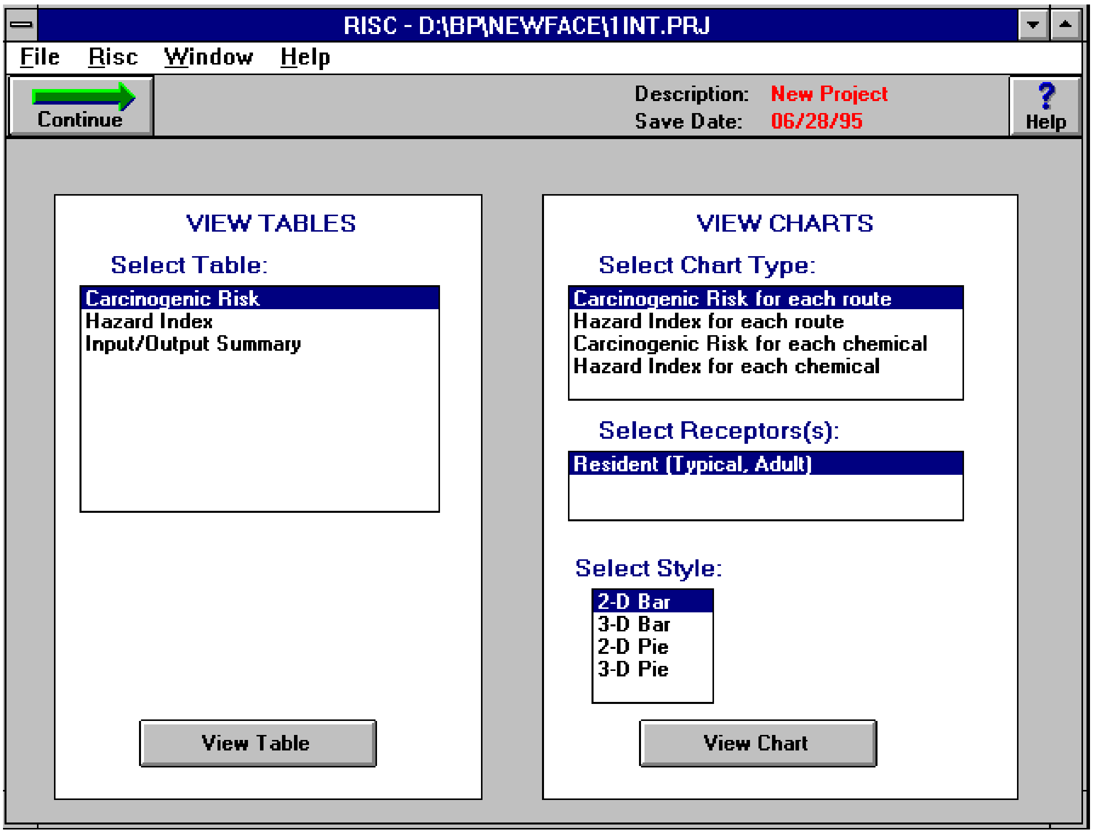
The results are displayed in Step 6: “View Results”, from the main menu. Step 6, “View Results,” is described in Chapter 9.

Chapter 9.0

Results



After a successful risk calculation has been performed, the results can be viewed in the form of tables and charts selected from the main screen of Step 6 (Figure 9-1).



RISC - D:\BP\NEWFACE\1INT.PRJ

Description: New Project
Save Date: 06/28/95

VIEW TABLES

Select Table:
- Carcinogenic Risk
- Hazard Index
- Input/Output Summary

VIEW CHARTS

Select Chart Type:
- Carcinogenic Risk for each route
- Hazard Index for each route
- Carcinogenic Risk for each chemical
- Hazard Index for each chemical

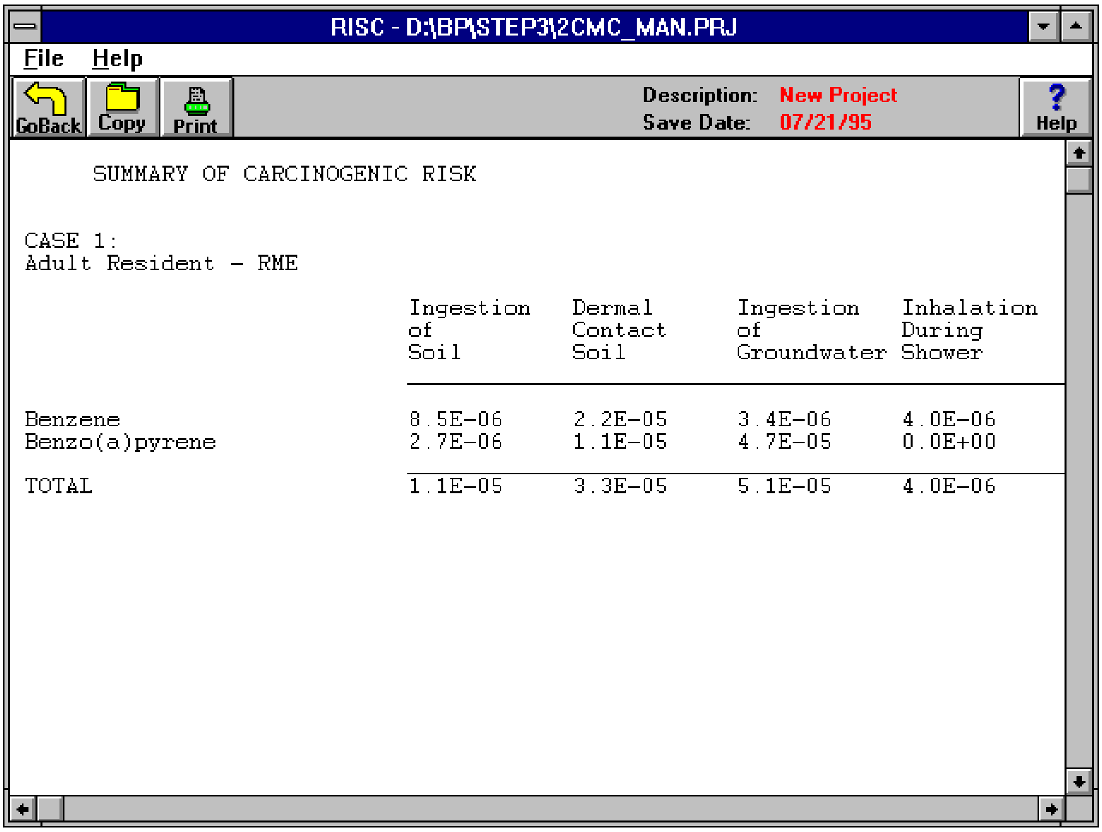
Select Receptors(s):
- Resident (Typical, Adult)

Select Style:
- 2-D Bar
- 3-D Bar
- 2-D Pie
- 3-D Pie

Figure 9-1. Menu for Viewing Results of a Deterministic Risk Assessment

9.1 DETERMINISTIC OUTPUT

Three different tables are available for all risk assessments: "Carcinogenic Risk", "Hazard Index", and the "Input/Output Summary" which lists the values used in the risk calculation. The tables are viewed by first selecting the table type from the "Select Table" box and then choosing the "View Table" button. Figure 9-2 shows an example of a "Carcinogenic Risk" table.



Description: New Project
Save Date: 07/21/95

```
     SUMMARY OF CARCINOGENIC RISK

CASE 1:
Adult Resident - RME

                             Ingestion    Dermal       Ingestion    Inhalation
                             of           Contact      of           During
                             Soil         Soil         Groundwater  Shower

Benzene                      8.5E-06      2.2E-05      3.4E-06      4.0E-06
Benzo(a)pyrene               2.7E-06      1.1E-05      4.7E-05      0.0E+00

TOTAL                        1.1E-05      3.3E-05      5.1E-05      4.0E-06
```

Figure 9-2. Example of Carcinogenic Risk Table

Note, the entire table is not shown in on the screen in Figure 9-2. The rest of the table may be viewed by using the vertical and horizontal scroll bars.

These tables may be copied and pasted into other applications for inclusion in reports. (This is discussed in section 9.3.) Examples of the "Carcinogenic Risk" and the "Input/Output Summary" tables (copied into Microsoft Word®) are shown in Tables

9-1 and 9-2 (at the end of this chapter). The "Input/Output Summary" lists all the input values used to calculate the risk and hazard index. This table is very useful as a concise summary of the entire risk analysis.

Charts are chosen similarly to the tables, however, there are more options for setting up charts (see Figure 9-1). Figure 9-3 shows "Carcinogenic Risk by each route" for the example presented in Tables 9-1 and 9-2. Most of the risk in this example is posed by ingestion of groundwater.

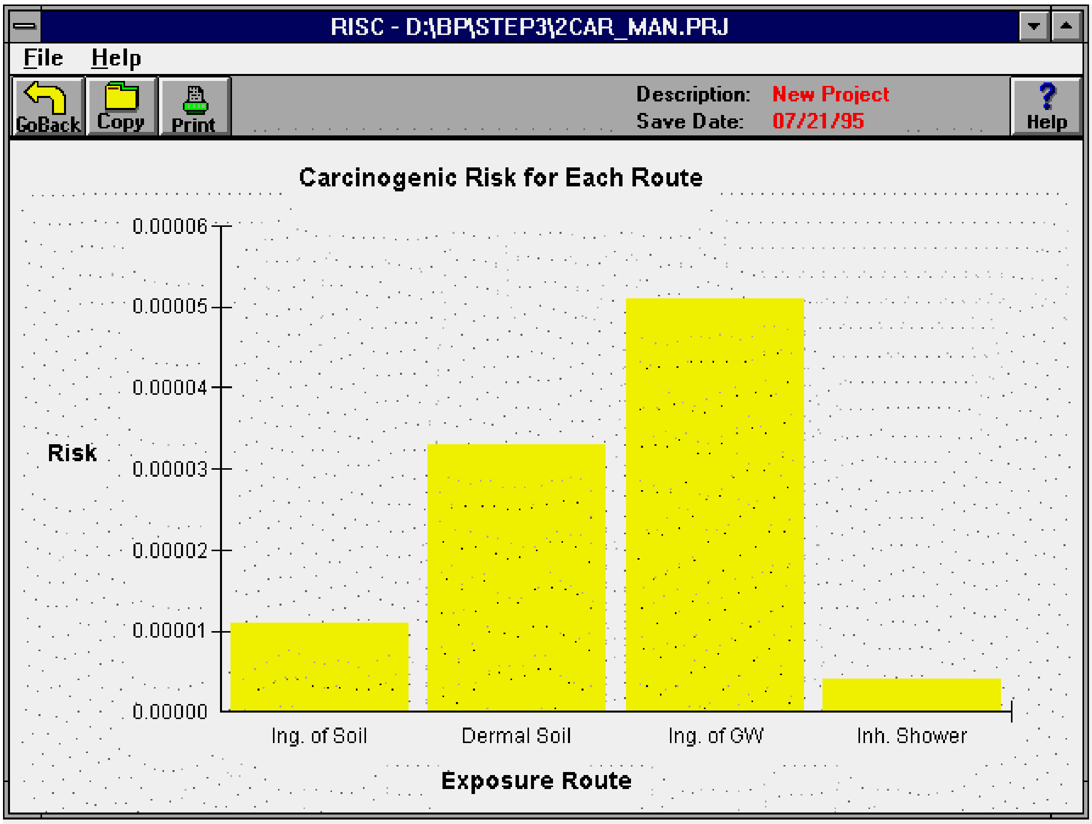


Figure 9-3. Chart of Carcinogenic Risk by Route

If more than one receptor is considered, (e.g. "Typical" and “RME” adult) the user has the option to view a chart of the results one at a time or for both receptors at once (select both receptors with the mouse). When both receptors are selected for plotting in one chart, the user may choose to either show the results in a "Clustered" or in a "Stacked" bar chart. Clustered bar charts are useful for making side-by-side comparisons of total risk or hazard between two receptors. Figure 9-4 shows an example of a "Clustered" bar chart comparing a “RME” and "Typical" residential adult receptor. Default values were used for all intake parameters.

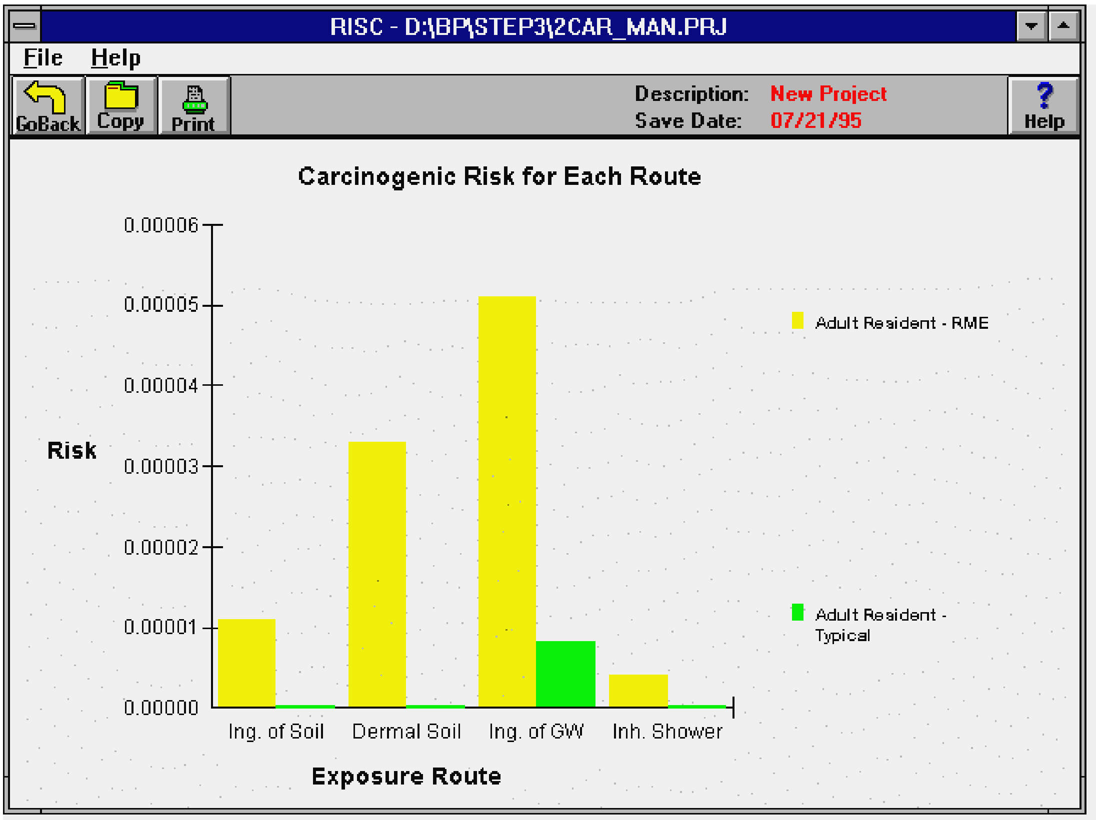


Figure 9-4. Chart of Carcinogenic Risk for Two Receptors

The results presented in Figure 9-4 were calculated using the example shown in Table 9-2 with a "Typical" receptor added. The total risk for the "Typical" residential adult receptor for this case is 8.8E-6 which is an order of magnitude less than the risk calculated for the RME receptor (9.9E-05). The clustered chart illustrates how the risk was distributed among the exposure routes and how the two receptors compare *risk-wise* for each route. Because the Y-axis is on a linear scale (as opposed to logarithmic) the bars indicating risk for the "Typical" receptor are quite small compared to the RME receptor.

Multiple receptor charts may also be presented using the "Stacked" option. This option is really only appropriate for cases when the additive risk to two receptors is being considered (e.g. an individual exposed as both a child and an adult). Figure 9-5 shows an example of a stacked chart for an RME adult and RME child.

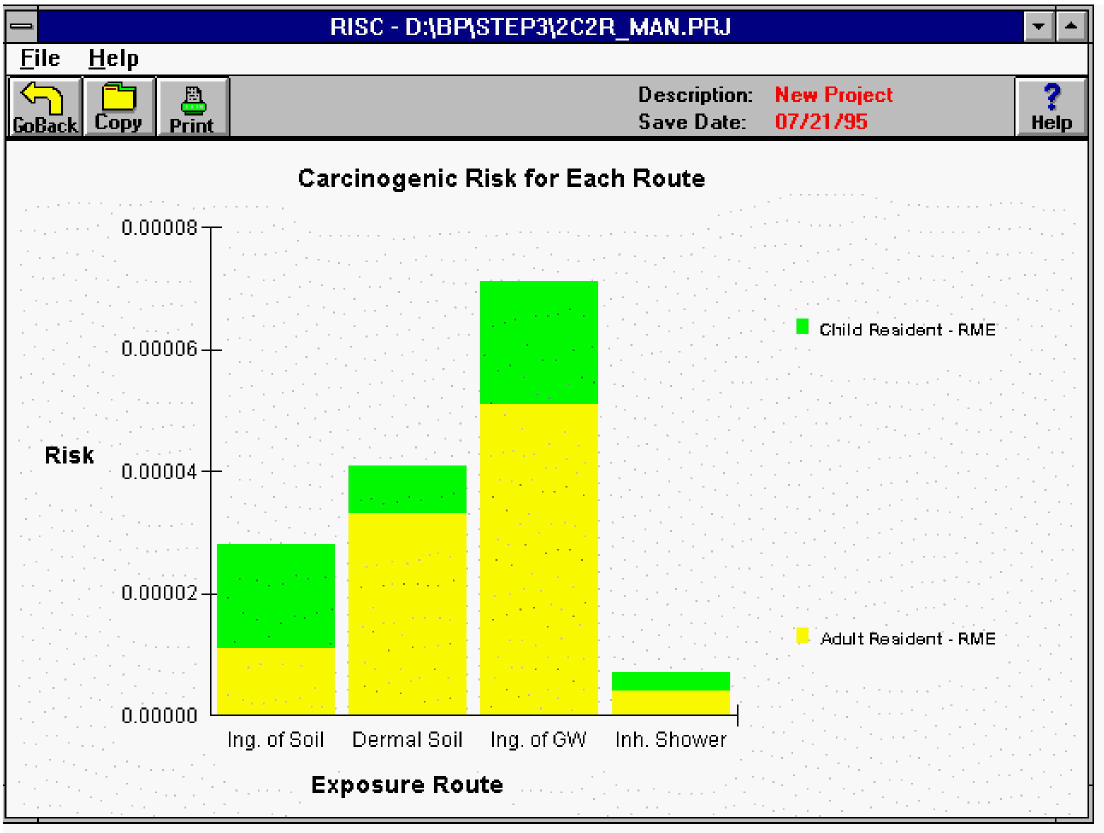


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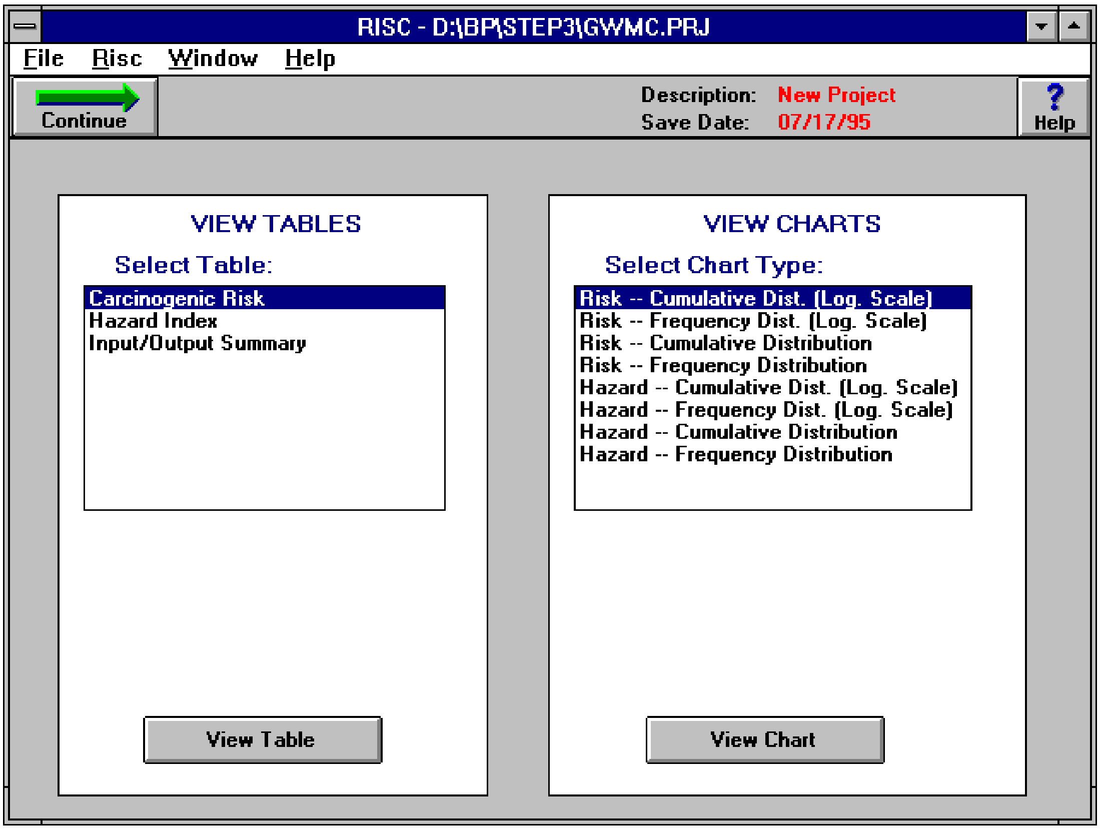
Figure 9-5. "Stacked" Chart for Additive Receptors

In this case the receptor is considered to be a child for 5 years and an adult for 30 years for a total exposure duration of 35 years. Since the behavior (and intake parameters) of children are different than adults, different risks will be calculated for the same length of exposure. The clustered option illustrates the contribution of both exposure periods to the total risk. In Figure 9-5, for example, just over one-half of the risk from ingestion of soil occurs while the receptor is a child (only 5 years of the 35 year exposure duration).

9.2 MONTE CARLO OUTPUT

When a Monte Carlo analysis is performed the types of tables and charts available are different than for the deterministic case. Figure 9-6 shows the options for the Monte Carlo analysis case.



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Carcinogenic Risk
Hazard Index
Input/Output Summary

Risk -- Cumulative Dist. (Log. Scale)
Risk -- Frequency Dist. (Log. Scale)
Risk -- Cumulative Distribution
Risk -- Frequency Distribution
Hazard -- Cumulative Dist. (Log. Scale)
Hazard -- Frequency Dist. (Log. Scale)
Hazard -- Cumulative Distribution
Hazard -- Frequency Distribution

Figure 9-6. Menu for Viewing Results of a Monte Carlo Risk Assessment

9.2.1 Monte Carlo Tables

There are three table options for Monte Carlo similar to the three table options for the deterministic case. For the former, the carcinogenic risk and hazard index tables present the statistics calculated from the Monte Carlo output. Tables 9-3 and 9-4 (at the end of this chapter) show the "Carcinogenic Risk" and "Input/Output Summary" tables for a residential adult. The "Input/Output Summary" table presents all the input distributions specified for the intake parameters.

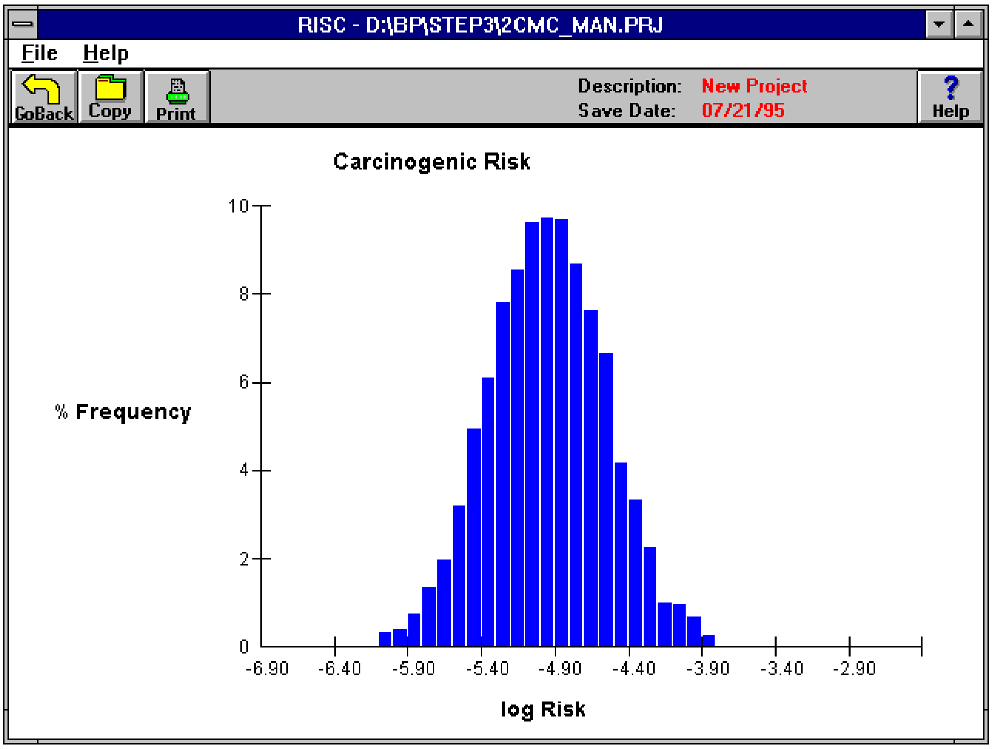
When using the Monte Carlo analysis an acceptable non-exceedence risk level must be decided. Typically this value is the 90th or 95th percentile although there is no universally accepted standard. The statistical summary table of risk (Table 9-3) indicates that the Monte Carlo output generated total risk values that ranged from a minimum of 3.11E-07 (about 3 in 10,000,000) to a maximum of 1.93E-04 (about 2 in 10,000). The 95% exceedence value is 4.05E-05. The deterministic example presented in Section 9.1 estimated a total risk of 9.9E-05 for the reasonable maximum exposure (RME) residential adult. One point of interest is to locate where the deterministic RME value falls on the range of Monte Carlo results. For this example, the RME value is above the 99th percentile but less than the maximum of the Monte Carlo results. This indicates that for this case, the risk estimated using the RME deterministic case would only be exceeded by less than 1% of the receptors exposed to this site.

9.2.2 Monte Carlo Charts

The charts available for a Monte Carlo analysis present summaries of *total* risk or *total* hazard, (not risk broken out from each route or chemical). These charts can be viewed as a frequency distribution or they can be viewed as a cumulative frequency distribution. Either type of chart may viewed on a linear or logarithmic scale.

9.2.2.1 Frequency Distributions

Frequency distributions are constructed from the Monte Carlo output by arranging the output values into classes and representing the frequency of occurrence in any class by the height of the bar. The frequency of occurrence corresponds to probability. Frequency distributions are sometimes called probability density functions (PDFs), however, a probability density function is a statistical term implying that the frequency distribution was constructed with an infinitely large data set and infinitely small class size (in essence a continuous curve). Frequency distributions are useful for evaluating the spread of the values and the shape of the "tails" (i.e. how narrow or wide they are). They are not as useful as cumulative distribution functions for evaluating probabilities of exceedence of a certain risk level. Figure 9-7 shows an example of a frequency distribution of total risk on a log scale.



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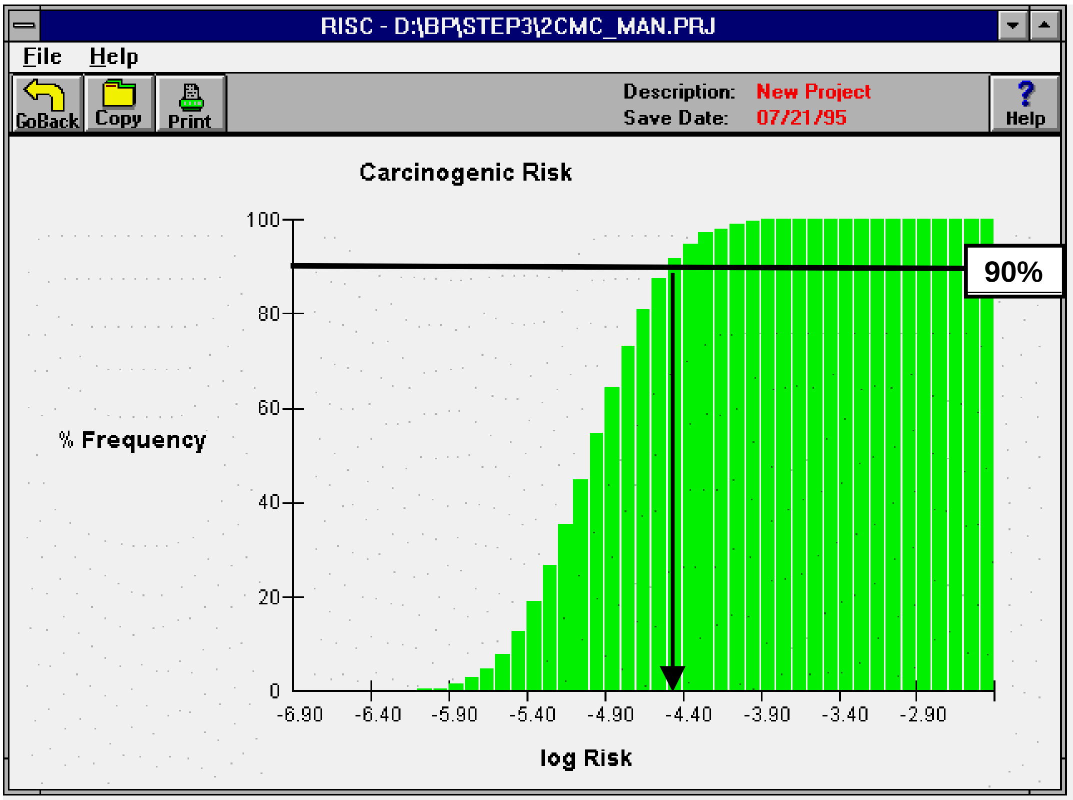
Save Date: 07/21/95

Figure 9-7. Frequency Distribution of Total Risk on a Logarithmic Scale

The most likely value (or mode) is the value that occurs most often (in other words, has the highest probability) in the set of values. In the histogram shown in Figure 9-7, the most likely value corresponds to a bar with a log risk of around -4.9. A log risk of -4.9 corresponds to a risk of 1.26E-5, which is very close to the 50th percentile of risk presented in Table 9-3. The most likely value is the center value of the class or bar with the highest probability, (in this case a log risk of -4.9) and does not necessarily equal the mean. (Consider a log-normal distribution where the most likely value occurs below the mean.)

9.2.2.2 Cumulative Frequency Distribution

Frequency distributions may also be presented in a cumulative form. A cumulative curve is typically scaled from 0 to 100% (or from 0 to 1 as a fraction) on the Y-axis, with Y-axis values representing the cumulative probability up to the corresponding X-axis value. For example, in a cumulative frequency distribution, the 50% cumulative value is the point of 50% probability. Fifty percent of the values in the distribution fall below this value and 50% are above. The 0 cumulative value is the minimum value and the 100% cumulative value is the maximum value of the distribution (100% of the values fall below this point). The most likely value can be found at that point where the slope of the Cumulative Probability vs. the Risk curve is greatest. Figure 9-8 shows a cumulative distribution of total risk on a log scale.



Description: New Project
Save Date: 07/21/95

Figure 9-8. Cumulative Risk on a Logarithmic Scale

Lines have been added to the chart in Figure 9-8 indicating the 90th percentile and the corresponding log risk value of -4.54 (or non-log value of 2.87E-5, as taken from the 90% value in Table 9-3). Ninety percent of the risk results for this Monte Carlo analysis fall below the total risk of 2.87E-5 (or about 3 in 10,000). Most of the output values fall in the range of -5.5 to -4.5 (the area where the curve is the steepest or the percentile increases fastest for the increase in risk). Only 10% of the values fall in the range -4.5 to -1.6.

9.3 TRANSFERRING TABLES AND CHARTS TO OTHER APPLICATIONS

Both the tables and charts can be transferred to another software application (such as a word processor) by clicking on the 'Copy' button at the top of the table or chart. Then the user can minimize or close the RISC main screen, open the new destination software, and choose "Paste" (or the Shift and Insert keys). When many routes of concern are being evaluated, the risk and hazard summary tables may be too wide to print in a portrait mode. To print these, the printer configuration should be changed using the printer control from the Windows® Control Panel. Many laser printers allow text to be printed in a landscape mode and will accept scaling factors. If the report is copied into another software package, the report can be re-formatted (font size may be reduced). The Carcinogenic Risk and Hazard Quotient Summary tables have tabs separating the data so that they can be transferred to a spreadsheet program directly (they are tab-delimited).

Table 9-1. Summary of Carcinogenic Risk

```
     SUMMARY OF CARCINOGENIC RISK


CASE 1:
Adult Resident - RME

                        Ingestion   Dermal      Ingestion   Inhalation
                        of          Contact     of          During
                        Soil        Soil        Groundwater Shower       TOTAL

____________________________________________________________________________

Benzene                 8.5E-06     2.2E-05     3.4E-06     4.0E-06     3.8E-05
Benzo(a)pyrene          2.7E-06     1.1E-05     4.7E-05     0.0E+00     6.1E-05

____________________________________________________________________________
TOTAL                   1.1E-05     3.3E-05     5.1E-05     4.0E-06     9.9E-05
```

Table 9-2. Input/Output Summary (Page 1 of 3)

```
Title:
New Project
07/21/95

Scenarios:
Adult Resident - RME

Routes:
INGESTION OF SOIL
DERMAL CONTACT WITH SOIL
INGESTION OF GROUNDWATER
INHALATION DURING SHOWER

Chemicals:
   Benzene
   Benzo(a)pyrene


SUMMARY OF INPUT PARAMETERS                     Scenario 1
-------------------------------------------------------------------

Lifetime and Body Weight
   Body Weight (kg)                               70.00
   Lifetime (years)                               70.00

INGESTION OF SOIL
   Soil Ingestion Rate (mg/day)                  100.00
   Exp. Frequency Soil (events/year)             350.00
   Exp. Duration Soil (years)                     30.00
   Absorption Adjustment Factor for
      Ingestion of Soil (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                .63

   Soil Bioavailability (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                1.0

DERMAL CONTACT WITH SOIL
   Fraction Skin Exposed to Soil (-)                .56
   Adherence Factor for Soil (mg/cm^2)             1.00
   Exposure Freq. Soil   (events/year)           350.00
   Exposure Duration Soil (years)                 30.00
   Absorption Adjustment Factor for
      Dermal Exposure to Soil (-)
                     Benzene                      2.00E-02
                     Benzo(a)pyrene               2.00E-02

   Soil Bioavailability (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                1.0

INGESTION OF GROUNDWATER
   Ingestion rate (l/day)                          2.00
   Exp. Freq Groundwater (events/year)           350.00
   Exp. Duration Groundwater (years)              30.00
   Absorption Adjustment Factor for
      Ingestion of water (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                1.1
```

Table 9-2. Input/Output Summary (Page 2 of 3)

```
INHALATION DURING SHOWER
   Volume of Bathroom (m^3)                        3.00
   Temperature of Shower Water (C)                48.00
   Shower Flow Rate (l/min)                       10.00
   Time in Shower (hour/day)                        .20
   Inhal. Rate in the Shower (m^3/hr)               .60
   Lung Retention Factor (-)                       1.00

Exp. Freq Groundwater (events/year)           350.00
   Exp. Duration Groundwater (years)              30.00
   Absorption Adjustment Factor for
      Inhalation (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                1.0

   Henry"s Law Constant (-)
                     Benzene                        .25
                     Benzo(a)pyrene               2.77E-05

   Molecular Weight (g/mole)
                     Benzene                       78.
                     Benzo(a)pyrene               2.52E+02


MEDIA CONCENTRATIONS
--------------------
Concentration in Groundwater (mg/l)
     Used in calculating carcinogenic risk and hazard index
                     Benzene                      1.00E-02
                     Benzo(a)pyrene               5.00E-04

Concentration in Soil (mg/kg)
     Used in calculating carcinogenic risk and hazard index
                     Benzene                      5.00E+02
                     Benzo(a)pyrene                1.0

SLOPE FACTORS AND REFERENCE DOSES
---------------------------------

Ingestion Slope Factor [1/(mg/kg-day)]
                     Benzene                      2.90E-02
                     Benzo(a)pyrene                7.3

Ingestion Reference Dose (mg/kg-day)
                     Benzene                        ND
                     Benzo(a)pyrene               3.00E-02

Inhalation Slope Factor [1/(mg/kg-day)]
                     Benzene                      2.90E-02
                     Benzo(a)pyrene                 ND

Inhalation Reference Dose (mg/kg-day)
                     Benzene                        ND
                     Benzo(a)pyrene                 ND

Dermal Slope Factor [1/(mg/kg-day)]
                     Benzene                      2.90E-02
                     Benzo(a)pyrene                7.3

Dermal Reference Dose (mg/kg-day)
                     Benzene                        ND
                     Benzo(a)pyrene               3.00E-02
```

Table 9-2. Input/Output Summary (Page 3 of 3)

```
SUMMARY OF RESULTS
---------------------------------------------------------

INGESTION OF SOIL
   Benzene
     CDI (mg/kg-day)               6.85E-04
     LADD (mg/kg-day)              2.94E-04
     Cancer Risk (-)               8.51E-06
     Hazard Index (-)              0.00E+00

   Benzo(a)pyrene
     CDI (mg/kg-day)               8.63E-07
     LADD (mg/kg-day)              3.70E-07
     Cancer Risk (-)               2.70E-06
     Hazard Index (-)              2.88E-05


DERMAL CONTACT WITH SOIL

   Benzene
     CDI (mg/kg-day)               1.76E-03
     LADD (mg/kg-day)              7.56E-04
     Cancer Risk (-)               2.19E-05
     Hazard Index (-)              0.00E+00

   Benzo(a)pyrene
     CDI (mg/kg-day)               3.53E-06
     LADD (mg/kg-day)              1.51E-06
     Cancer Risk (-)               1.10E-05
     Hazard Index (-)              1.18E-04

INGESTION OF GROUNDWATER

   Benzene
     CDI (mg/kg-day)               2.74E-04
     LADD (mg/kg-day)              1.17E-04
     Cancer Risk (-)               3.41E-06
     Hazard Index (-)              0.00E+00

   Benzo(a)pyrene
     CDI (mg/kg-day)               1.51E-05
     LADD (mg/kg-day)              6.46E-06
     Cancer Risk (-)               4.71E-05
     Hazard Index (-)              5.02E-04

INHALATION DURING SHOWER

   Concentration in Bathroom Air (mg/m^3)
                  Benzene                      .195
                  Benzo(a)pyrene              2.055E-05
   Fraction Volatilized from Shower Water (-)
                  Benzene                      .488
                  Benzo(a)pyrene              1.027E-03
   Total Mass Volatilized per Shower (mg)
                  Benzene                      .586
                  Benzo(a)pyrene              6.164E-05
   Benzene
     CDI (mg/kg-day)               3.21E-04
     LADD (mg/kg-day)              1.38E-04
     Cancer Risk (-)               3.99E-06
     Hazard Index (-)              0.00E+00

   Benzo(a)pyrene
     CDI (mg/kg-day)               3.38E-08
     LADD (mg/kg-day)              1.45E-08
     Cancer Risk (-)               0.00E+00
     Hazard Index (-)              0.00E+00
```

Table 9-3. Summary Statistics of Carcinogenic Risk for a Monte Carlo Analysis

```
SUMMARY STATISTICS OF CARCINOGENIC RISK
              (by route)
   Route of Concern                Min.        5%      Mean       75%       90%       95%       99%      Max.   Std.Dev.
 ------------------------------------------------------------------------------------------------------------------------
 INGESTION OF SOIL             7.04E-10  2.49E-08  6.39E-07  6.71E-07  1.55E-06  2.45E-06  5.36E-06  3.72E-05  1.24E-06
 DERMAL CONTACT WITH SOIL      2.07E-09  2.48E-08  6.92E-07  7.54E-07  1.69E-06  2.67E-06  5.94E-06  2.13E-05  1.26E-06
 INGESTION OF GROUNDWATER      1.34E-07  1.23E-06  1.16E-05  1.40E-05  2.57E-05  3.72E-05  7.37E-05  1.91E-04  1.40E-05
 INHALATION DURING SHOWER      1.90E-09  3.20E-08  6.97E-07  7.96E-07  1.73E-06  2.62E-06  5.65E-06  1.81E-05  1.12E-06
 ------------------------------------------------------------------------------------------------------------------------
 TOTAL                         3.11E-07  2.02E-06  1.36E-05  1.66E-05  2.87E-05  4.05E-05  7.88E-05  1.93E-04  1.49E-05
 ------------------------------------------------------------------------------------------------------------------------

         SUMMARY STATISTICS OF CARCINOGENIC RISK
              (by chemical)
  Chemical                        Min.        5%      Mean       75%       90%       95%       99%      Max.   Std.Dev.
 ------------------------------------------------------------------------------------------------------------------------
 Benzene                       6.35E-08  4.01E-07  2.42E-06  3.03E-06  5.06E-06  7.01E-06  1.22E-05  3.34E-05  2.42E-06
 Benzo(a)pyrene                2.09E-07  1.41E-06  1.12E-05  1.36E-05  2.43E-05  3.52E-05  6.92E-05  1.78E-04  1.31E-05
 ------------------------------------------------------------------------------------------------------------------------
 TOTAL                         3.11E-07  2.02E-06  1.36E-05  1.66E-05  2.87E-05  4.05E-05  7.88E-05  1.93E-04  1.49E-05
 ------------------------------------------------------------------------------------------------------------------------
```

Table 9-4. Input/Output Summary for a Monte Carlo Analysis (Page 1 of 2)

```
Title:
New Project
07/21/95

Scenarios:
Resident -- Adult

Routes:
INGESTION OF SOIL
DERMAL CONTACT WITH SOIL
INGESTION OF GROUNDWATER
INHALATION DURING SHOWER

Chemicals:
   Benzene
   Benzo(a)pyrene


 Number of Monte Carlo runs:       5000

SUMMARY OF INPUT PARAMETERS        Distribution    Mean   Std Dev    Min      Max
-------------------------------------------------------------------------------------

Lifetime and Body Weight

Body Weight (kg)                     Normal      7.20E+01 1.59E+01 2.40E+01 1.25E+02
Lifetime (years)                     Constant    7.00E+01    NA       NA       NA

INGESTION OF SOIL

Soil Ingestion Rate (mg/day)         Lognormal   4.04E+01 3.73E+01 1.50E+00 6.67E+02
Exp. Frequency Soil (events/year)    Triangular  4.00E+01    NA    1.00E+01 3.50E+02
Exp. Duration Soil (years)           Lognormal   1.14E+01 1.37E+01 0.00E+00 1.00E+02
   Absorption Adjustment Factor for
      Ingestion of Soil (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                .63

   Soil Bioavailability (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                1.0

DERMAL CONTACT WITH SOIL

Fraction Skin Exposed to Soil (-)    Triangular  1.00E-01    NA    0.00E+00 5.60E-01
Adherence Factor for Soil (mg/cm^2)  Triangular  2.00E-01    NA    2.00E-01 1.00E+00
Exposure Freq. Soil   (events/year)  Triangular  4.00E+01    NA    1.00E+01 3.50E+02
Exposure Duration Soil (years)       Lognormal   1.14E+01 1.37E+01 0.00E+00 1.00E+02
   Absorption Adjustment Factor for
      Dermal Exposure to Soil (-)
                     Benzene                      2.00E-02
                     Benzo(a)pyrene               2.00E-02

   Soil Bioavailability (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                1.0

INGESTION OF GROUNDWATER

Ingestion rate (l/day)               Lognormal   1.27E+00 6.00E-01 1.00E-01 3.00E+00
Exp. Freq Groundwater (events/year)  Constant    3.50E+02    NA       NA       NA
Exp. Duration Groundwater (years)    Lognormal   1.14E+01 1.37E+01 0.00E+00 7.00E+01
   Absorption Adjustment Factor for
      Ingestion of water (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                1.1
```

Table 9-4. Input/Output Summary for a Monte Carlo Analysis (Page 2 of 2)

```
INHALATION DURING SHOWER

Volume of Bathroom (m^3)             Triangular  2.90E+00    NA    2.00E+00 6.00E+00
Temperature of Shower Water (C)      Triangular  4.50E+01    NA    3.50E+01 5.00E+01
Shower Flow Rate (l/min)             Lognormal   8.00E+00 2.70E+00 0.00E+00 3.00E+01
Time in Shower (hour/day)            Triangular  1.10E-01    NA    3.00E-02 3.30E-01
Inhal. Rate in the Shower (m^3/hr)   Constant    6.00E-01    NA       NA       NA
Lung Retention Factor (-)            Constant    1.00E+00    NA       NA       NA
Exp. Freq Groundwater (events/year)  Constant    3.50E+02    NA       NA       NA
Exp. Duration Groundwater (years)    Lognormal   1.14E+01 1.37E+01 0.00E+00 7.00E+01
   Absorption Adjustment Factor for
      Inhalation (-)
                     Benzene                       1.0
                     Benzo(a)pyrene                1.0

   Henry"s Law Constant (-)
                     Benzene                       .25
                     Benzo(a)pyrene               2.77E-05

   Molecular Weight (g/mole)
                     Benzene                       78.
                     Benzo(a)pyrene               2.52E+02


MEDIA CONCENTRATIONS
--------------------
Concentration in Groundwater (mg/l)
     Used in calculating carcinogenic risk and hazard index
       Benzene                       Constant    1.00E-02    NA       NA       NA
       Benzo(a)pyrene                Constant    5.00E-04    NA       NA       NA

Concentration in Soil (mg/kg)
     Used in calculating carcinogenic risk and hazard index
       Benzene                       Constant    5.00E+02    NA       NA       NA
       Benzo(a)pyrene                Constant    1.00E+00    NA       NA       NA

SLOPE FACTORS AND REFERENCE DOSES
---------------------------------

Ingestion Slope Factor [1/(mg/kg-day)]
                     Benzene                      2.90E-02
                     Benzo(a)pyrene                7.3

Ingestion Reference Dose (mg/kg-day)
                     Benzene                        ND
                     Benzo(a)pyrene               3.00E-02

Inhalation Slope Factor [1/(mg/kg-day)]
                     Benzene                      2.90E-02
                     Benzo(a)pyrene                 ND

Inhalation Reference Dose (mg/kg-day)
                     Benzene                        ND
                     Benzo(a)pyrene                 ND

Dermal Slope Factor [1/(mg/kg-day)]
                     Benzene                      2.90E-02
                     Benzo(a)pyrene                7.3

Dermal Reference Dose (mg/kg-day)
                     Benzene                        ND
                     Benzo(a)pyrene               3.00E-02


   Monte Carlo Output is summarized in separate tables.
 ---------------------------------------------
```

Chapter
10.0

Example Risk Assessment Scenarios

This chapter presents three risk assessment scenarios and discusses how to use RISC to evaluate the scenarios. These examples are designed to be worked through by the user on the computer. There are also saved project files shipped with the software for each of these three examples.

The first example is for a former gas station that is planned to be re-developed with single family homes. In the second example, residents adjacent to an existing gas station use groundwater to irrigate their yards and gardens (the indoor water is provided by a municipality). The gas station has impacted groundwater in the past. The third scenario illustrates a simple ecological screening model using the surface model in RISC to estimate surface water concentrations in a stream adjacent to contaminated groundwater. These surface water concentrations will be compared with ambient water quality criteria. The three examples are described in detail in the following sections.

10.1 EXAMPLE 1: FORMER GAS STATION REDEVELOPED WITH SINGLE FAMILY HOUSING

This example is saved in a project file called "Example1.prj". The reader is encouraged to work through the example and enter in the information for themselves.

In this scenario, it is assumed that a former gas station site containing contaminated soil (both at the ground surface and at depth) might be re-developed at some point in the future for single-family houses. There are two questions to be answered for this site: (1) what is the human health risk from the site if the soil is left as is?, and (2) what clean-up levels would be protective of human health at this site?

Benzene, ethylbenzene and toluene have been detected in the top foot of soil and at depth. Three soil borings were made and samples collected at 0.5, 3.0, and 6.0 meters below ground surface. The table below shows the analytical results. It is suspected that the surficial contamination arose from surface spills or hose leaks and the contamination at depth resulted from a leaky storage tank. The fuel tank has been removed along with any stained soil from the pit. (The soil samples were collected after the stained soil was removed.) Groundwater is at 6 meters below ground surface and is not potable (due to contamination from a neighboring silicon fabrication plant).

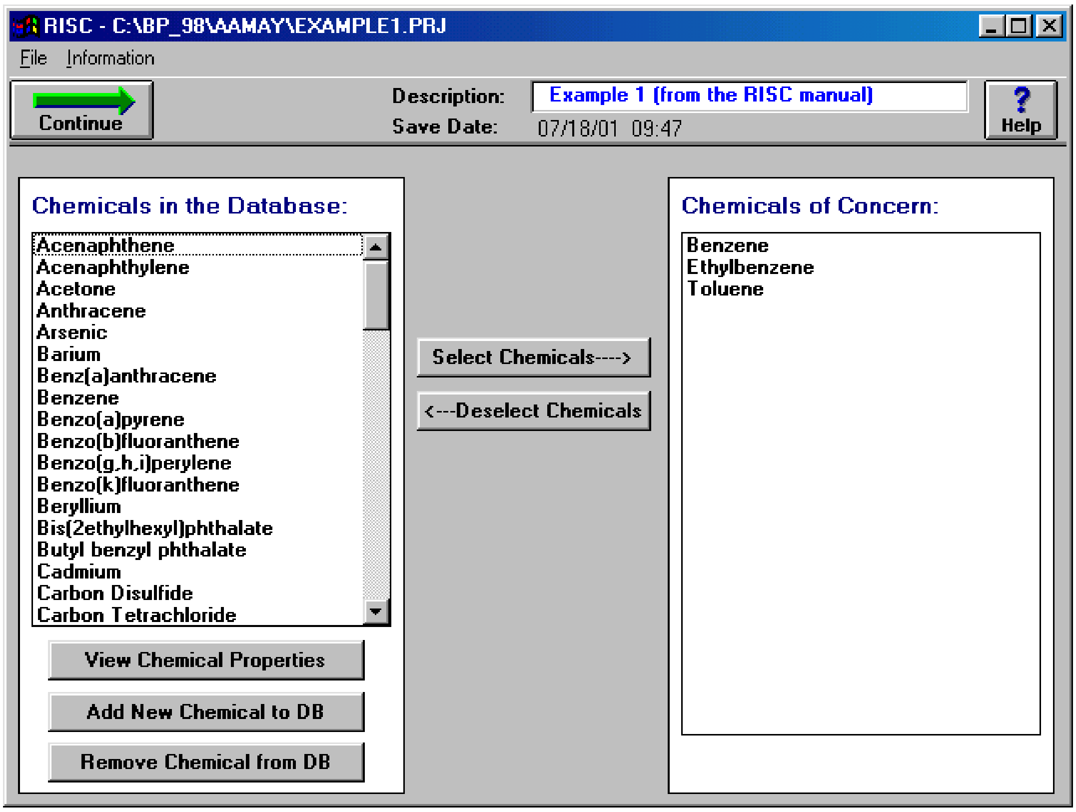
Chemical Concentrations Detected at Former Gas Station Site
Example #1

Sample Description	Units	Benzene Concentration	Ethylbenzene Concentration	Toluene Concentration
Soil Boring #1	mg/kg soil			
0.5 m depth		ND (0.005)	0.012	ND (0.005)
3.0 m depth		2.6	0.047	17
6.0 m depth		0.68	ND (0.005)	5.8
Soil Boring #2	mg/kg soil			
0.5 m depth		0.01	0.008	0.03
3.0 m depth		6	4.5	37
6.0 m depth		1.2	ND (0.005)	8.2
Soil Boring #3	mg/kg soil			
0.5 m depth		ND (0.005)	ND (0.005)	ND (0.005)
3.0 m depth		0.086	0.11	0.74
6.0 m depth		0.006	ND (0.005)	0.009
Creek Sample #1	mg/l water	0.007	ND (0.0005)	0.012
Creek Sample #2	mg/l water	0.016	ND (0.0005)	0.032

( ) = detection limit

Step 1: Choose Chemicals of Concern *(Example #1)*

Benzene, ethylbenzene, and toluene were the only chemicals detected from an analysis that included BTEX, MTBE, the PAHs, and heavy metals. These three chemicals are the chemicals of concern. The screen in Step 1 should look like the following after the chemicals of concern have been selected.



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

Chemicals in the Database:
Acenaphthene
Acenaphthylene
Acetone
Anthracene
Arsenic
Barium
Benz(a)anthracene
Benzene
Benzo(a)pyrene
Benzo(b)fluoranthene
Benzo(g,h,i)perylene
Benzo(k)fluoranthene
Beryllium
Bis(2ethylhexyl)phthalate
Butyl benzyl phthalate
Cadmium
Carbon Disulfide
Carbon Tetrachloride

Chemicals of Concern:
Benzene
Ethylbenzene
Toluene

Example #1: Step 1

Step 2: Identify Appropriate Exposure Pathways and Determine Method for Estimating Receptor Point Concentrations *(Example #1)*

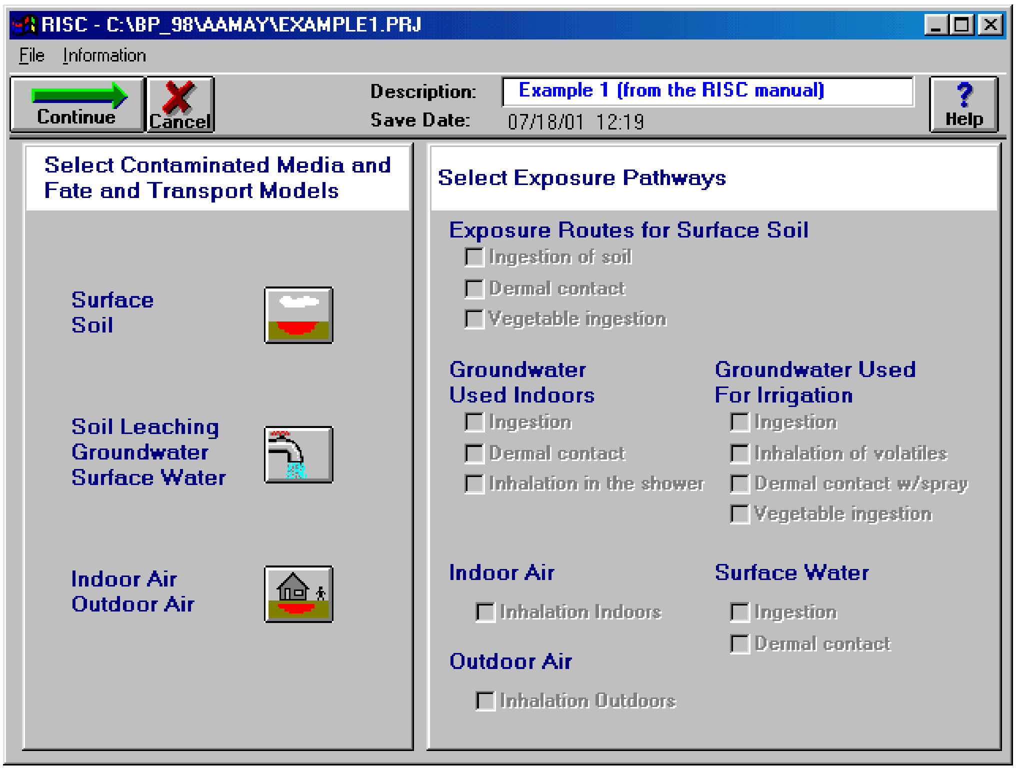
In this step, potential exposure pathways for a residential exposure at this site will be chosen. It is assumed that a single-family house (with a backyard) will be built on the former gas station site with no vapor membrane under the house. Both children and adults may live in the house and use the garden. There are restrictions preventing the residents from installing a well and using groundwater in this area. The next table lists the potential exposure pathways, contaminated media and receptor contact media.

Exposure Pathways, Source Media, and Receptor Contact Media
Example #1

Exposure Pathway	Source Media	Receptor Contact Media
Ingestion of soil	Surficial soil	Surficial soil (top 50 cm might be reasonable for a residential exposure)
Dermal contact with soil	Surficial soil	Surficial soil (top 50 cm might be reasonable for a residential exposure)
Ingestion of vegetables grown in contaminated soil	Surficial soil	Surficial soil (top 50 cm might be reasonable for a residential exposure)
Volatilization from soil to indoor air	Soil (any depth)	Indoor air

The above exposure pathways could apply to both children and adult residents.

After determining the potential exposure pathways, the next step is to decide how to estimate receptor point concentrations. Two of the exposure routes (ingestion of soil and dermal contact with soil), are direct exposure routes. That is, the source media is also the media that the receptor may contact. The contaminants in soil, however, may also volatilize into indoor air, so the concentrations in air need to be estimated. Fate and transport models are used to estimate the receptor point concentrations in indoor air. For estimating indoor air concentrations, the vapor transport model from soil into buildings will be used, the maximum soil concentration found at the relevant depth where the basement will be located will be used for the source. The following screens show the choices made in Step 2.



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 12:19

Select Contaminated Media and Fate and Transport Models

Select Exposure Pathways

Exposure Routes for Surface Soil
☐ Ingestion of soil
☐ Dermal contact
☐ Vegetable ingestion

Groundwater Used Indoors
☐ Ingestion
☐ Dermal contact
☐ Inhalation in the shower

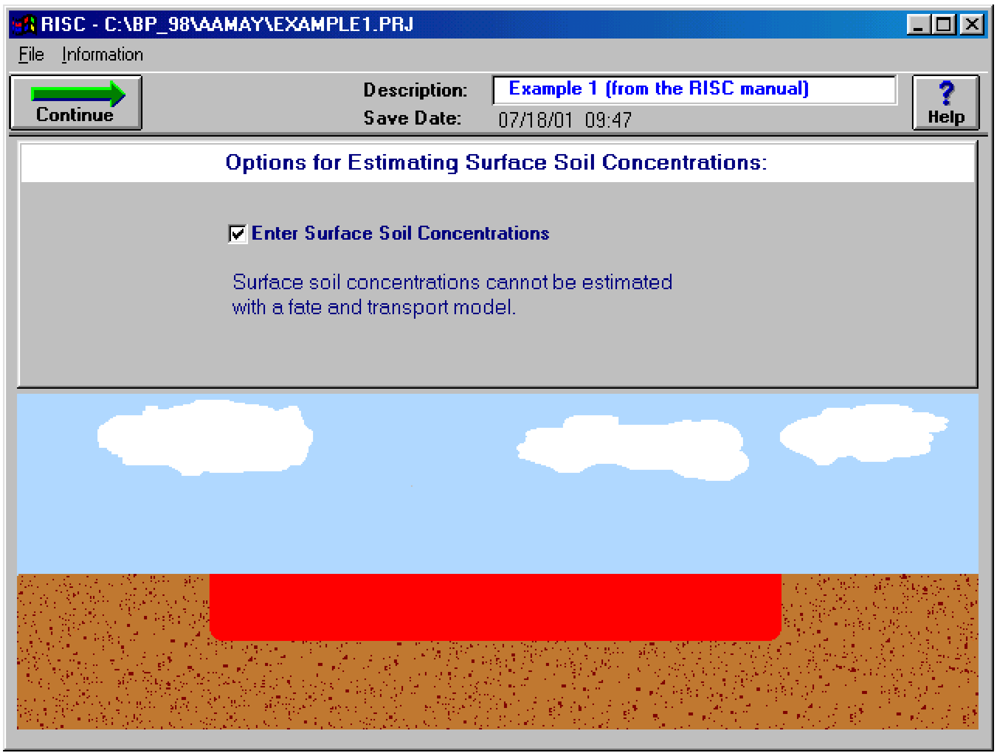
Groundwater Used For Irrigation
☐ Ingestion
☐ Inhalation of volatiles
☐ Dermal contact w/spray
☐ Vegetable ingestion

Indoor Air
☐ Inhalation Indoors

Outdoor Air
☐ Inhalation Outdoors

Surface Water
☐ Ingestion
☐ Dermal contact

Example #1: Step 2, Before Choosing any Media and Exposure Pathways



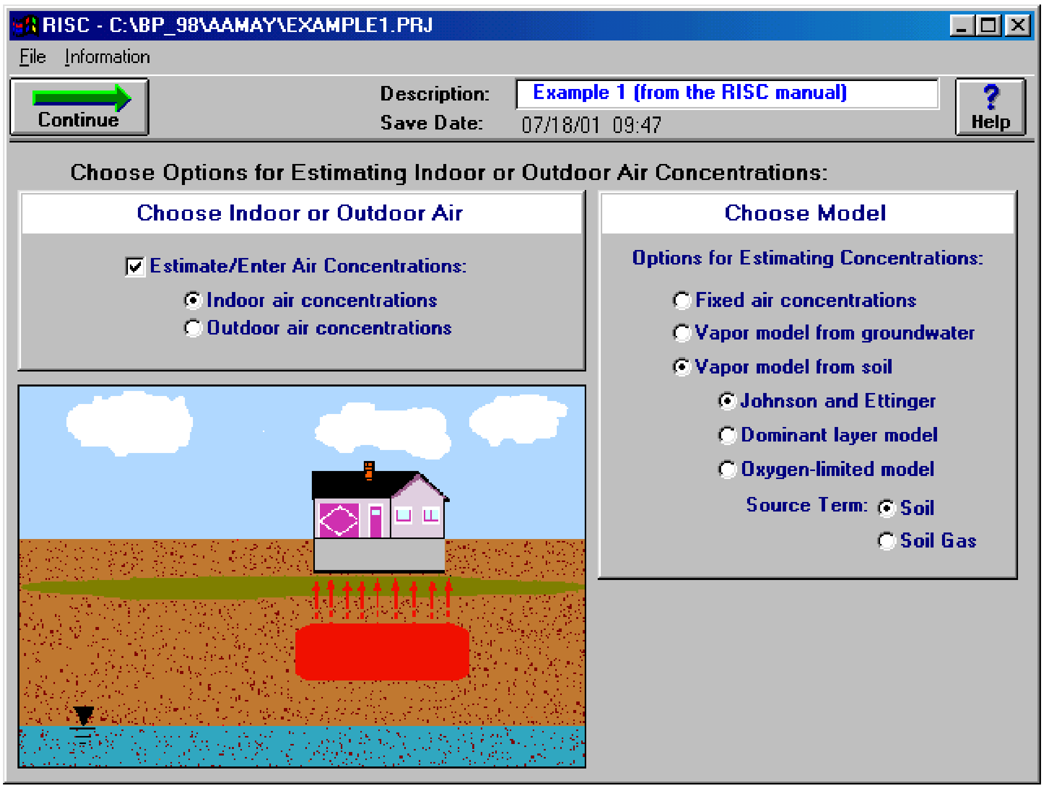
Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

Options for Estimating Surface Soil Concentrations:

☑ Enter Surface Soil Concentrations

Surface soil concentrations cannot be estimated with a fate and transport model.

Example #1: Step 2, Choosing Surface Soil as a Contaminated Media



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

Choose Options for Estimating Indoor or Outdoor Air Concentrations:

Choose Indoor or Outdoor Air

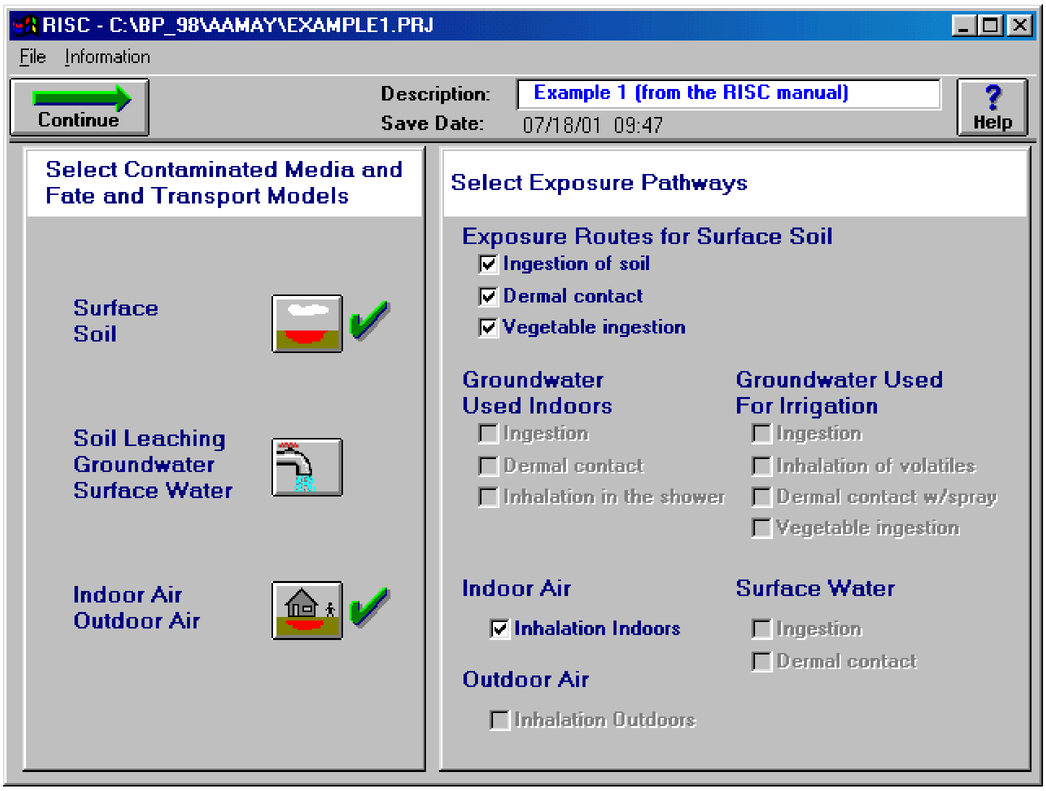
☑ Estimate/Enter Air Concentrations:
- ● Indoor air concentrations
- ○ Outdoor air concentrations

Choose Model

Options for Estimating Concentrations:
- ○ Fixed air concentrations
- ○ Vapor model from groundwater
- ● Vapor model from soil
  - ● Johnson and Ettinger
  - ○ Dominant layer model
  - ○ Oxygen-limited model

Source Term: ● Soil ○ Soil Gas

Example #1: Step 2, Choosing Indoor Air Model



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

Select Contaminated Media and Fate and Transport Models

Surface Soil ✓

Soil Leaching Groundwater Surface Water

Indoor Air Outdoor Air ✓

Select Exposure Pathways

Exposure Routes for Surface Soil
- ☑ Ingestion of soil
- ☑ Dermal contact
- ☑ Vegetable ingestion

Groundwater Used Indoors
- ☐ Ingestion
- ☐ Dermal contact
- ☐ Inhalation in the shower

Groundwater Used For Irrigation
- ☐ Ingestion
- ☐ Inhalation of volatiles
- ☐ Dermal contact w/spray
- ☐ Vegetable ingestion

Indoor Air
- ☑ Inhalation Indoors

Outdoor Air
- ☐ Inhalation Outdoors

Surface Water
- ☐ Ingestion
- ☐ Dermal contact

Example #1: Step 2, Choosing Exposure Pathways

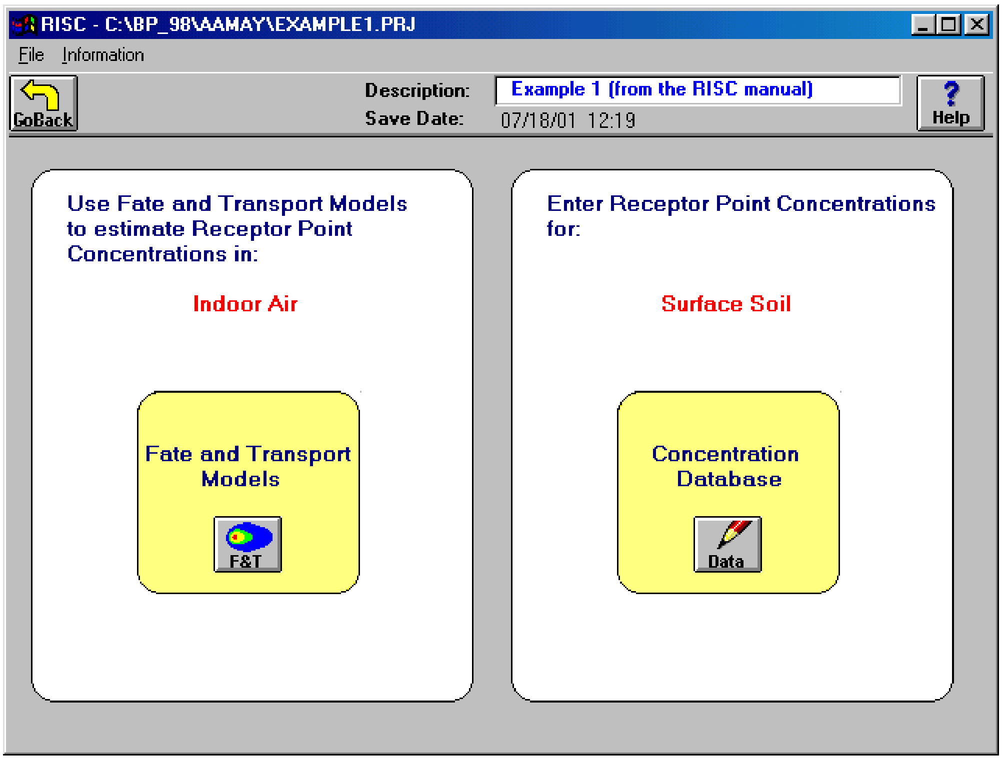
Step 3: Estimate Receptor Point Concentrations *(Example #1)*

The receptor point concentrations for the direct contact media (surficial soil) will be taken from the analytical data. Since so few samples were collected, the maximum values detected in the direct contact media will be used. The table below lists the receptor point concentrations used for surface soil.

Example 1: Receptor Point Concentrations in Surficial Soil

Chemical	Surface Soil Concentration [mg/kg]
Benzene	0.01
Ethylbenzene	0.12
Toluene	0.03

The receptor point concentrations for surface soil will be entered into the screens in Step 3. The information for the indoor air model will also be entered in Step 3 and the indoor air concentrations will be estimated. The following screens illustrate this process; first, the receptor point concentrations will be entered for the surface soil, then, the indoor air model will be run.



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 12:19

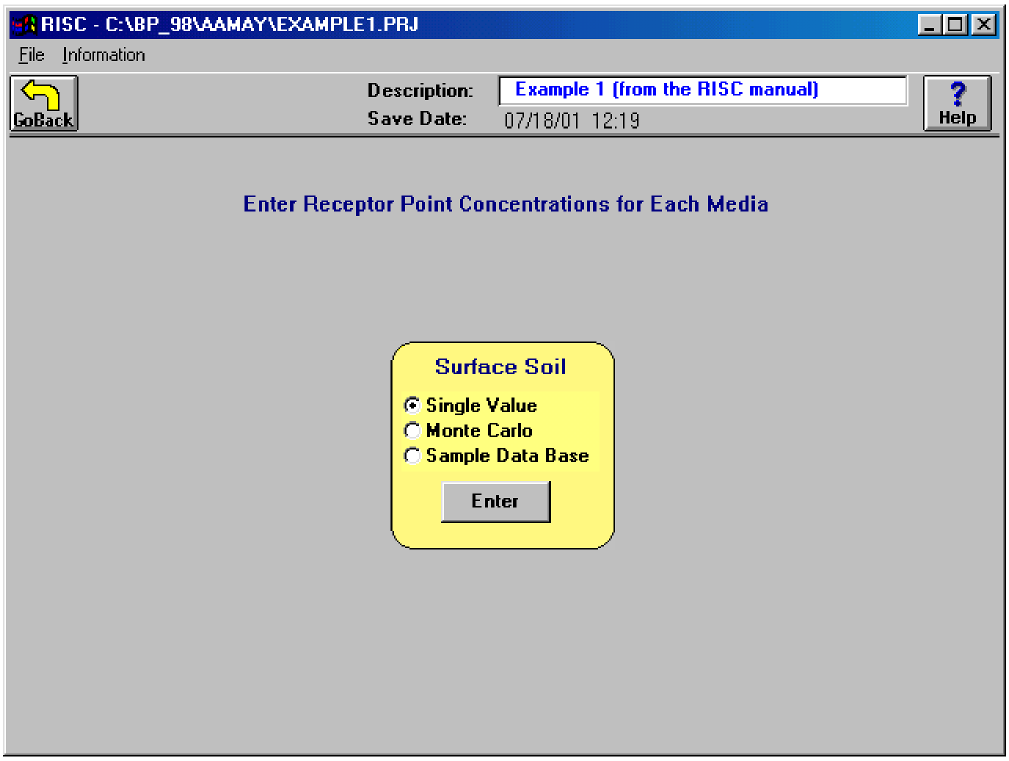
Use Fate and Transport Models to estimate Receptor Point Concentrations in:

Indoor Air

Enter Receptor Point Concentrations for:

Surface Soil

Example 1: Main Screen of Step 3

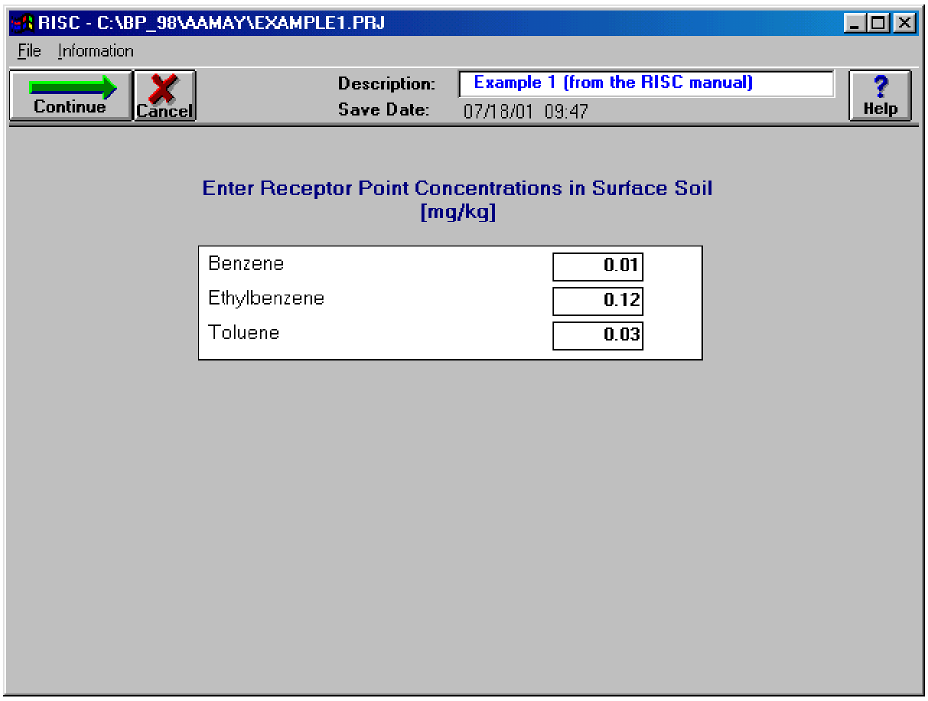


Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 12:19

Enter Receptor Point Concentrations for Each Media

Surface Soil
● Single Value
○ Monte Carlo
○ Sample Data Base

Example 1: Choose the "Single Value" Option



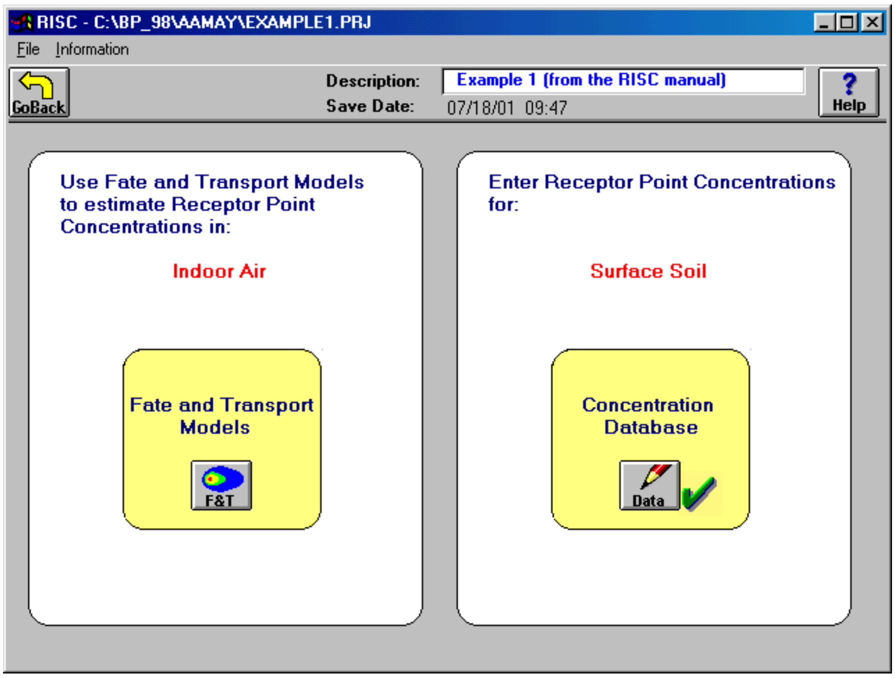
Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

Enter Receptor Point Concentrations in Surface Soil
[mg/kg]

Benzene	0.01
Ethylbenzene	0.12
Toluene	0.03

Example 1: Entering Surface Soil Concentrations

The next step is to use the fate and transport models to estimate concentrations in indoor and outdoor air. Select “Use Fate and Transport Models” from the following screen:



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

Use Fate and Transport Models to estimate Receptor Point Concentrations in:

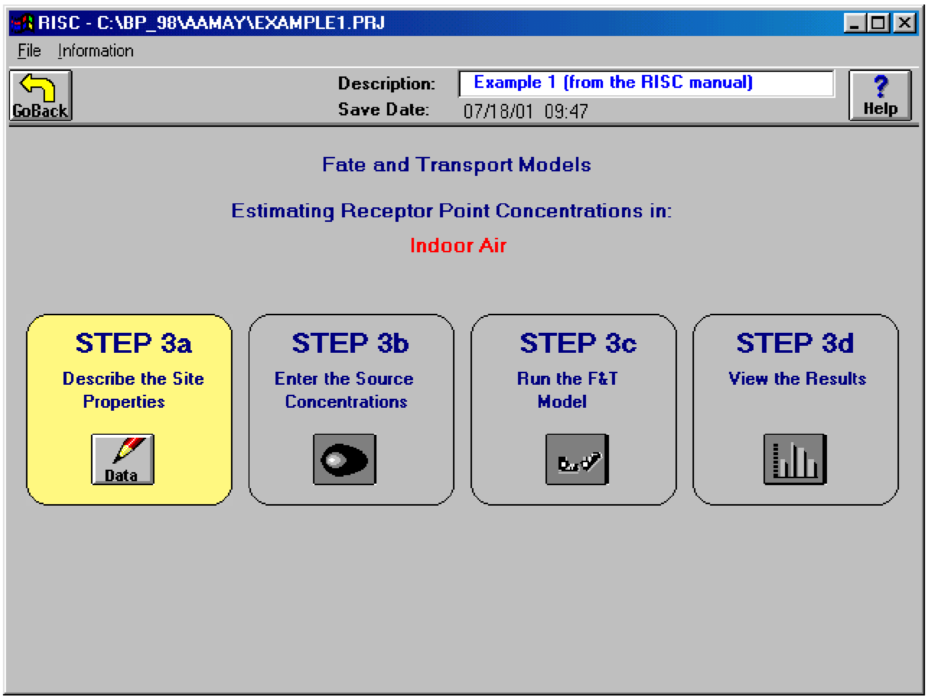
Indoor Air

Enter Receptor Point Concentrations for:

Surface Soil

Example 1: Select “Fate and Transport Models”

Then select “Step 3a: Describe the Site Properties”:



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

Fate and Transport Models

Estimating Receptor Point Concentrations in:
Indoor Air

STEP 3a
Describe the Site Properties

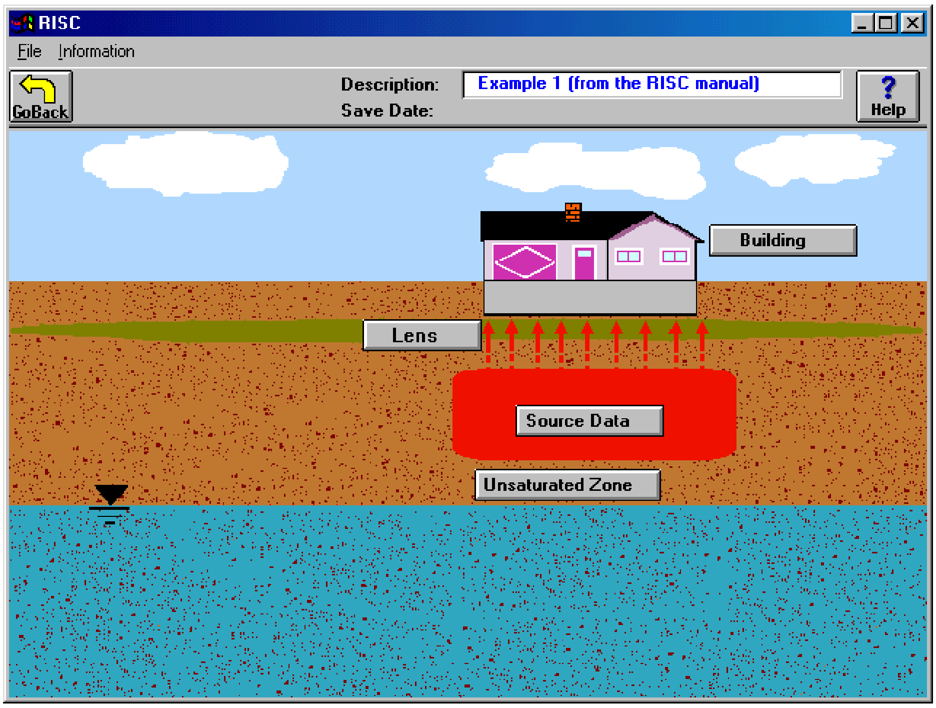
STEP 3b
Enter the Source Concentrations

STEP 3c
Run the F&T Model

STEP 3d
View the Results

Example 1: Select "Describe the Site Properties

The next screen, uniquely generated for the defined exposure pathways, identifies all of the parameter groups for this problem: building, lens, source data, and unsaturated zone.



Description: Example 1 (from the RISC manual)
Save Date:

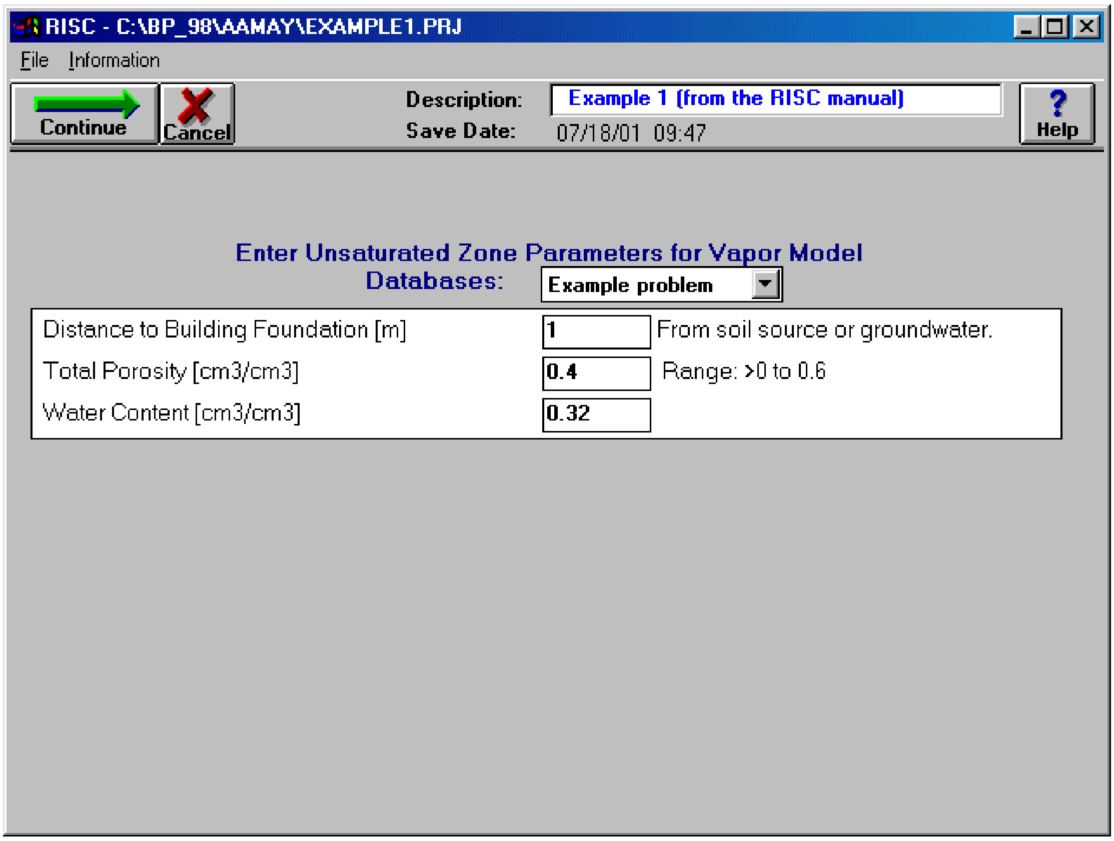
Example 1: Input Data Groups for the Indoor Air Model

Unsaturated Zone Data

At the site, the soil bulk density was measured and found to be 1.62 g/cm^3. Total porosity was measured in several samples and found to range from 0.3 to 0.45 cm^3 voids/cm^3 soil. Fraction organic carbon was measured in one soil sample from the 3 meter depth and found to be 0.007 g OC/g soil. Moisture content and soil conductivity were not measured so they will be estimated from the literature based on the soil type observed at the site. (Note that the moisture content under the house is not estimated by this indoor air model and must be entered explicitly by the user.) By visual observation, the soils samples were very wet so the moisture content under the (proposed) house is set to 0.32 cm^3/cm^3 (80% of the porosity is assumed saturated). Note, the soil samples were collected from an area that was originally under pavement (that was recently removed) so conditions under a new house are expected to be similar.

The boring logs for adjacent water wells and site observation indicate that the soil consists predominantly of silty clay. The input parameters which are needed for modeling can be obtained from default values in the soils database (available from the unsaturated zone parameters screen), if they are not specifically known. It is assumed that a house may be built anywhere on the site so the shortest distance to a hypothetical basement will be used. Assuming the bottom of the basement is 2 meters below grade, the bulk of the contamination could be within 1 meter of the foundation.

In this indoor air model, degradation of contaminants in the vapor phase is ignored. Entering the unsaturated zone parameters into the model yields:



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

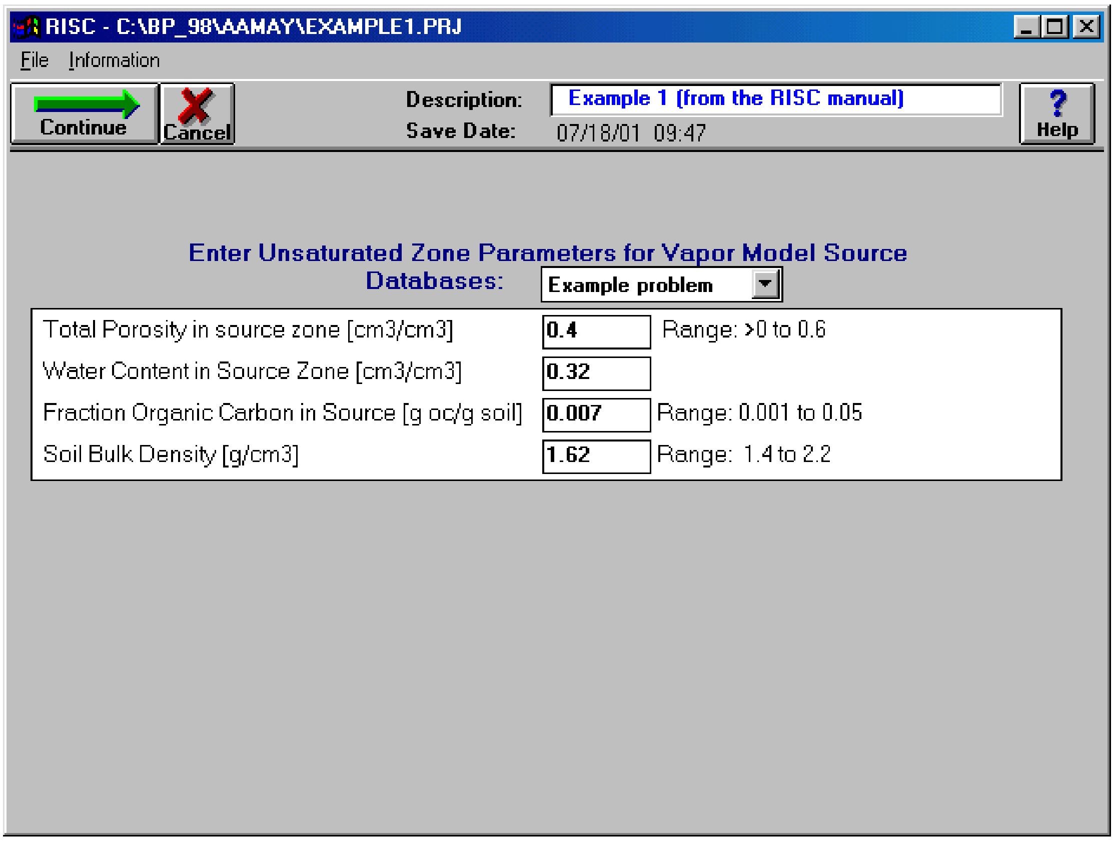
Enter Unsaturated Zone Parameters for Vapor Model
Databases: Example problem

Distance to Building Foundation [m] 1 From soil source or groundwater.
Total Porosity [cm3/cm3] 0.4 Range: >0 to 0.6
Water Content [cm3/cm3] 0.32

Example 1: Entering Unsaturated Zone Parameters

Source Data

The source geometry is defined based on several considerations, including the size of the former gas station, visual extent of contamination, and size of building. The source should be no larger than the footprint of the building or the cross-sectional area of the foundation available for vapor flux. In this example, based on visual observation, the source size is estimated to be approximately 12 meters by 8 meters. The bulk of the contamination occurs at the bottom of the tank, 3 m below ground surface (bgs). The Johnson-Ettinger indoor air model assumes that the source is constant (i.e. infinite), therefor the vertical extent is not specified. The porosity, water content, fraction organic carbon, and soil bulk density are entered to reflect the conditions in the source area. These parameters are used to estimate the partitioning into the vapor phase (including any solubility limitations) at the source.



Description: Example 1 (from the RISC manual)

Save Date: 07/18/01 09:47

Enter Unsaturated Zone Parameters for Vapor Model Source

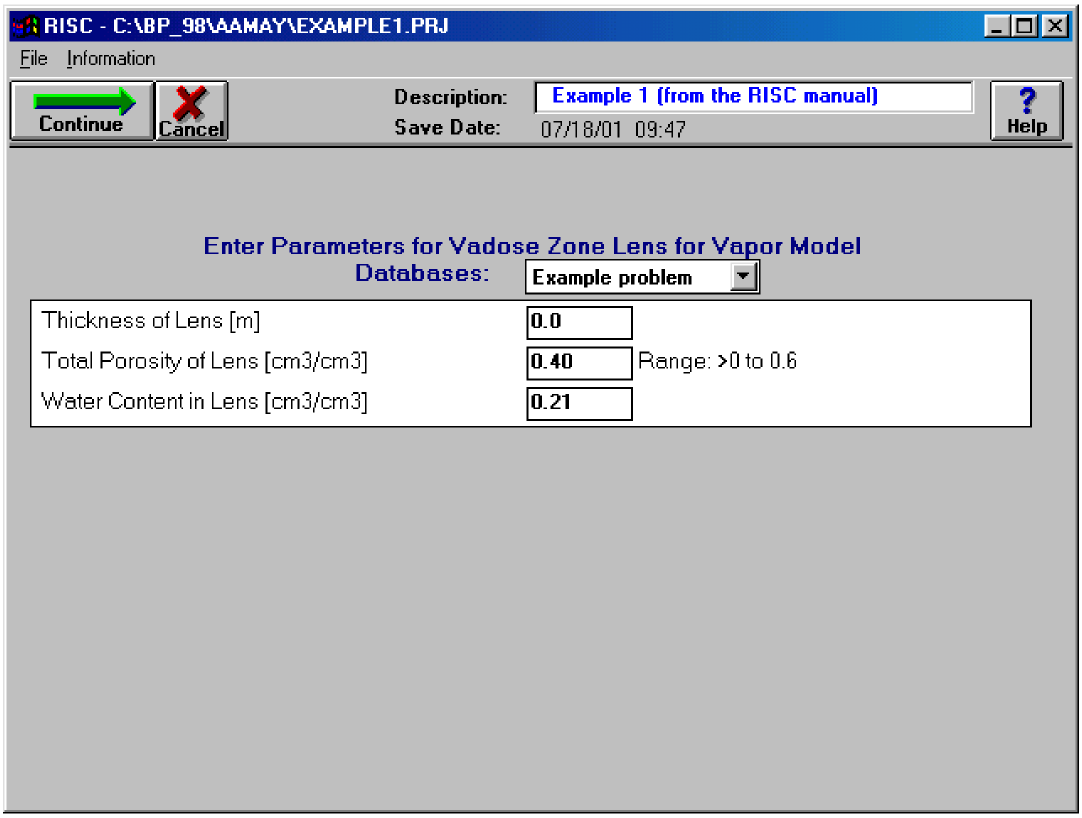
Databases: Example problem

Total Porosity in source zone [cm3/cm3]	0.4	Range: >0 to 0.6
Water Content in Source Zone [cm3/cm3]	0.32	
Fraction Organic Carbon in Source [g oc/g soil]	0.007	Range: 0.001 to 0.05
Soil Bulk Density [g/cm3]	1.62	Range: 1.4 to 2.2

Example 1: Entering the Vapor Model Source Data

Lens

The soil borings do not reveal a continuous lens that would affect vapor transport at this site. The lens thickness is therefore set equal to zero.



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

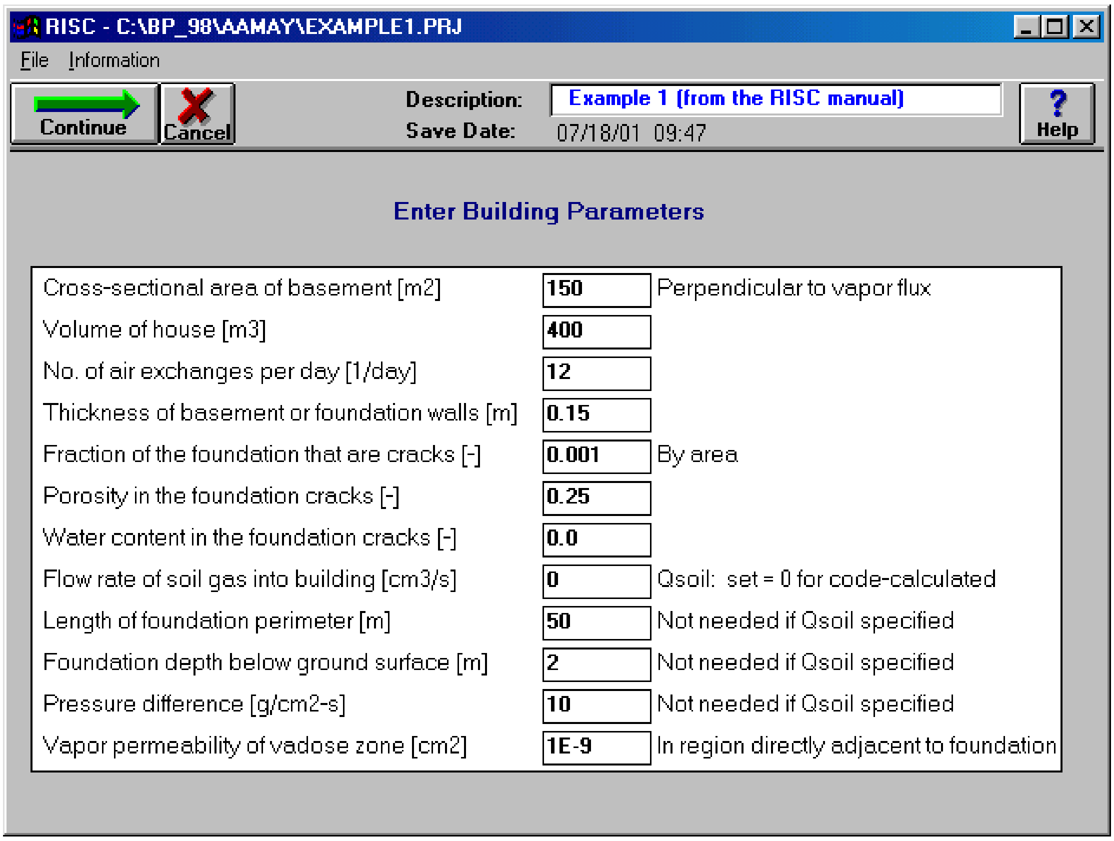
Enter Parameters for Vadose Zone Lens for Vapor Model
Databases: Example problem

Thickness of Lens [m]	0.0	
Total Porosity of Lens [cm3/cm3]	0.40	Range: >0 to 0.6
Water Content in Lens [cm3/cm3]	0.21	

Example 1: Entering Lens Data

Building Data

Since the house will be new construction, the amount of cracks in the basement will assumed to be 0.001 (0.1%). The remainder of the parameters are left at their default values since these represent fairly conservative values for single family residential houses.



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

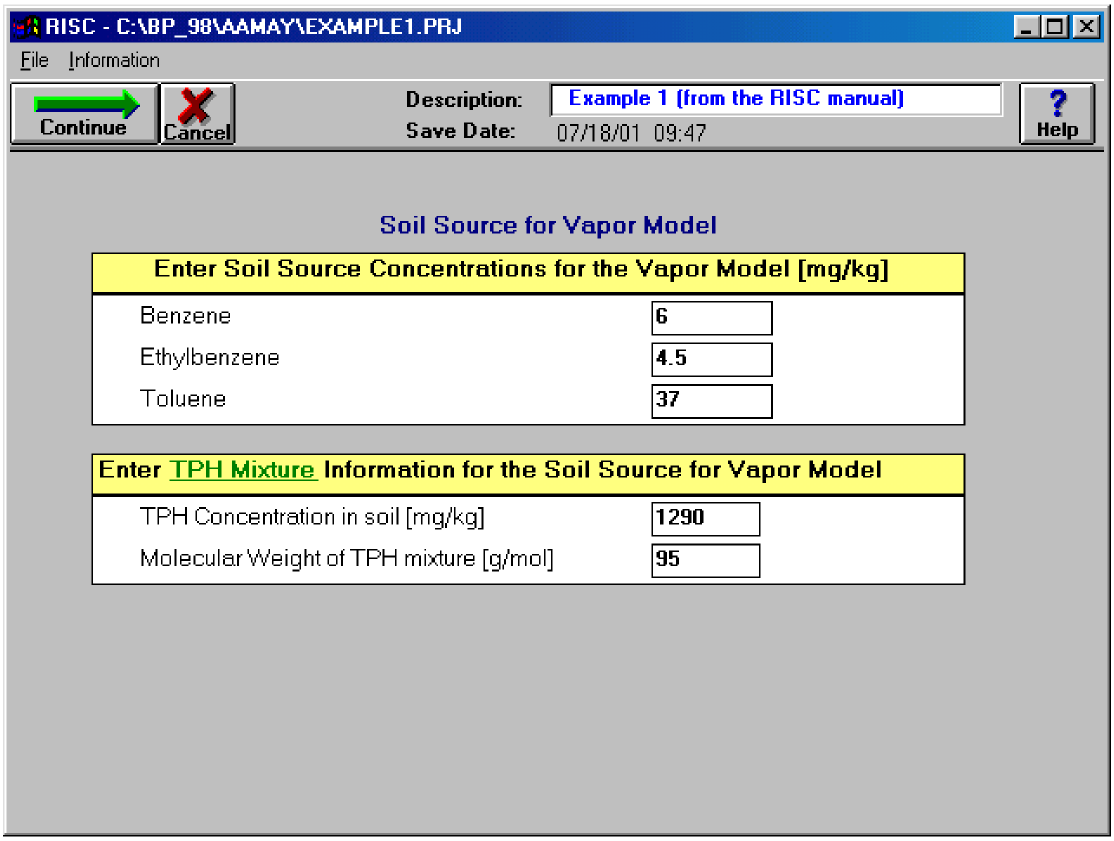
Enter Building Parameters

Cross-sectional area of basement [m2]	150	Perpendicular to vapor flux
Volume of house [m3]	400	
No. of air exchanges per day [1/day]	12	
Thickness of basement or foundation walls [m]	0.15	
Fraction of the foundation that are cracks [-]	0.001	By area
Porosity in the foundation cracks [-]	0.25	
Water content in the foundation cracks [-]	0.0	
Flow rate of soil gas into building [cm3/s]	0	Qsoil: set = 0 for code-calculated
Length of foundation perimeter [m]	50	Not needed if Qsoil specified
Foundation depth below ground surface [m]	2	Not needed if Qsoil specified
Pressure difference [g/cm2-s]	10	Not needed if Qsoil specified
Vapor permeability of vadose zone [cm2]	1E-9	In region directly adjacent to foundation

Example 1: Enter Building Parameters

Source Concentrations

The maximum detected concentrations at 3 m depth are assumed for the source concentrations since that is closest to the depth of the basement foundation. If additional spatial data were available, the total contaminant mass in the soil could be roughly estimated and the average concentration representing that mass could be used. TPH was measured at this site and the average concentration was 1290 mg/kg. An average value for the molecular weight of gasoline is 95 g/mol.



Description: Example 1 (from the RISC manual)

Save Date: 07/18/01 09:47

Soil Source for Vapor Model

Enter Soil Source Concentrations for the Vapor Model [mg/kg]	
Benzene	6
Ethylbenzene	4.5
Toluene	37

Enter TPH Mixture Information for the Soil Source for Vapor Model	
TPH Concentration in soil [mg/kg]	1290
Molecular Weight of TPH mixture [g/mol]	95

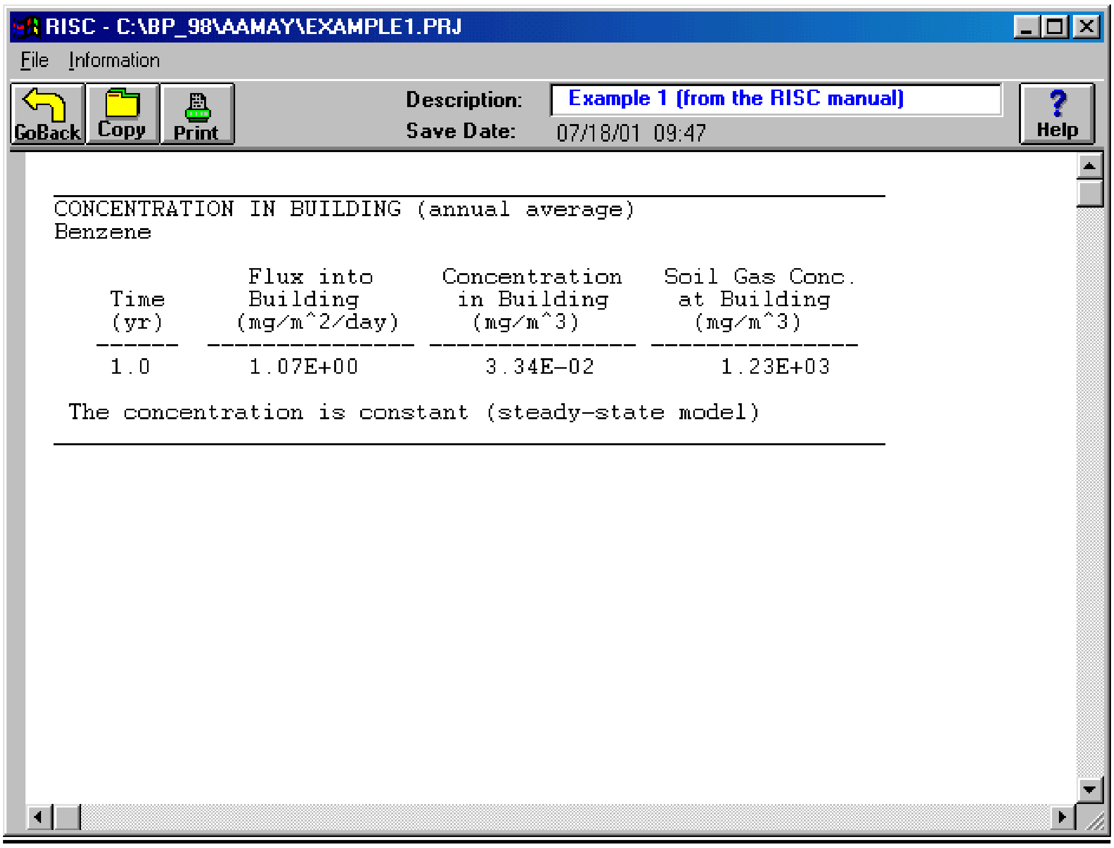
Example 1: Step 3b, Entering Source Concentrations

Run the Fate and Transport Model

At this point all the data required to run the model has been entered. Select "Step 3c: Run the F&T Model". The simulation time is not needed because the indoor air model is assumes that the system is already at steady-state (e.g. there is no change in concentration).

View the Results

Under “Step 3d: View the Results”, a number of different tables and charts are available for viewing. The maximum concentration of benzene in indoor air is estimated to be 3.34E-2 mg/m^3 whereas the concentration in the soil gas just below the foundation is 1.23E+01 (see figure below). Note, the concentration plot for indoor air yields straight lines (constant indoor air concentrations) because the indoor air model assumes steady-state conditions.



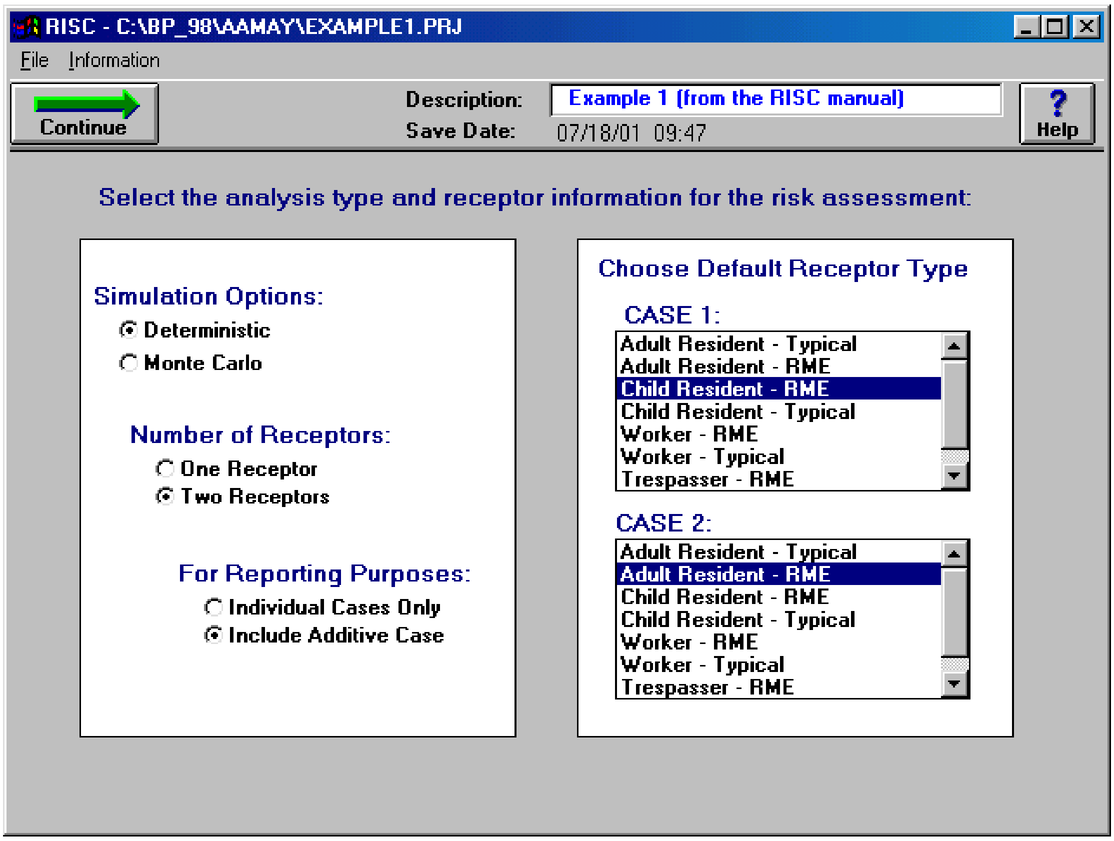
Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

```
CONCENTRATION IN BUILDING (annual average)
Benzene

                 Flux into      Concentration    Soil Gas Conc.
    Time          Building       in Building      at Building
    (yr)        (mg/m^2/day)      (mg/m^3)         (mg/m^3)
   ------     ---------------  ---------------  ---------------
    1.0          1.07E+00         3.34E-02          1.23E+03

 The concentration is constant (steady-state model)
```

Example 1: The Vapor Model Results for Benzene

Step 4: Describe the Receptors *(Example #1)*

The receptors of concern will be a residential child and adult. The additive receptor (child growing into an adult at the same residence) will also be considered for the carcinogenic scenario. Under Step 4a: Choose Receptors and Analysis Type, select the following options: “Deterministic”, “Two Receptors”, and “Include Additive Case”. The two receptors considered in this initial screening will be a “child resident – RME” and an “Adult Resident – RME”.



Description: Example 1 (from the RISC manual)

Save Date: 07/18/01 09:47

Select the analysis type and receptor information for the risk assessment:

Simulation Options:

● Deterministic
○ Monte Carlo

Number of Receptors:

○ One Receptor
● Two Receptors

For Reporting Purposes:

○ Individual Cases Only
● Include Additive Case

Choose Default Receptor Type

CASE 1:

- Adult Resident - Typical
- Adult Resident - RME
- **Child Resident - RME**
- Child Resident - Typical
- Worker - RME
- Worker - Typical
- Trespasser - RME

CASE 2:

- Adult Resident - Typical
- **Adult Resident - RME**
- Child Resident - RME
- Child Resident - Typical
- Worker - RME
- Worker - Typical
- Trespasser - RME

Example 1: Step 4, Choosing Analysis Type and Receptor Types

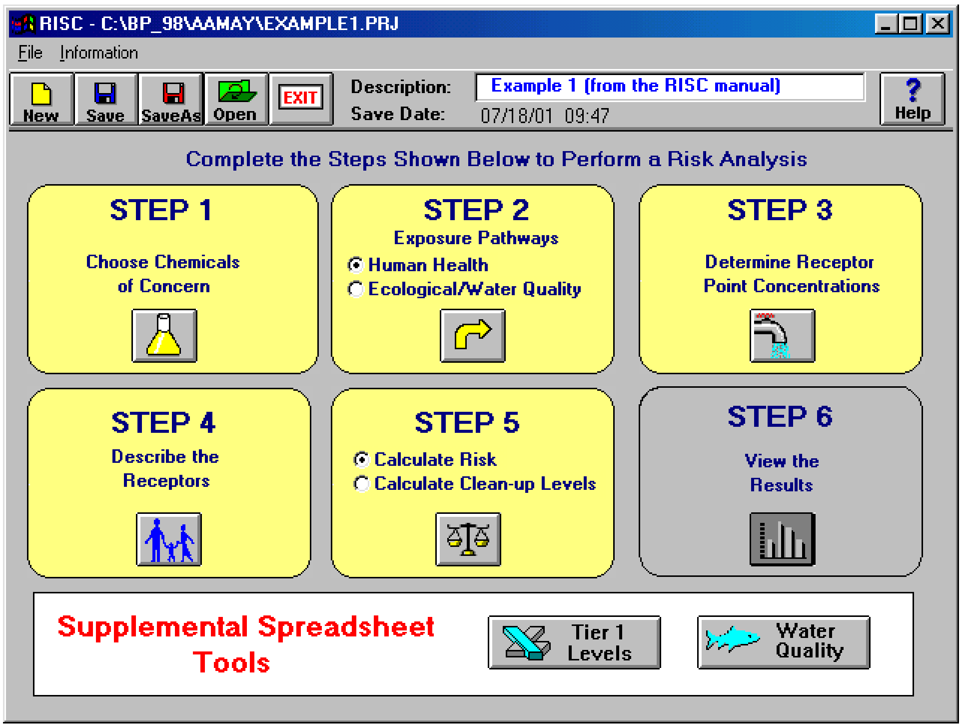
The exposure duration for the child and adult are modified to be 6 and 24 years, respectively, so that when added, a 30-year exposure results. The input parameter values assumed for this scenario are shown in the following table. This table was generated by copying the “Input/Output Summary” table (from Step 6: Results) into this Microsoft Word document. The font was changed to “Courier New” to maintain the formatting.

Example 1: Input Parameter Values for the Residential Scenario

```
Title:
Example 1 (from the RISC manual)
07/18/01  09:47

Scenarios:
Child Resident - RME
Adult Resident - RME

Routes:
INGESTION OF SOIL
DERMAL CONTACT WITH SOIL
INHALATION OF INDOOR AIR
INGESTION OF ROOT VEGETABLES
INGESTION OF ABOVE GROUND VEGETABLES

SCENARIO:
SUMMARY OF INPUT PARAMETERS                         1         2
----------------------------------------------------------------------

LIFETIME AND BODY WEIGHT
   Body Weight (kg)                              15.        70.
   Lifetime (years)                              70.        70.

INGESTION OF SOIL
   Soil Ingestion Rate (mg/day)                 2.00E+02   1.00E+02
   Exp. Frequency Soil (events/year)            3.50E+02   3.50E+02
   Exp. Duration Soil (years)                    6.0        24.
   Soil Bioavailability (-)
              Benzene                              1.0       1.0
              Ethylbenzene                         1.0       1.0
              Toluene                              1.0       1.0

DERMAL CONTACT WITH SOIL
   Total Skin Surface Area (cm^2)               7.28E+03   2.30E+04
   Fraction Skin Exposed to Soil (-)            0.55       0.25
   Adherence Factor for Soil (mg/cm^2)          0.20       0.20
   Exposure Freq. Soil   (events/year)          3.50E+02   3.50E+02
   Exposure Duration Soil (years)                6.0        24.
   Soil Bioavailability (-)
              Benzene                              1.0       1.0
              Ethylbenzene                         1.0       1.0
              Toluene                              1.0       1.0

INHALATION OF INDOOR AIR
   Inhalation rate (m^3/hr)                     0.62       0.83
   Time indoors (hours/day)                      24.        24.
   Lung Retention Factor (-)                     1.0        1.0
   Exp. Freq. Indoor Air (events/yr)            3.50E+02   3.50E+02
   Exp. Duration Indoor Air (yr)                 6.0        24.
INGESTION OF ROOT VEGETABLES
INGESTION OF ABOVE GROUND VEGETABLES
   Root Veg. Ingestion Rate (g/day)              48.        88.
   Above Ground Veg. Ing. Rate(g/day)            56.       1.27E+02
   Fraction Organic Carbon in Soil g/g          5.00E-02   5.00E-02
   Exp. Frequency Veg. (events/year)            3.50E+02   3.50E+02
   Exp. Duration Veg. Intake (years)             6.0        24.
   Fraction grown in home garden (-)            0.25       0.25
```

Step 5: Calculate Risk *(Example #1)*

In this step, the carcinogenic risk and hazard index are calculated for the screening level assessment.



RISC - C:\BP_98\AAMAY\EXAMPLE1.PRJ

Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

STEP 2 Exposure Pathways
● Human Health
○ Ecological/Water Quality

STEP 5
● Calculate Risk
○ Calculate Clean-up Levels

Example 1: Ready to Calculate Risk

STEP 6: View the Results *(Example #1)*

The following two tables show the screening level results for carcinogenic risk and hazard index for this example. The total carcinogenic risk for the additive case was estimated to be 2.4E-8 from surface soil and 1.6E-4 from the indoor air pathway. The total carcinogenic risk is 1.6E-4 and the driver for the carcinogenic risk is inhalation of indoor air. The total hazard indices for the child and adult receptors were estimated to be 0.56 and 0.16, respectively. Most of the risk comes from the indoor air pathway.

The hazard indices are not added together for the child and adult cases because non-carcinogenic effects are not considered additive over a lifetime. Although the USEPA is in the process of finalizing an assessment of the non-carcinogenic effects of benzene, its non-carcinogenic toxicity will be ignored in this example. The next example however takes this effect into account.

Example 1: Summary of Carcinogenic Risk (page 1 of 2)

```
     SUMMARY OF CARCINOGENIC RISK
     For Surface Soil

CASE 1:
Child Resident - RME
                                   Ingestion   Dermal      Ingestion   Ingestion
                                   of          Contact     of Root     AboveGround
                                   Soil        Soil        Vegetables  Vegetables   TOTAL
                                   ____________________________________________________________
Benzene                            3.2E-10     1.3E-10     1.4E-10     7.9E-09     8.5E-09
                                   ____________________________________________________________
TOTAL                              3.2E-10     1.3E-10     1.4E-10     7.9E-09     8.5E-09

CASE 2:
Adult Resident - RME
                                   Ingestion   Dermal      Ingestion   Ingestion
                                   of          Contact     of Root     AboveGround
                                   Soil        Soil        Vegetables  Vegetables   TOTAL
                                   ____________________________________________________________
Benzene                            1.4E-10     1.6E-10     2.1E-10     1.5E-08     1.6E-08
                                   ____________________________________________________________
TOTAL                              1.4E-10     1.6E-10     2.1E-10     1.5E-08     1.6E-08

CASE 3:
Cases 1 and 2 Added Together
                                   Ingestion   Dermal      Ingestion   Ingestion
                                   of          Contact     of Root     AboveGround
                                   Soil        Soil        Vegetables  Vegetables   TOTAL
                                   ____________________________________________________________
Benzene                            4.5E-10     2.8E-10     3.5E-10     2.3E-08     2.4E-08
                                   ____________________________________________________________
TOTAL                              4.5E-10     2.8E-10     3.5E-10     2.3E-08     2.4E-08
```

Example 1: Summary of Carcinogenic Risk (page 2 of 2)

```
     SUMMARY OF CARCINOGENIC RISK
     For Vapor Model Soil Source


CASE 1:
Child Resident - RME
                                   Inhalation
                                   of
                                   Indoor Air   TOTAL
                                   ________________________
Benzene                            7.4E-05     7.4E-05
                                   ________________________
TOTAL                              7.4E-05     7.4E-05

CASE 2:
Adult Resident - RME
                                   Inhalation
                                   of
                                   Indoor Air   TOTAL
                                   ________________________
Benzene                            8.4E-05     8.4E-05
                                   ________________________
TOTAL                              8.4E-05     8.4E-05

CASE 3:
Cases 1 and 2 Added Together
                                   Inhalation
                                   of
                                   Indoor Air   TOTAL
                                   ________________________
Benzene                            1.6E-04     1.6E-04
                                   ________________________
TOTAL                              1.6E-04     1.6E-04
```

Example 1: Summary of Hazard Index (page 1 of 2)

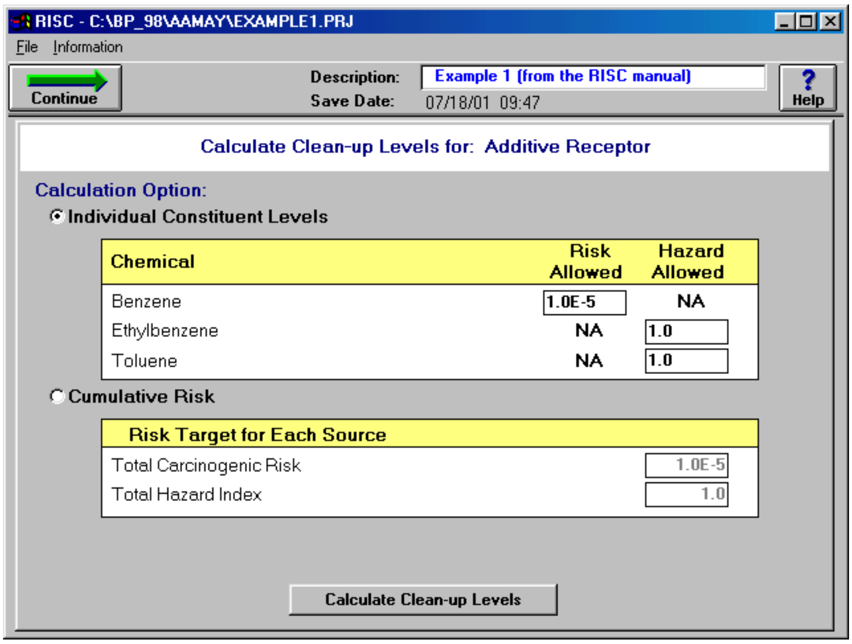
```
     SUMMARY OF HAZARD QUOTIENTS
     For Surface Soil


CASE 1:
Child Resident - RME
                                   Ingestion   Dermal      Ingestion   Ingestion
                                   of          Contact     of Root     AboveGround
                                   Soil        Soil        Vegetables  Vegetables   TOTAL
                                   ____________________________________________________________
Ethylbenzene                       1.5E-05     6.1E-06     4.5E-06     1.0E-04     1.3E-04
Toluene                            1.9E-06     7.7E-07     6.9E-07     1.9E-05     2.2E-05
                                   ____________________________________________________________
TOTAL                              1.7E-05     6.9E-06     5.1E-06     1.2E-04     1.5E-04

CASE 2:
Adult Resident - RME
                                   Ingestion   Dermal      Ingestion   Ingestion
                                   of          Contact     of Root     AboveGround
                                   Soil        Soil        Vegetables  Vegetables   TOTAL
                                   ____________________________________________________________
Ethylbenzene                       1.6E-06     1.9E-06     1.7E-06     4.9E-05     5.4E-05
Toluene                            2.1E-07     2.4E-07     2.7E-07     9.1E-06     9.8E-06
                                   ____________________________________________________________
TOTAL                              1.8E-06     2.1E-06     2.0E-06     5.8E-05     6.4E-05
```

Example 1: Summary of Hazard Index (page 2 of 2)

```
     SUMMARY OF HAZARD QUOTIENTS
     For Vapor Model Soil Source


CASE 1:
Child Resident - RME
                                   Inhalation
                                   of
                                   Indoor Air   TOTAL
                                   ________________________
Ethylbenzene                       7.3E-03     7.3E-03
Toluene                            5.5E-01     5.5E-01
                                   ________________________
TOTAL                              5.6E-01     5.6E-01

CASE 2:
Adult Resident - RME
                                   Inhalation
                                   of
                                   Indoor Air   TOTAL
                                   ________________________
Ethylbenzene                       2.1E-03     2.1E-03
Toluene                            1.6E-01     1.6E-01
                                   ________________________
TOTAL                              1.6E-01     1.6E-01


 NOTE:  A zero hazard index may indicate that a RfD
        was not entered for that chemical.
```

Determining Clean-up Levels

Clean-up levels for this example can be calculated by returning to “Step 5: Calculate Clean-up Levels”. In this example, clean-up levels will be calculated so that the risk from each chemical does not exceed an individual target for that chemical, rather than the cumulative case from all chemicals.



Description: Example 1 (from the RISC manual)
Save Date: 07/18/01 09:47

Calculate Clean-up Levels for: Additive Receptor

Calculation Option:

● Individual Constituent Levels

Chemical	Risk Allowed	Hazard Allowed
Benzene	1.0E-5	NA
Ethylbenzene	NA	1.0
Toluene	NA	1.0

○ Cumulative Risk

Risk Target for Each Source	
Total Carcinogenic Risk	1.0E-5
Total Hazard Index	1.0

Example 1: Specifying Target Risk Levels

The results of the clean-up level calculation (shown in the table below) indicate that the clean-up levels for benzene, ethylbenzene and toluene in *surface soil* are 4.1, 950 and 1,400 mg/kg, respectively. All of these levels exceed the measured concentrations from the upper soil samples. For *subsurface soil,* (soil that could potentially be a vapor source for indoor air), the site concentrations for all three chemicals would need to be reduced to meet the estimated clean-up levels. The calculated clean-up levels are 0.38, 1.6, and 22 mg/kg for benzene, ethylbenzene and toluene, respectively.

Example 1: Summary Of Clean-Up Levels (part 1 of 2)

```
   Clean-up Levels in Surface Soil                    SSTLs
   Receptor:  Additive Receptor Case                 [mg/kg]
________________________________________________________________________
     Benzene                                         4.1E+00
     Ethylbenzene                                    9.5E+02
     Toluene                                         1.4E+03
_______________________________________________________________________
     The exposure routes that depend on this source are:
        Ingestion of soil
        Dermal contact with soil
        Ingestion of root vegetables
        Ingestion of above ground vegetables
```

Example 1: Summary Of Clean-Up Levels (part 2 of 2)

```
Vapor Model Soil Source
--------------------------------------

   Exposure pathways depending on this source:
              Inhalation of indoor air

                                       Summary of Original Source Concentrations
                                       for Vapor Model Soil Source
                                       ______________________________________

                                       Original   TPH        Mass       Effective  Residual
                                       Source     Conc.      Fraction   Solubility Conc.
                                       [mg/kg]    [mg/kg]    [-]        [mg/l]     [mg/kg]
   ________________________________________________________________________________________

    Benzene                            6.0E+00    1.3E+03    4.7E-03    8.1E+00    1.1E+03
    Ethylbenzene                       4.5E+00    1.3E+03    3.5E-03    5.9E-01    4.6E+02
    Toluene                            3.7E+01    1.3E+03    2.9E-02    1.5E+01    7.7E+02
   ________________________________________________________________________________________

                                       Site-Specific Target Levels (SSTLs)
                                       for Vapor Model Soil Source
                                       ______________________________________
                                                  TPH        Mass
                                       SSTL       Conc.      Fraction
                                       [mg/kg]    [mg/kg]    [-]
   ________________________________________________________________________

    Benzene                            3.8E-01    8.1E+01    4.7E-03
    Ethylbenzene                       1.6E+00    4.6E+02    3.5E-03
    Toluene                            2.2E+01    7.7E+02    2.9E-02
   ________________________________________________________________________
```

10.2 EXAMPLE 2: IRRIGATION AND VOLITILIZATION FROM GROUNDWATER

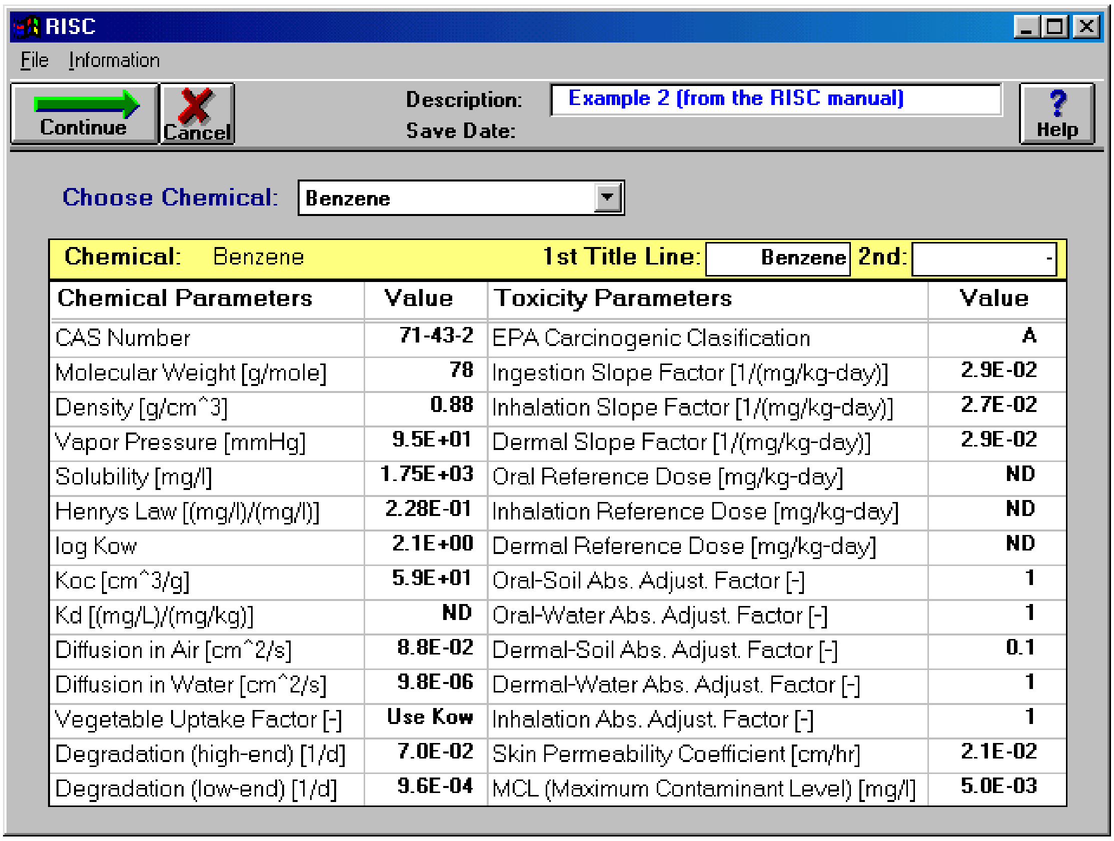
This example is saved in the project file named “Example2.prj”. The reader is encouraged to work through the example and enter in the information for themselves.

A potential human scenario often overlooked in creating risk-based cleanup goals is the ‘irrigation’ scenario. This refers to residential use of contaminated well water for watering lawns or gardens at homes that have their potable water supplied by their municipality. Exposure may occur from ingestion, dermal contact, or vapor inhalation by a child playing under the sprinkler, from vapor inhalation by an adult gardening downwind of the sprinkler, and from adult or child ingestion of vegetables grown in a garden irrigated by the sprinkler. In this example, target levels for benzene in groundwater are derived for reasonable exposure assumptions associated with a receptor living as both a child and then as an adult in the house over a 30-year duration.

In this example benzene is considered both as a carcinogen and non-carcinogen (i.e. it has both a slope factor and reference dose) because the example site is located within USEPA Region 9 and the overseeing regulatory agency in this case uses the toxicity factors used by Region 9. This means that the RISC chemical database will need to be modified in Step 1.

Step 1: Identify Chemicals of Concern *(Example #2)*

Since groundwater contamination of backyard wells is often associated with migration of dissolved petroleum hydrocarbon constituents from a remote source, the most soluble and toxic VOCs present the greatest risk. Benzene, MTBE, ethylbenzene, toluene and xylenes are probably the most soluble and toxic chemicals commonly found in petroleum mixtures. Benzene is often a driver for groundwater clean-ups because of its carcinogenicity and this is the only chemical considered in this example. Select benzene as a chemical of concern in Step 1. The RISC chemical database only contains values of slopes factors for benzene since these are the only toxicity values listed in the Integrated Risk and Information System (IRIS, see Chapter 12 for more information). In order to evaluate the non-carcinogenic effects, reference doses need to be added to the database. In Step 1, select "View Chemical Properties". Select "Benzene" from the list of chemicals at the top. The screen should look like the following figure.



Description: Example 2 (from the RISC manual)
Save Date:

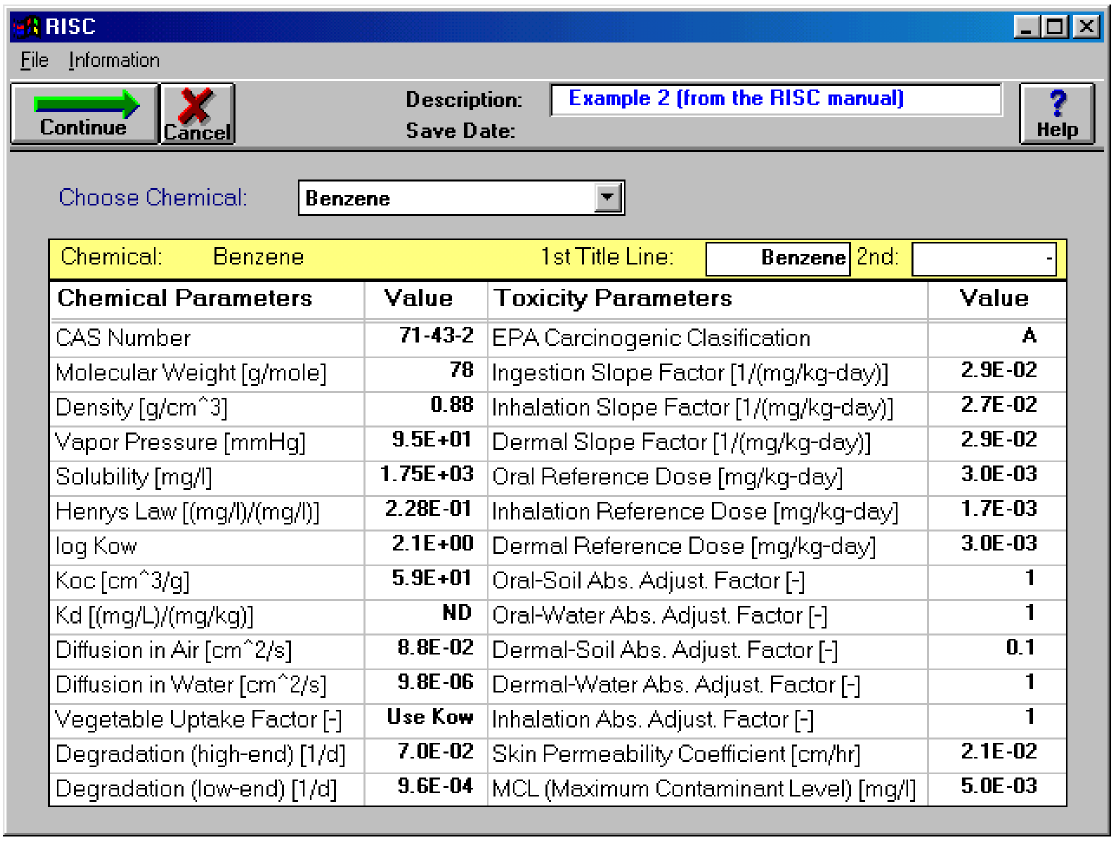
Choose Chemical: Benzene

Chemical: Benzene 1st Title Line: Benzene 2nd:

Chemical Parameters	Value	Toxicity Parameters	Value
CAS Number	71-43-2	EPA Carcinogenic Clasification	A
Molecular Weight [g/mole]	78	Ingestion Slope Factor [1/(mg/kg-day)]	2.9E-02
Density [g/cm^3]	0.88	Inhalation Slope Factor [1/(mg/kg-day)]	2.7E-02
Vapor Pressure [mmHg]	9.5E+01	Dermal Slope Factor [1/(mg/kg-day)]	2.9E-02
Solubility [mg/l]	1.75E+03	Oral Reference Dose [mg/kg-day]	ND
Henrys Law [(mg/l)/(mg/l)]	2.28E-01	Inhalation Reference Dose [mg/kg-day]	ND
log Kow	2.1E+00	Dermal Reference Dose [mg/kg-day]	ND
Koc [cm^3/g]	5.9E+01	Oral-Soil Abs. Adjust. Factor [-]	1
Kd [(mg/L)/(mg/kg)]	ND	Oral-Water Abs. Adjust. Factor [-]	1
Diffusion in Air [cm^2/s]	8.8E-02	Dermal-Soil Abs. Adjust. Factor [-]	0.1
Diffusion in Water [cm^2/s]	9.8E-06	Dermal-Water Abs. Adjust. Factor [-]	1
Vegetable Uptake Factor [-]	Use Kow	Inhalation Abs. Adjust. Factor [-]	1
Degradation (high-end) [1/d]	7.0E-02	Skin Permeability Coefficient [cm/hr]	2.1E-02
Degradation (low-end) [1/d]	9.6E-04	MCL (Maximum Contaminant Level) [mg/l]	5.0E-03

Example 2. Chemical Properties in the RISC Database for Benzene

Note, the Oral, Inhalation, and Dermal Reference Dose boxes contain NDs. USEPA Region 9 uses a reference dose of 3.0E-3 mg/kg-d for the oral pathway and 1.7E-3 mg/kg-d for the inhalation pathway. It will be assumed that the dermal reference dose is equal to the oral value. Enter "3.0E-3" in the oral and dermal reference dose boxes and "1.7E-3" in the inhalation reference dose box. The Chemical Properties screen should now look like the next figure.



Description: Example 2 (from the RISC manual)

Save Date:

Choose Chemical: Benzene

Chemical: Benzene 1st Title Line: Benzene 2nd:

Chemical Parameters	Value	Toxicity Parameters	Value
CAS Number	71-43-2	EPA Carcinogenic Clasification	A
Molecular Weight [g/mole]	78	Ingestion Slope Factor [1/(mg/kg-day)]	2.9E-02
Density [g/cm^3]	0.88	Inhalation Slope Factor [1/(mg/kg-day)]	2.7E-02
Vapor Pressure [mmHg]	9.5E+01	Dermal Slope Factor [1/(mg/kg-day)]	2.9E-02
Solubility [mg/l]	1.75E+03	Oral Reference Dose [mg/kg-day]	3.0E-03
Henrys Law [(mg/l)/(mg/l)]	2.28E-01	Inhalation Reference Dose [mg/kg-day]	1.7E-03
log Kow	2.1E+00	Dermal Reference Dose [mg/kg-day]	3.0E-03
Koc [cm^3/g]	5.9E+01	Oral-Soil Abs. Adjust. Factor [-]	1
Kd [(mg/L)/(mg/kg)]	ND	Oral-Water Abs. Adjust. Factor [-]	1
Diffusion in Air [cm^2/s]	8.8E-02	Dermal-Soil Abs. Adjust. Factor [-]	0.1
Diffusion in Water [cm^2/s]	9.8E-06	Dermal-Water Abs. Adjust. Factor [-]	1
Vegetable Uptake Factor [-]	Use Kow	Inhalation Abs. Adjust. Factor [-]	1
Degradation (high-end) [1/d]	7.0E-02	Skin Permeability Coefficient [cm/hr]	2.1E-02
Degradation (low-end) [1/d]	9.6E-04	MCL (Maximum Contaminant Level) [mg/l]	5.0E-03

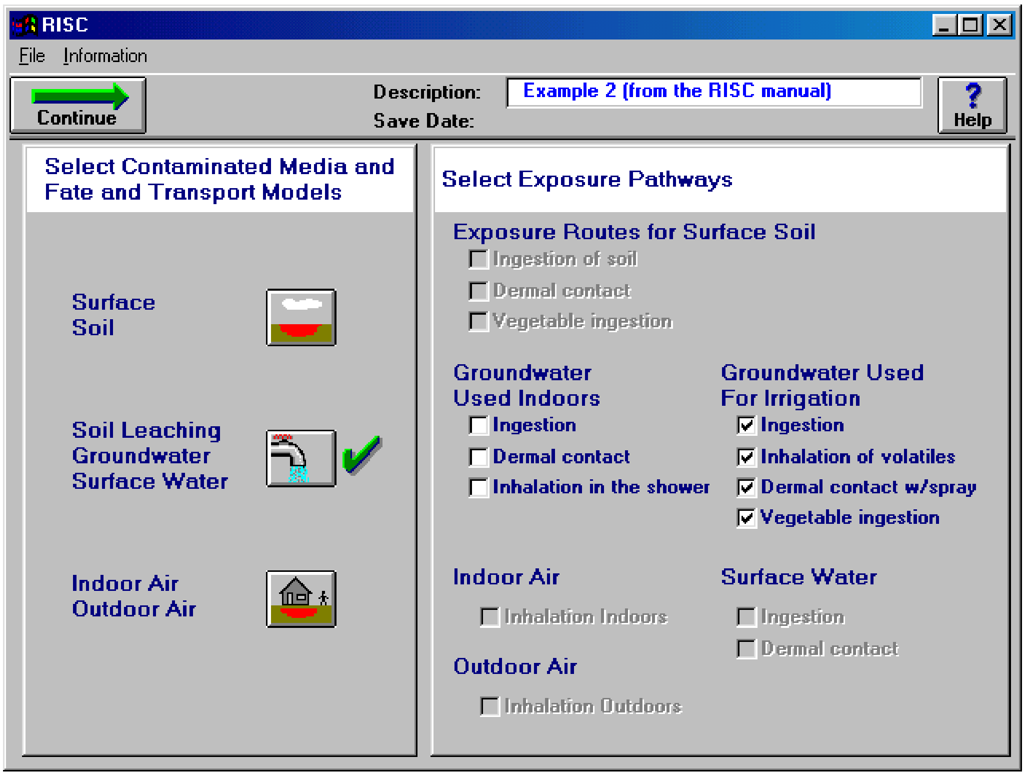
Example 2. Chemical Properties Database Screen for Benzene After Entering Reference Doses

Click on the "Continue" button. A warning message will appear saying that the values in the chemical database have been changed. Click on "OK." In the main Step 1 screen, make sure that benzene is selected as a chemical of concern and then select Continue to go to the Main Menu.

Step 2: Identify Appropriate Exposure Pathways and Determine Method for Estimating Receptor Point Concentrations *(Example #2)*

For a child, whose exposure duration is typically defined as 6 years (ages 0 to 6), the behavioral assumption is that the child may play in the sprinkler and eat vegetables from the garden. The relevant routes of exposure for the irrigation water are: inhalation of vapor emissions, dermal contact with the water, ingestion of water while playing, and ingestion of vegetables irrigated with the water. For an adult, the behavioral assumption is that he/she may be gardening or attending the lawn in a location downwind of the contaminated vapors being emitted from the sprinkler drops. No dermal contact or ingestion of the water is assumed. The relevant exposure routes are thus inhalation of vapor emissions and the ingestion of home-grown vegetables.

All of the above pathways are "direct" pathways, that is fate and transport models (with the exception of the shower model) will not be used to estimate concentrations in the media. The screen for Step 2 should look like this:



Description: Example 2 (from the RISC manual)
Save Date:

Select Contaminated Media and Fate and Transport Models

Surface Soil

Soil Leaching Groundwater Surface Water ✓

Indoor Air Outdoor Air

Select Exposure Pathways

Exposure Routes for Surface Soil
☐ Ingestion of soil
☐ Dermal contact
☐ Vegetable ingestion

Groundwater Used Indoors
☐ Ingestion
☐ Dermal contact
☐ Inhalation in the shower

Groundwater Used For Irrigation
☑ Ingestion
☑ Inhalation of volatiles
☑ Dermal contact w/spray
☑ Vegetable ingestion

Indoor Air
☐ Inhalation Indoors

Outdoor Air
☐ Inhalation Outdoors

Surface Water
☐ Ingestion
☐ Dermal contact

Example 2: Choosing Exposure Pathways

Step 3: Determine Receptor Point Concentrations *(Example #2)*

The goal of this example is to develop a clean-up level for benzene in groundwater, not to calculate risk, so the concentration entered in Step 3 is not important. Accept the default concentration of "0.0" for benzene in groundwater.

Step 4: Describe the Receptors *(Example #2)*

Three receptors are considered in this example: a child, an adult, and a receptor that is a child for 6 years and an adult for 24 years (the additive case). In Step 4a: Choose

Receptors and Analysis Type, choose two receptors, a child RME and an adult RME, and select the additive case, exactly as was done in the previous example.

In this example, the scenario for the irrigation pathways (direct water contact, ingestion, and vapor inhalation) assumes the residents (child or adult) may be outside twice a week during the warm weather season, which may last for half the year or 27 weeks. It is assumed the child plays under the sprinkler for 30 minutes per event; the adult gardens 2 hours during each of the days outside.

Dermal Contact and Ingestion of Groundwater—Child

For the child, 100% of their skin surface area is assumed to get wet and they are assumed to ingest 0.50 ml/hr.

Volatilization and Inhalation of Vapors—Child and Adult

The inputs for this model are similar to those of the shower model. In the shower model however the air is assumed to be stagnant whereas in this model an outdoor box is assumed to be ventilated by the wind. An average wind speed of 2 m/s and sprinkler flowrate of 30 l/min is assumed. The width of the box is defined by the dimension that the receptor is playing or working in; it is assumed to be 9 m. The height of the receptor, assumed to be 2 m, defines the third dimension. This model conservatively assumes the receptor is always downwind of the source.

Other input parameters that are changed from shower defaults are: drop time of the water droplets, drop size diameter, and water temperature. The drop time is assumed to be ten seconds (after which volatilization is assumed not to occur). This drop time is lengthened (from the shower default of 2 seconds) to account for volatilization occurring from water before it soaks into the soil. The drop size is assumed to be 0.2 cm and the water temperature 25^{o} C.

Vegetable Intake—Child and Adult

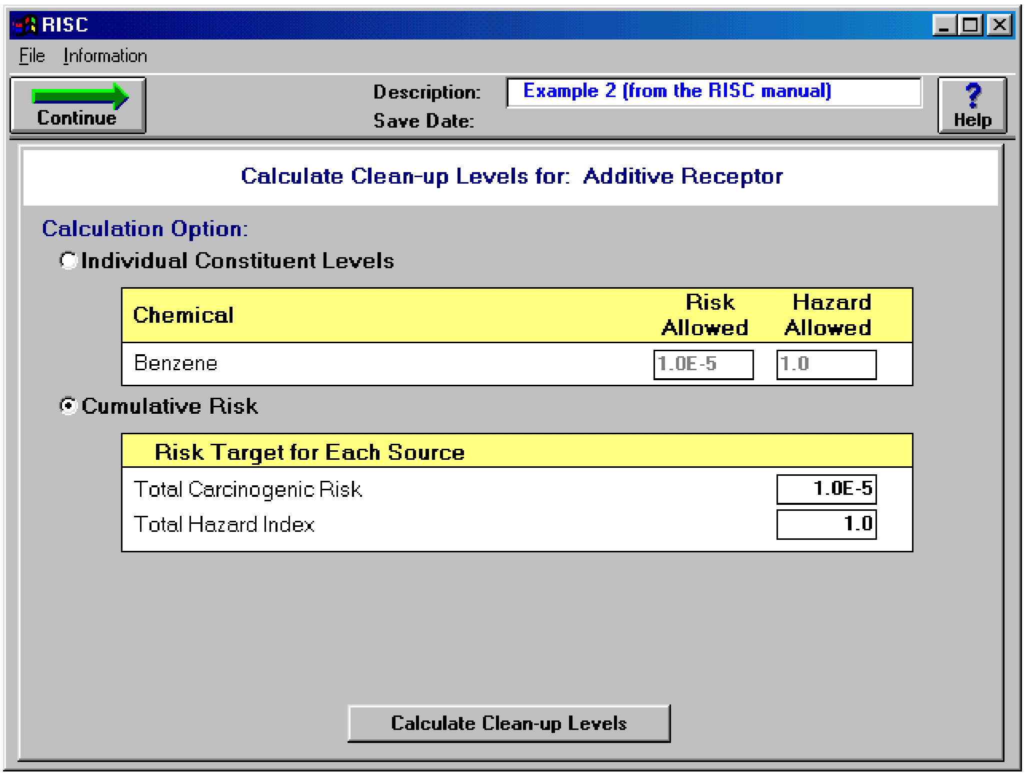
The EPA Exposure Factors Handbook (1996) was used to obtain default vegetable ingestion rates. It is assumed that the adult consumes 127 grams (1.82 g/kg bodyweight-day) of above ground vegetables and 87.5 (1.25 g/kg bodyweight-day) of root vegetables for a total of 215 grams of vegetables total per day. It is assumed that the child consumes 55.8 grams (3.72 g/kg bodyweight-day) of above ground vegetables and 48.5 (3.23 g/kg bodyweight-day) of root vegetables for a total of about 105 grams of vegetables total per day. This same reference states that the fraction of homegrown vegetables, averaged over the whole year (accounting for those months outside the growing season), is 24%. The fraction organic carbon (FOC) in soil is required to estimate partitioning into the above ground vegetables. The FOC is assumed to equal 0.05 g OC/g soil. The input parameter values used in this example are summarized in the next table.

Example 2: Input Parameters Used to Calculate Clean-Up Levels
(excerpted from "Input/Output Summary Table" in Step 6)

```
SCENARIO:
SUMMARY OF INPUT PARAMETERS                         1         2
---------------------------------------------------------------------

LIFETIME AND BODY WEIGHT
   Body Weight (kg)                             15.0       70.0
   Lifetime (years)                             70.0       70.0

INGESTION OF ROOT VEGETABLES
INGESTION OF ABOVE GROUND VEGETABLES
   Root Veg. Ingestion Rate (g/day)             48.5       87.5
   Above Ground Veg. Ing. Rate(g/day)           55.8       127.
   Fraction Organic Carbon in Soil g/g        5.000E-02  5.000E-02
   Exp. Frequency Veg. (events/year)           350.       350.
   Exp. Duration Veg. Intake (years)            6.00       24.0
   Fraction grown in home garden (-)           0.240      0.240

INHALATION OF GW SPRAY
   Width of Sprinkler Spray (m)                 9.00       9.00
   Height of Breathing Zone (m)                 2.00       2.00
   Average Windspeed (m/s)                      2.00       2.00
   Temperature of Irrigation Water (C)          25.0       25.0
   Sprinkler Flow Rate (l/min)                  30.0       30.0
   Droplet Diameter Sprinkler (cm)             0.200      0.200
   Droplet Droptime for Sprinkler (s)           10.0       10.0
   Time in Sprinkler (hour/day)                0.500       2.00
   Inhal. Rate Outdoors (m^3/hr)               0.830      0.830
   Lung Retention Factor (-)                   1.00        1.00
   Exp. Freq Irrigation (events/year)           54.0       54.0
   Exp. Duration Groundwater (years)            6.00       24.0

DERMAL CONTACT WITH IRRIG. WATER
   Total Skin Surface Area (cm^2)             7.280E+03  2.300E+04
   Fraction Skin Exposed to Water (-)          1.00        0.00
   Time in Irrigation Water (hour/day)         0.500       2.00
   Exp. Freq Irrigation (events/year)           54.0       54.0
   Exp. Duration Groundwater (years)            6.00       24.0

INGESTION OF IRRIGATION WATER
   Ingestion rate (ml/hr)                       50.0       0.00
   Exp. Freq Irrigation (events/year)           54.0       54.0
   Exp. Duration Groundwater (years)            6.00       24.0
```

Step 5: Calculate Clean-Up Levels *(Example #2)*

In Step 5, choose the “Calculate Clean-Up Levels” option and click on the button. For this example, a target cancer risk level of $1x10^{-5}$ is adopted as well as a hazard quotient of one. Since this example has just one chemical of concern, the option of “Cumulative Risk” or “Individual Constituent Levels” will generate the same results. When the "Calculate Clean-up Levels" button is chosen, a warning message will prompt the user to save their work so far. The reason is that the new clean-up levels will overwrite the concentrations stored in Step 3. In this example, the receptor point concentrations were equal to zero. For scenarios using fate and transport models, calculating clean-up levels in Step 5 will overwrite the source concentrations entered in Step 3.



Description: Example 2 (from the RISC manual)

Save Date:

Calculate Clean-up Levels for: Additive Receptor

Calculation Option:

○ Individual Constituent Levels

Chemical	Risk Allowed	Hazard Allowed
Benzene	1.0E-5	1.0

● Cumulative Risk

Risk Target for Each Source	
Total Carcinogenic Risk	1.0E-5
Total Hazard Index	1.0

Example 2: Specifying Target Risk in Example #2

Step 6: View the Results *(Example #2)*

In “Step 6: View the Results”, summary tables of carcinogenic risk, hazard index, input/output parameters, and clean-up levels may be viewed.

The calculated groundwater clean-up level is shown in the following table.

Example 2:   Summary of Clean-up Levels for the Irrigation Scenario

```
    SUMMARY OF CLEAN-UP LEVELS
    --------------------------


   Clean-up Levels in Groundwater                   SSTLs    Solubility
   Receptor:  Additive Receptor Case               [mg/l]      [mg/l]

_____________________________________________________________________________

   Benzene                                        5.1E-01     1.8E+03
_____________________________________________________________________________

   The exposure routes that depend on this source are:
        Ingestion of root vegetables
        Ingestion of above ground vegetables
        Inhalation of irrigation water spray
        Dermal contact with irrigation water
        Ingestion of irrigation water
```

In this case, the carcinogenic component drove the clean-up level calculations so the clean-up level presented is for the additive receptor. This can be verified by looking at the two risk summary tables. The table summarizing carcinogenic risk indicates that the target risk of 1E-5 was met exactly for the additive receptor whereas the total hazard index was below the target of 1.0 for both receptors.

The next two tables present summaries of carcinogenic risk and hazard indices, respectively.

Example 2: Summary of Carcinogenic Risk by Route after Calculating Clean-up Levels

CASE 1:
Child Resident - RME

	Ingestion of Root Vegetables	Ingestion AboveGround Vegetables	Inhalation of GW Spray	Dermal Contact Irrig.Water	Ingestion of Irrig. Water	TOTAL
Benzene	2.0E-06	1.1E-06	4.9E-08	9.6E-07	3.2E-07	4.5E-06
TOTAL	2.0E-06	1.1E-06	4.9E-08	9.6E-07	3.2E-07	4.5E-06

CASE 2:
Adult Resident - RME

	Ingestion of Root Vegetables	Ingestion AboveGround Vegetables	Inhalation of GW Spray	Dermal Contact Irrig.Water	Ingestion of Irrig. Water	TOTAL
Benzene	3.1E-06	2.2E-06	1.7E-07	0.0E+00	0.0E+00	5.5E-06
TOTAL	3.1E-06	2.2E-06	1.7E-07	0.0E+00	0.0E+00	5.5E-06

CASE 3:
Cases 1 and 2 Added Together

	Ingestion of Root Vegetables	Ingestion AboveGround Vegetables	Inhalation of GW Spray	Dermal Contact Irrig.Water	Ingestion of Irrig. Water	TOTAL
Benzene	5.1E-06	3.4E-06	2.2E-07	9.6E-07	3.2E-07	1.0E-05
TOTAL	5.1E-06	3.4E-06	2.2E-07	9.6E-07	3.2E-07	1.0E-05

Example 2: Summary of Hazard Index by Route after Calculating Clean-up Levels

```
     SUMMARY OF HAZARD QUOTIENTS
     For Groundwater


CASE 1:
Child Resident - RME
                                   Ingestion   Ingestion   Inhalation  Dermal      Ingestion
                                   of Root     AboveGround of          Contact     of Irrig.
                                   Vegetables  Vegetables  GW Spray    Irrig.Water Water         TOTAL
                                   ________________________________________________________________________
Benzene                            2.7E-01     1.5E-01     1.2E-02     1.3E-01     4.2E-02     6.1E-01
                                   ________________________________________________________________________
TOTAL                              2.7E-01     1.5E-01     1.2E-02     1.3E-01     4.2E-02     6.1E-01

CASE 2:
Adult Resident - RME
                                   Ingestion   Ingestion   Inhalation  Dermal      Ingestion
                                   of Root     AboveGround of          Contact     of Irrig.
                                   Vegetables  Vegetables  GW Spray    Irrig.Water Water         TOTAL
                                   ________________________________________________________________________
Benzene                            1.0E-01     7.5E-02     1.1E-02     0.0E+00     0.0E+00     1.9E-01
                                   ________________________________________________________________________
TOTAL                              1.0E-01     7.5E-02     1.1E-02     0.0E+00     0.0E+00     1.9E-01
```

10.3 EXAMPLE 3: SURFACE WATER ECOLOGICAL RISK

This example is saved in a project file called “Example3.prj”. The reader is encouraged to work through the example and enter in the information for themselves.

In this example, a site adjacent to a medium-sized stream in New Zealand has free product gasoline in the ground water. The edge of the free product is estimated to be approximately 18 meters up-gradient of the stream. Dissolved phase concentrations in groundwater have not been measured at this site (the groundwater samples contained free product), so the dissolved phase concentrations at the downgradient edge of the source will be estimated using conservative gasoline composition and solubility assumptions.

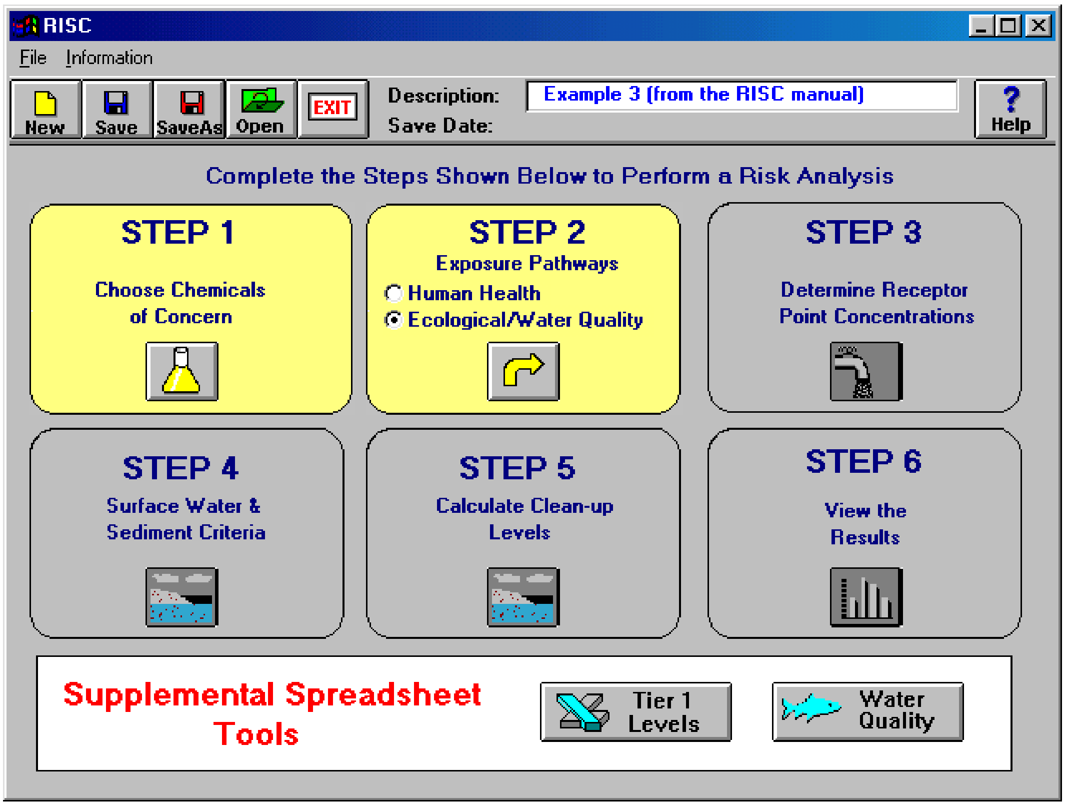
The goal of this assessment is to predict the movement of the dissolved-phase contaminants emanating from the free product towards the stream. The surface water mixing model will be used to estimate concentrations in the surface water and those concentrations will be compared with the Australia/New Zealand Environment and Conservation Council (ANZECC) surface water quality criteria numbers for the protection of ecological species.

Step 1: Identify Chemicals of Concern *(Example #3)*

The main chemicals of concern are the soluble and mobile components of the free product, including benzene, toluene, xylenes, and naphthalene. These will be the chemicals of concern for this example.

Step 2: Identify Appropriate Exposure Pathways *(Example #3)*

Before entering Step 2, select the "Ecological/Water Quality" option. The next figure shows what the main screen looks like before selecting Step 2.



Description: Example 3 (from the RISC manual)
Save Date:

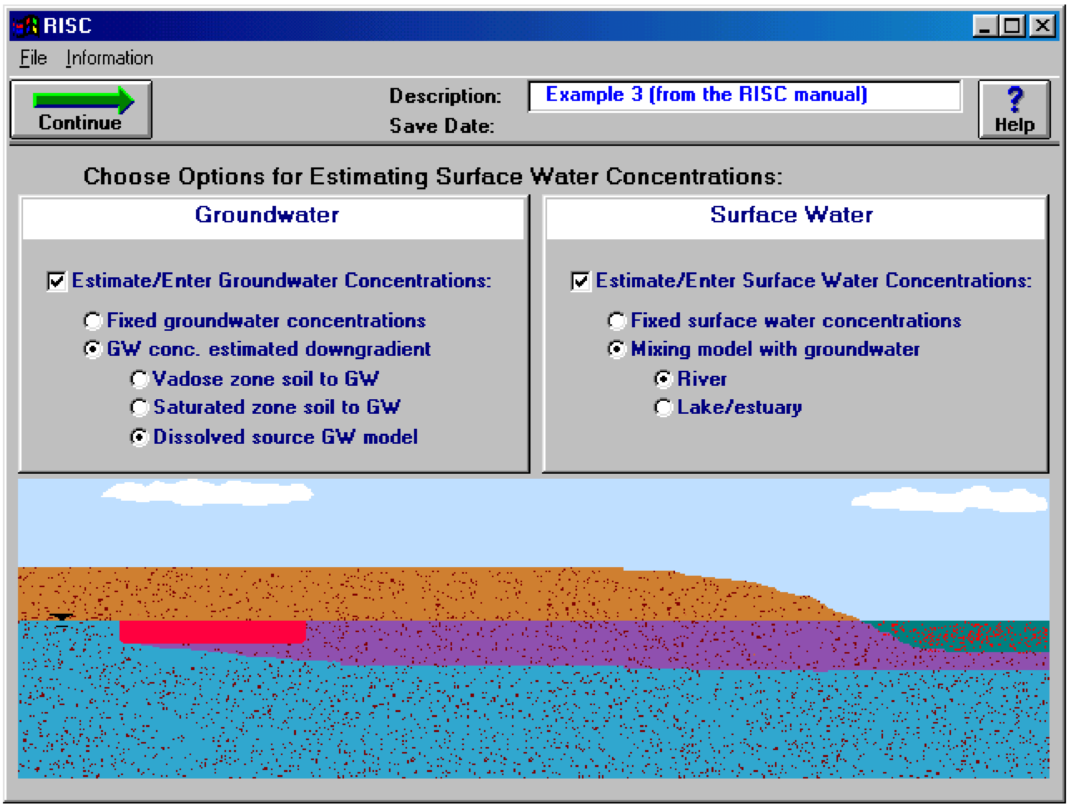
○ Human Health
● Ecological/Water Quality

Example 3: The Main Screen With the "Ecological/Water Quality" Option Selected

Choosing Models in Step 2

The Dissolved Phase Transport (groundwater) model will be used to model the movement of the chemicals of concern from the source to the surface water edge, followed by the surface water mixing model for estimating the concentrations in the stream. The Dissolved Phase Model is chosen to model the groundwater transport because the groundwater source will be assumed to be non-depleting (due to the potentially large amount of free product compared to dissolved phase chemicals leaving the source). At the edge of the surface water body, the river mixing model will be used to estimate concentrations in the stream.

The next figure shows the model selections made in Step 2 to estimate surface water concentrations.



Description: Example 3 (from the RISC manual)

Save Date:

Choose Options for Estimating Surface Water Concentrations:

Groundwater

☑ Estimate/Enter Groundwater Concentrations:

- ○ Fixed groundwater concentrations
- ● GW conc. estimated downgradient
  - ○ Vadose zone soil to GW
  - ○ Saturated zone soil to GW
  - ● Dissolved source GW model

Surface Water

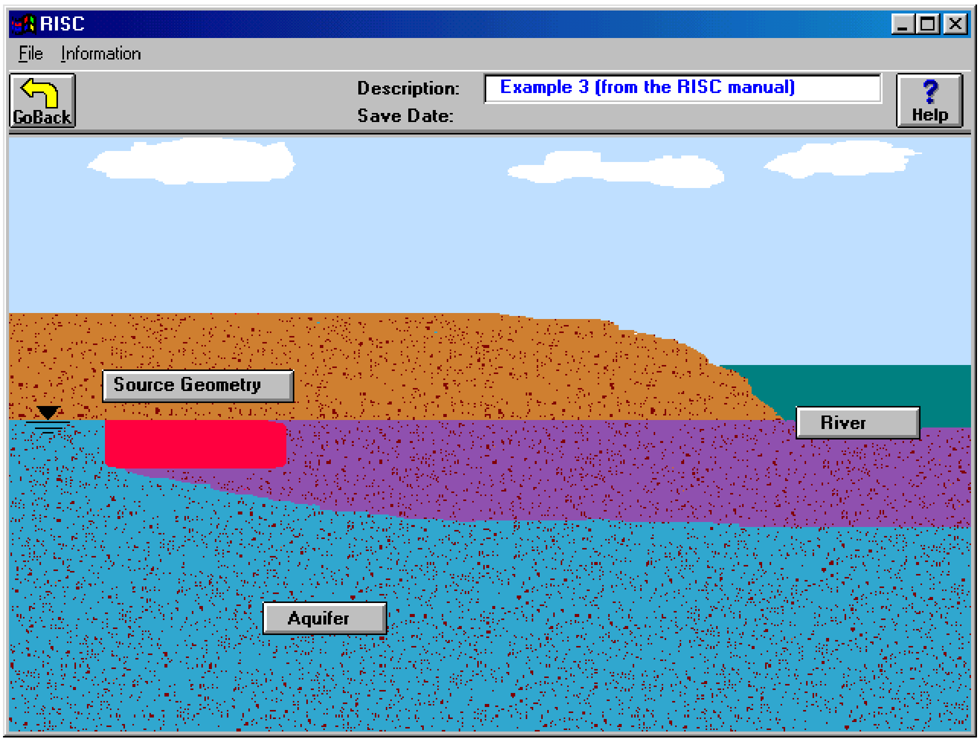
☑ Estimate/Enter Surface Water Concentrations:

- ○ Fixed surface water concentrations
- ● Mixing model with groundwater
  - ● River
  - ○ Lake/estuary

Example 3: Choosing Options for Estimating Surface Water Concentrations

Step 3: Determine Receptor Point Concentrations *(Example 3)*

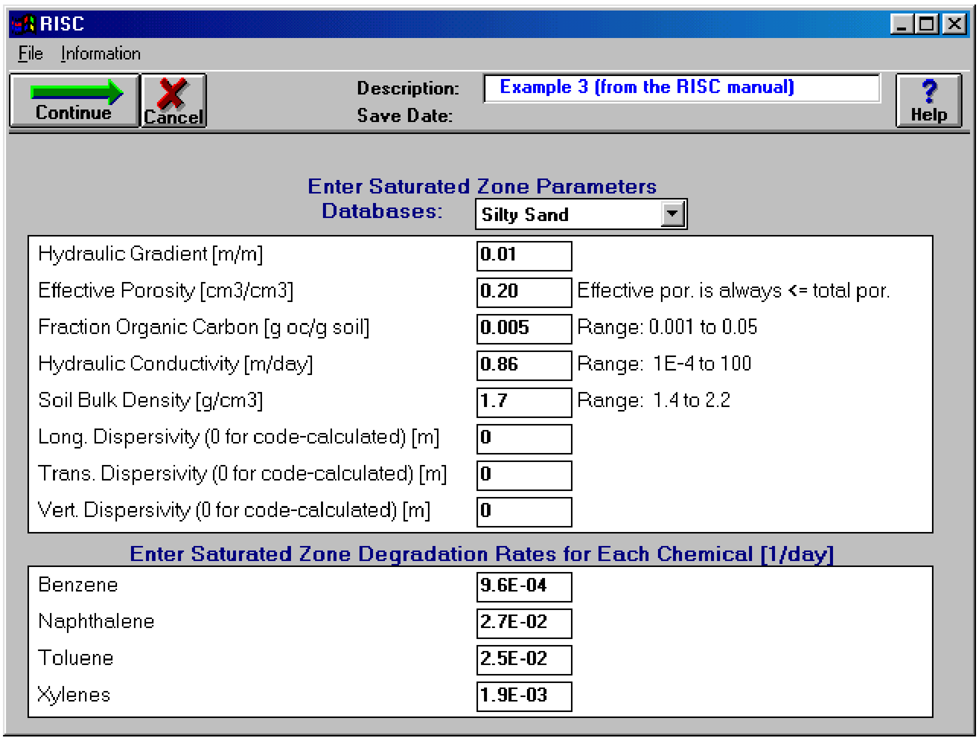
The input parameter values for the groundwater model are obtained from the RISC database for silty sands (the regional aquifer has been characterized as predominantly silty sands). The default values for degradation rates from the RISC chemical database rates are used in this example. The input values used for this example are listed in the following figures from Step 3a. The first figure shows how the site properties schematic should look in Step 3a. The input values used in the models follow.



Description: Example 3 (from the RISC manual)

Save Date:

Example 3: Site Properties Schematic



Description: Example 3 (from the RISC manual)

Save Date:

Enter Saturated Zone Parameters

Databases: Silty Sand

Hydraulic Gradient [m/m]	0.01	
Effective Porosity [cm3/cm3]	0.20	Effective por. is always <= total por.
Fraction Organic Carbon [g oc/g soil]	0.005	Range: 0.001 to 0.05
Hydraulic Conductivity [m/day]	0.86	Range: 1E-4 to 100
Soil Bulk Density [g/cm3]	1.7	Range: 1.4 to 2.2
Long. Dispersivity (0 for code-calculated) [m]	0	
Trans. Dispersivity (0 for code-calculated) [m]	0	
Vert. Dispersivity (0 for code-calculated) [m]	0	

Enter Saturated Zone Degradation Rates for Each Chemical [1/day]

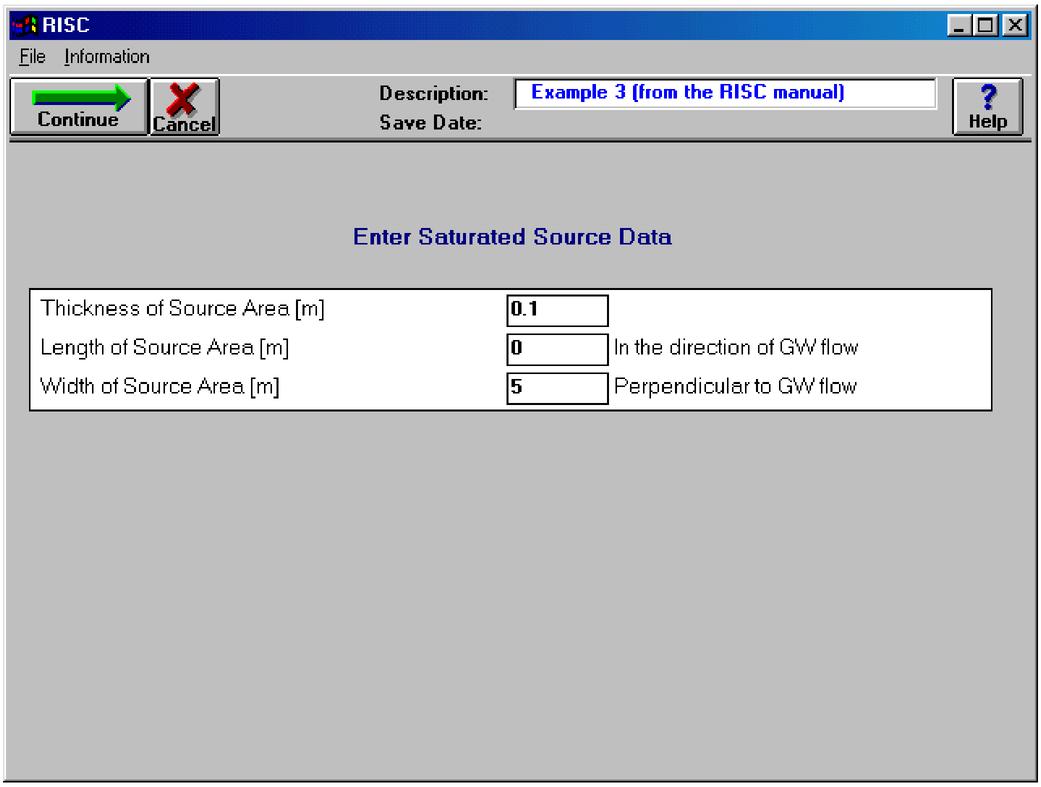
Benzene	9.6E-04
Naphthalene	2.7E-02
Toluene	2.5E-02
Xylenes	1.9E-03

Example 3: Saturated Zone Parameters

Saturated Source Parameters

The free product has been roughly been estimated to be about 0.1 m thick. The width of the product perpendicular to the direction of groundwater flow has been estimated to be less than 5 meters. These two dimensions form the vertical plane that will be the dissolved phase source. The model will set all of the groundwater exiting this plane equal to the source concentration specified in the source inputs. The length of the source area should be equal to zero to specify a vertical planar source. The next figure shows the saturated source data input screen.

> If the groundwater concentrations had been measured at a location between the source and the surface water edge, these concentrations could have been used as the source term. The thickness of the source should be adjusted to equal the length of the screen of the sampling well. The source concentration should be set equal to the measured concentration in the well and the distance to the surface water body should be adjusted to the distance to the well. The width of the source would have to be estimated.



Description: Example 3 (from the RISC manual)

Save Date:

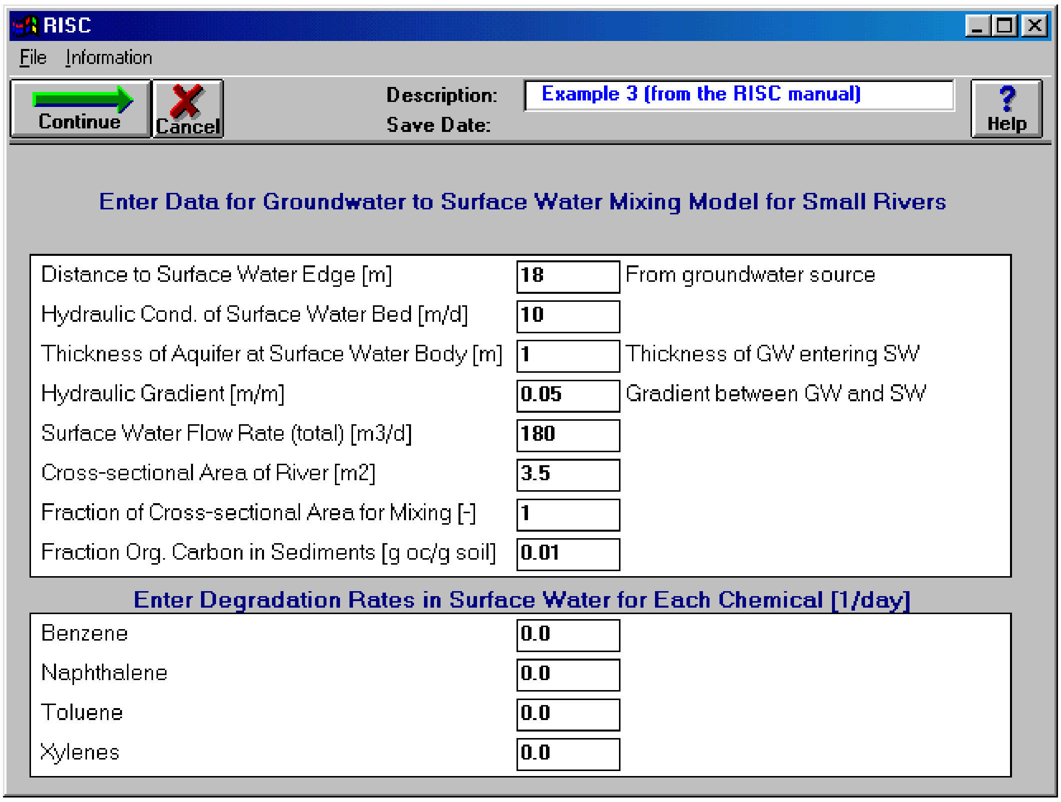
Enter Saturated Source Data

Thickness of Source Area [m]	0.1	
Length of Source Area [m]	0	In the direction of GW flow
Width of Source Area [m]	5	Perpendicular to GW flow

Example 3: Saturated Source Parameters

River Data

The next figure shows the data used in this example for the surface water input values.



Description: Example 3 (from the RISC manual)
Save Date:

Enter Data for Groundwater to Surface Water Mixing Model for Small Rivers

Distance to Surface Water Edge [m]	18	From groundwater source
Hydraulic Cond. of Surface Water Bed [m/d]	10	
Thickness of Aquifer at Surface Water Body [m]	1	Thickness of GW entering SW
Hydraulic Gradient [m/m]	0.05	Gradient between GW and SW
Surface Water Flow Rate (total) [m3/d]	180	
Cross-sectional Area of River [m2]	3.5	
Fraction of Cross-sectional Area for Mixing [-]	1	
Fraction Org. Carbon in Sediments [g oc/g soil]	0.01	

Enter Degradation Rates in Surface Water for Each Chemical [1/day]

Benzene	0.0
Naphthalene	0.0
Toluene	0.0
Xylenes	0.0

Example 3: Surface Water Mixing Model Data

In Step 3b, the groundwater model source concentrations must be specified. The following assumptions are made about the free product composition:

- Benzene, 3%;
- Naphthalene, 1%;
- Toluene, 10%; and
- Xylenes, 12%.

These assumptions translate to the dissolve phase source concentrations shown in the following table.

Example 3: Source Concentration for the Groundwater Model

Chemical	Solubility [mg/l]	Mole Fraction [-]	Source Concentration [mg/l]
Benzene	1750	0.03	53
Naphthalene	31	0.01	0.31
Toluene	526	0.1	53
Xylenes	198	0.12	24

In Step 3c, the model was run for 75 years. The maximum concentrations in surface water are presented in the next section.

Step 4: Surface Water and Sediment Criteria *(Example 3)*

In Step 4, the ANZECC water quality criteria are selected for comparison with the calculated maximum surface water concentrations. The following table presents the results.

Example 3. Maximum Surface Water Concentrations and ANZECC Criteria Results for Example 3

Surface Water Concentrations and Selected Freshwater Criteria (ug/l)

	Maximum Modeled SW Conc.	Australia/NZ ANZECC ug/l
Benzene	72	230
Naphthalene	5.8E-04	0.3
Toluene	0.146	170
Xylenes	22	61

The maximum modeled surface water concentrations did not exceed the ANZECC criteria for the three chemicals that have criteria (benzene, naphthalene and toluene).

Sensitivity Analysis *(Example 3)*

It is important to perform sensitivity analyses to bracket the range of possible surface water concentrations. One scenario that might be important to consider is the seasonal differences in stream flow rates. Depending on the location of the stream, the variation in flow rates could be substantial. Note, that the groundwater gradient may also be different.

A sensitivity analysis is performed for this example. The streamflow used in the previous analysis corresponds to the wet flow rate of an average year. The flow rate in the dry season is approximately 1/5 of the wet season flow (36 m^3/d). One thing to potentially consider when using low flow rates is the species for which the surface water criteria was developed; can the species live, or does it live, in streams with that low of a flow rate and can it live in the stream during that time of year? Another thing to consider is that the groundwater gradient may change during various times of the year or from year to year. For this sensitivity analysis, it is assumed that the hydraulic gradient in the aquifer is 0.006 m/m in the dry season (it was 0.01 in the wet season).

The thickness of the NAPL typically increases in the dry season so its thickness will be increased from 0.1 m to 0.15 m.

The next table shows the results from Step 4 for this sensitivity analysis comparing the maximum modeled surface water concentrations with the ANZECC criteria. In this scenario, the benzene and xylenes concentrations exceed their criteria by about 115 and 26μg/l, respectively.

Example 3. Results for Sensitivity Analysis
Maximum Surface Water Concentrations and ANZECC Criteria

Surface Water Concentrations and Selected Freshwater Criteria (ug/l)

	Maximum Modeled SW Conc.	**Australia/NZ ANZECC ug/l**
Benzene	345	230
Naphthalene	1.6E-04	0.3
Toluene	0.053	170
Xylenes	87	61

If the water table drops, the thickness of the aquifer at the surface water boundary (an input parameter in the "River" section) may also be less than during the wet season. The same is true for the hydraulic gradient between the groundwater and surface water. In this scenario, if the thickness of the aquifer intersecting the river is changed from 1 m to 0.6 m and the hydraulic gradient between the aquifer and river is changed from 0.05 to 0.03 m/m the model predicts the following results.

Example 3. Results for Sensitivity Analysis with Reduced Aquifer Thickness and Reduced Gradient at River Edge

Surface Water Concentrations and Selected Freshwater Criteria (ug/l)

	Maximum Modeled SW Conc.	**Australia/NZ ANZECC ug/l**
Benzene	185	230
Naphthalene	7.7E-05	0.3
Toluene	0.025	170
Xylenes	46	61

Chapter 11.0

Chemical Database

The RISC software contains a large chemical database that can be accessed through Step 1: Select Chemicals of Concern. The chemical database contains physical and chemical parameters used in fate and transport modeling, toxicity values, and absorption adjustment factors for 86 chemicals potentially found at oil and gas sites. The database can be modified by the user through the RISC interface. This procedure is described in Chapters 3.2 through 3.5 of this document.

Table 11-1 (at the end of this chapter) shows the chemicals in the RISC database and their various properties. The primary reference consulted for chemical properties was the U.S. EPA’s Soil Screening Guidance Technical Background Document (1996). This document contains default values of Henry’s Law coefficient, K_{oc}, log K_{ow}, diffusion coefficients in air and water, and solubility for most of the chemicals in the RISC database.

For the TPH fractions, all of the chemical parameters (except for the skin permeability coefficient) were obtained from the TPH Criteria Working Group document entitled “A Risk-Based Approach for the Management of Total Petroleum Hydrocarbons in Soil” (TPHCWG, 1997).

11.1 PHYSICAL/CHEMICAL PROPERTIES

11.1.1 Density

The density of the chemical is presented in g/cm^3. The density of water is 1 g/cm^3. Currently density is not used in the RISC equations. It may be used in future updates.

The density values in the chemical database were obtained from the following reference:

1. Verschueren (1983)

11.1.2 Vapor Pressure (saturated)

The vapor pressure of a liquid or solid is the pressure of the gas in equilibrium with the liquid or solid at a given temperature. Chemicals with relatively low vapor pressures, high adsorptivity onto solids, or high solubility in water are less likely to vaporize and become airborne than chemicals with high vapor pressures or with less affinity for solution in water or adsorption to solids and sediments (Verschueren, 1983). Vapor pressures are expressed either in mm Hg (or just mm) or in atmospheres (atm.) If vapor pressures for certain compounds are not available, they can be derived graphically from their boiling points and the boiling point/vapor pressure relationship for homologous series. (See Verschueren, 1983, for an example using chlorinated benzenes and phenols as the homologous series.)

The vapor pressure values in the RISC database are presented in mm of mercury (mmHg). Vapor pressures for the contaminants in the database were obtained from Verschueren (1983). Vapor pressures in units of atmospheres can be converted to mmHg by the following equation:

$$VP(mmHg) = VP(atm) \times \frac{760\ \ mmHg}{atm} \qquad \textbf{(11-1)}$$

where

VP(mmHg) = vapor pressure in units of mmHg

VP(atm) = vapor pressure in units of atm

760 = conversion factor for mmHg to atm

Vapor pressure is an indication of volatility and is used to calculate the saturated vapor pressure for the Tier 1 spreadsheet. This value is compared with the soil gas RBSL in the vadose zone. If the soil gas RBSL exceeds the saturated vapor pressure, then a ">VP" is substituted into the RBSL table for the soil gas number. This indicates that the target risk level cannot be reached at saturated conditions.

The vapor pressure values in the chemical database were obtained from the following references (by order of preference):

1. Howard and Meylen (1997)
2. Verschueren (1983)

11.1.3 Solubility

Solubility in water indicates a chemicals likelihood to mix and transport with water in the environment (e.g. leaching from vadose zone soils to groundwater and transporting with groundwater flow). Chemicals with high solubility in water tend to remain dissolved in water and not to partition into soil or bioconcentrate in organisms. Further, they are less likely to volatilize from water (also dependent on vapor pressure and Henry’s Law constant) and are generally more likely to biodegrade (Howard, 1989).

The following references were used (by order of preference):

1. U.S. EPA’s Soil Screening Guidance: Technical Background Document (1996).
2. Howard and Meylen (1997)

Solubility values are required for all of the fate and transport models except the Dissolved Phase Transport model. For this model, it is important to check that the source concentrations do not exceed solubility. For contaminants that are part of a mixture, the effective solubility will be lower than the pure phase solubility.

11.1.4 Henry’s Law Coefficient

The Henry’s Law Coefficient, H, is the air/water partition coefficient. Henry’s Law relates the chemical concentration in the gas phase to its concentration in the water phase (Howard, 1989). The conversion from the dimensional form of Henry's Law coefficient to the dimensionless form is given by:

$$H' = \frac{H}{RT} \tag{11-2}$$

where

H' = the non-dimensional form of Henry's Law constant [(mg/l)/(mg/l)]

H = Henry's Law constant [atm-m^3/mol]

R = the universal gas constant, [atm-m^3/mol-K] (R = 8.2×10^{-5})

T = absolute temperature [K] (20 ^{o}C = 293 K)

For Henry's Law, the following references were used (by order of preference):

1. U.S. EPA's Soil Screening Guidance: Technical Background Document (1996).
2. Howard and Meylen (1997)

Henry's Law is used in all of the fate and transport models (except the Dissolved Phase Transport model).

11.1.5 Log Octanol/Water Partition Coefficient (log K_{ow})

The octanol/water partition coefficient is the ratio of the chemical concentration in octanol divided by the concentration in water. Log K_{ow} is used to estimate the vegetable uptake factor for organic chemicals. It is not used in any of the fate and transport models in Version 4 of RISC. In future versions it will be used for the ecological risk component because it is an important indicator of bioaccumulation in organisms.

The values for log K_{ow} were obtained from:

1. U.S. EPA's Soil Screening Guidance: Technical Background Document (1996).

2. Howard and Meylen (1997)
3. Howard's (1989) Handbook of Fate and Exposure Data (Volumes 1 - 3)

11.1.6 Organic Carbon Partition Coefficient (K_{oc})

The organic carbon partition coefficient is an important chemical transport property describing an organic chemical's affinity for sorption to organic carbon (the higher the K_{oc}, the higher the sorption). Experimentally measured K_{oc} values for gasoline constituents are not readily available in the literature (Lyman et al., 1992). They have been included for many chemicals in the database; however, if the user needs to add new chemicals, the K_{oc} may not be easily found. Lyman et al. (1992) suggests the following algorithms for estimating K_{oc}. One equation uses the octanol/water partition coefficient, K_{ow} , while the other uses the chemical solubility, S.

$$\log K_{oc} = 0.779 \log K_{ow} + 0.46 \tag{11-3}$$

$$\log K_{oc} = -0.602 \log S + 0.656 \tag{11-4}$$

where

S = liquid phase solubility for chemical [mg/l]

K_{oc} = chemical-specific organic carbon partition coefficient [l/kg]

K_{ow} = chemical-specific octanol/water partition coefficient [l/kg]

For gasoline constituents with low K_{ow} values, solubility-based relationships are probably superior to those based on K_{ow} (Lyman et al., 1992). For the organic carbon partition coefficient (K_{oc}), the following references were used (by order of preference):

1. U.S. EPA's Soil Screening Guidance: Technical Background Document (1996).
2. U.S. EPA: Basics of Pump and Treat Groundwater Remediation Technology (1990)

For inorganic chemicals, the K_{oc} values are assumed to be zero and the K_d parameter is used to estimate partitioning between the sorbed and dissolved phases. K_{oc} is used in all the fate and transport models except volatilization from groundwater.

11.1.7 Inorganic Partition Coefficient (K_d)

The K_d parameter is used for inorganic chemicals (usually metals) to estimate the relationship of the dissolved and sorbed phases of the chemical. Unlike K_{oc} for organic chemicals, the sorption of metals is highly site-specific and usually dependent on water pH so the K_d value should be adjusted in the chemical database if site-specific data is available. The following reference was used for the K_d values in the RISC database (a pH of 7.0 was assumed):

1. U.S. EPA's Soil Screening Guidance: Technical Background Document (1996).

Most of the inorganic chemicals in the RISC database have a K_d value of zero because of the site-specific nature of the parameter. This means that the chemicals will be treated by the models as if they are non-retarded. For many pathways this is a conservative assumption.

11.1.8 Diffusion Coefficients in Air and Water

Diffusion coefficients in air and water were obtained predominantly from:

1. U.S. EPA's Soil Screening Guidance: Technical Background Document (1996).
2. U.S. EPA: Hazardous Waste Treatment, Storage and Disposal Facilities (TSDF) –Air Emission Models (1987)

The diffusion coefficients in air and in water are used by all of the models estimating volatilization or transport of vapors to estimate the effective diffusion coefficient. The diffusion coefficient in water is used by the Dissolved Phase Transport model.

11.1.9 Degradation Rates

The degradation rates are used in all of the fate and transport models in RISC with the exception of the Johnson and Ettinger and the Volatilization from Groundwater vapor models. The degradation rates in the RISC database represent the "high-end" and "low-end" degradation rates presented in Howard (1991) for groundwater. These were obtained for a limited number of chemicals. These values should not be construed as absolute minimum and maximum rates. Degradation rates are highly site-specific and can also vary across a plume because of available dissolved oxygen and nutrients in the groundwater.

The degradation rates represent the minimum and maximum values found by Howard (1991) in the published literature at the time the reference was published. There have been many new studies published since 1991.

The degradation rates may be modified in Step 3 of RISC for use in the fate and transport models. This is the only chemical-specific parameter that can be modified outside of Step 1 (the chemical database).

The degradation rates are also used in the Tier 1 spreadsheet to calculate the RBSLs when using the Green-Ampt and Domenico models.

11.1.10 Vegetable Uptake Factor

Baes et al (1984) presents soil-to-plant concentration factors (called B_v by Baes) for the elements of the periodic table. Eleven chemicals in RISC have values for B_v entered in the database (Table 11-1). These B_v values are used by RISC to estimate the uptake factors for both root and above-ground vegetables. The vegetable model is described in detail in Appendix O. The following relationships are used if the uptake factor is entered in the chemical database (excerpted from Appendix O):

For soil:

$$B_{va} = B_{vBaes} \times (1 - 0.85) \quad \textbf{(11-5)}$$

$$B_{vr} = B_{vBaes} \times (1 - 0.85) \quad \textbf{(11-6)}$$

For water:

$$RCF = B_{vBaes} \times (1 - 0.85) \times K_d \quad \textbf{(11-7)}$$

$$ABCF = B_{vBaes} \times (1 - 0.85) \times K_d \tag{11-8}$$

where:

B_{vr} = soil-to-root uptake factor [mg chemical/kg **wet weight** root vegetable per mg chemical/kg soil]

B_{va} = soil-to-above-ground vegetable uptake factor [mg chemical/kg **wet weight** above-ground vegetable per mg chemical/kg soil]

B_{vBaes} = soil-to-plant concentration factor [mg chemical/kg **dry weight** vegetable per mg chemical/kg dry soil]

$(1 - 0.85)$ = adjustment from dry weight to wet weight vegetable where 0.85 is the assumed moisture content of the vegetable

RCF = root concentration factor [mg chemical/kg produce per mg chemical/l water]

$ABCF$ = above-ground concentration factor [mg chemical/kg vegetable per mg chemical/l water]

K_d = equilibrium partitioning coefficient [l/kg or ml/g]

The chemicals that have B_v*'s* entered in the database are inorganic, (i.e. they are not expected to have K_{ow} or K_{oc} values). If a chemical does not have a K_d, K_{oc}, or a K_{ow} entered in the database, the uptake factors from water are assumed to be equal to zero.

For organic chemicals, the vegetable uptake factors will be calculated from K_{ow} or K_d using the equations found in Appendix O.

11.2 TOXICOLOGICAL PROPERTIES

11.2.1 USEPA Carcinogenic Classification

USEPA’s Carcinogenic Classification, or Weight-of-Evidence Classification, is a system for characterizing the extent to which the available data indicate that an agent is a human carcinogen. The evidence is characterized separately for human studies and animal studies as sufficient, limited, inadequate, no data, or evidence of no effect (USEPA, 1989a).

The carcinogenicity classification values for each chemical were obtained from USEPA's Integrated Risk and Information System (IRIS). The USEPA classification system for weight of evidence is shown below.

Table 11-2. USEPA's Carcinogenic Classification

Group (Classification)	Description
A	Human carcinogen
B1 or B2	Probable human carcinogen: B1 indicates that limited human data are available. B2 indicates sufficient evidence in animals but inadequate or no evidence in humans.
C	Possible human carcinogen
D	Not classifiable as to human carcinogenicity (may be a hazard, however).
E	Evidence of non-carcinogenicity for humans.

11.2.2 Toxicity Parameters

The slope factor (or potency factor) is the toxicity parameter (developed by USEPA) to evaluate carcinogenic risk. The reference dose, or *RfD*, is the toxicity parameter used to evaluate non-carcinogenic risk. Values for both toxicity parameters were obtained from the USEPA's Region 9 Preliminary Remediation Goals (USEPA, 1999). The introduction section to the Region 9 Preliminary Remediation Goals lists the following order of preference for obtaining toxicological constants:

1. IRIS (U.S. EPA's on-line Integrated Risk Information System)
2. NCEA (U.S. EPA's National Center for Exposure Assessment)
3. Health Effects Assessment Summary Table (HEAST) (USEPA, 1995)

4. Withdrawn from IRIS or HEAST and under review (but previously published value still being used), and
5. Obtained from other USEPA documents.

Many chemicals do not have toxicity values for both inhalation and oral exposure routes. The USEPA's Region 9 Preliminary Remediation Goals (USEPA, 1999) notes the following:

> *Route-to-route extrapolations were frequently used when there were no toxicity values available for a given route of exposure. Oral cancer slope factors and reference doses were used for both oral and inhaled exposures for organic compounds lacking inhalation values. Inhalation slope factors and inhalation reference doses were used for both inhaled and oral exposure for organic compounds lacking oral values. Route extrapolations were not performed for inorganics due to portal of entry effects and known differences in absorption efficiency for the two routes of exposure. An additional route extrapolation is the use of oral toxicity values for evaluating dermal exposures.*

11.2.3 Inhalation Conversion Factors

As of January 1991, IRIS and NCEA databases (used as toxicology sources by the PRG table) no longer present inhalation reference doses (RfDi) or inhalation slope factors (SFi). Rather, reference concentrations (RfCs) for non-carcinogenic effects and unit risk factors (URFs) for carcinogenic effects are used. For purposes of estimating risk and calculating risk-based concentrations, inhalation reference doses and inhalation slope factors are preferred. This is not a problem for most chemicals because the inhalation toxicity criteria are easily converted. To calculate an RfDi from a RfC, the following equation is used:

$$RfDi\left(\frac{mg}{kg \cdot d}\right) = RfC\left(\frac{mg}{m^3}\right) \times \frac{20m^3}{d} \times \frac{1}{70kg} \qquad \textbf{(11-9)}$$

Likewise, to calculate an SFi from a URF, the following equation is used:

$$SFi\left(\frac{kg \cdot d}{mg}\right) = URF\left(\frac{m^3}{\mu g}\right) \times \frac{d}{20m^3} \times 70kg \times \frac{10\mu g}{mg} \qquad \textbf{(11-10)}$$

11.2.4 Absorption Adjustment Factors (AAFs)

Absorption adjustment factors are used to account for the differences between applied and absorbed dose. For the most part, the AAFs are equal to 1; i.e., the dose is not adjusted.

Dermal AAFs (sometimes called dermal absorption values) were obtained from USEPA’s Region 9's Preliminary Remediation Goals (USEPA, 1996). Note that this is the previous version of the PRG table. The current PRG table (1999) presents dermal absorption values for non-volatile organics (AAF = 0.10) and a few select chemicals only (arsenic, cadmium, chlordane, 2,4-D, DDT, lindane, TCDD, PAHs, PCBs, and pentachlorophenols) as recommended in the "Risk Assessment Guidance for Superfund Volume I: Human Health Evaluation Manual (Part E, Supplemental Guidance for Dermal Risk Assessment) Interim Guidance" (U.S. EPA 1999). The dermal absorption factors have been withdrawn for all other chemicals (inorganics and VOCs) in the current PRG table, effectively eliminating dermal contact with soil as an exposure pathway of concern for these chemicals. Since many states have not adopted this approach yet, the previous absorption coefficients were maintained in the RISC database.

The default values used for dermal-soil AAFs for organic chemicals is 0.1 and for inorganic chemicals is 0.01. The following chemicals have chemical-specific dermal-soil AAFs: arsenic (0.03), cadmium (0.001), PAHs (0.1), and PCBs (0.14).

11.2.5 Skin Permeability Coefficient

The permeability coefficient is used to evaluate the amount of intake for dermal contact with water exposure pathways. The value is presented in terms of flux, normalized for concentration, and represents the rate at which a chemical penetrates the skin. Dermal permeability coefficients are presented in USEPA’s Dermal Exposure Assessment guidance (1992). For chemicals not listed in the guidance, permeability was estimated from:

$$\log K_p = -2.72 + 0.71 \log K_{ow} - 0.0061 MW \qquad \textbf{(11-6)}$$

where

K_p = skin permeability coefficient [cm/hr]

K_{ow} = chemical-specific octanol/water partition coefficient [l/kg]

MW = molecular weight [g/mol]

For the TPH groups, the skin permeability coefficient was estimated using the above equation.

11.3 TECHNICAL DETAILS OF THE CHEMICAL DATABASE

Table 11-1 presents the chemical database. This table is contained in the Tier 1 spreadsheet (Tier 1.xls).

11.3.1 Chemical Database Format

The chemical database used in RISC is contained in a tab-delimited text file, 'CHEMICAL.TXT' (originally created from the Tier 1 spreadsheet). Changes to the database should be made through the RISC interface in Step 1. The modifications should also be made in the Tier 1 spreadsheet since the spreadsheet and the RISC software do not share data and are not directly linked.

11.3.2 Restoring the Original Chemical Database

There are two choices for reinstalling the original chemical database for RISC: (1) reinstall the software from the installation file, or (2) delete the file named 'CHEMICAL.TXT'. The second method notifies the RISC software to create a new chemical database from the backup file 'CHEMBACK.TXT'.

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Acenaph thene**	**Acenaph thylene**	**Acetone**	**Anthracene**	**Arsenic**	**Barium**	**Benz(a) anthracene**	**Benzene**
CAS Number	-	83-32-9	208-96-8	67-64-1	120-12-7	7440-38-2	7440-39-3	56-55-3	71-43-2
Molecular Weight	g/mol	154.2	152.2	58.08	178.2	74.9	137.3	228.0	78
Density	g/cm^3	1.07	0.90	0.79	1.25	ND	ND	1.27	0.88
Vapor Pressure	mmHg	2.3E-03	9.1E-04	2.3E+02	2.7E-06	0.0E+00	0.0E+00	3.1E-08	9.5E+01
Solubility	mg/L	4.24E+00	3.93E+00	1.00E+06	4.34E-02	ND	ND	9.40E-03	1.75E+03
Henry's Law Constant (no NDs)	-	6.36E-03	4.67E-03	1.59E-03	2.67E-03	0.00E+00	0.00E+00	1.37E-04	2.28E-01
Koc (for organics -- ND for inorganics)	ml/g	7.1E+03	4.8E+03	5.8E-01	3.0E+04	ND	ND	4.0E+05	5.9E+01
Kd (partition coefficient for inorganics)	ml/g	ND	ND	ND	ND	2.9E+01	3.0E+01	ND	ND
log Kow -- Octanol/Water Partition Coefficient	L/kg	3.9E+00	3.9E+00	-2.4E-01	4.6E+00	ND	ND	5.7E+00	2.1E+00
Diffusion Coeff. in Air	cm^2/s	4.2E-02	5.4E-02	1.2E-01	3.2E-02	ND	ND	5.1E-02	8.8E-02
Diffusion Coefficient in Water	cm^2/s	7.7E-06	6.6E-06	1.1E-05	7.7E-06	ND	ND	9.0E-06	9.8E-06
Degradation Rate -- high end of range	1/day	2.8E-02	8.2E-03	ND	7.0E-03	ND	ND	3.4E-03	7.0E-02
Degradation Rate -- low end of range	1/day	3.4E-03	5.8E-03	ND	7.5E-04	ND	ND	5.1E-04	9.6E-04
Uptake Factor for Plants	-	Use Kow	Use Kow	Use Kow	Use Kow	4.00E-02	1.50E-01	Use Kow	Use Kow
Toxicity Parameters									
EPA Classification	-	ND	D	D	D	A	D	B2	A
Slope Factor Oral	1/(mg/kg-d)	ND	ND	ND	ND	1.5E+00	ND	7.3E-01	2.9E-02
Slope Factor Inhalation	1/(mg/kg-d)	ND	ND	ND	ND	1.5E+01	ND	3.1E-01	2.7E-02
RfD Oral	mg/kg-d	6.0E-02	ND	1.0E-01	3.0E-01	3.0E-04	7.0E-02	ND	ND
RfD Inhalation	mg/kg-d	6.0E-02	ND	1.0E-01	3.0E-01	ND	1.4E-04	ND	ND
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.1	0.1	0.1	0.03	0.01	0.1	0.1
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	1.5E-01	9.6E-02	5.7E-04	2.2E-01	1.0E-03	1.0E-03	8.1E-01	2.1E-02
Maximum Contaminant Levels in Groundwater									
MCL (Maximum Contaminant Level)	mg/l	ND	ND	ND	ND	5.0E-02	2.0E+00	ND	5.0E-03

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Benzo(a) pyrene**	**Benzo(b) fluoranthene**	**Benzo(g,h,i) perylene**	**Benzo(k) fluoranthene**	**Beryllium**	**Bis(2 ethylhexyl) phthalate**	**Butyl benzyl phthalate**
CAS Number	-	50-32-8	205-99-2	191-24-2	207-08-9	7440-41-7	117-81-7	85-68-7
Molecular Weight	g/mol	252.3	252.3	276.3	252.3	9.0	390.6	312.4
Density	g/cm^3	1.35	1.35	1.35	1.35	ND	0.99	1.10
Vapor Pressure	mmHg	5.5E-09	5.0E-07	1.0E-10	9.7E-10	0.0E+00	9.8E-06	8.3E-06
Solubility	mg/L	1.62E-03	1.50E-03	2.60E-04	8.00E-04	ND	3.40E-01	2.69E+00
Henry's Law Constant (no NDs)	-	4.63E-05	4.55E-03	1.09E-05	3.40E-05	0.00E+00	4.18E-06	5.17E-05
Koc (for organics -- ND for inorganics)	ml/g	1.0E+06	1.2E+06	7.8E+06	1.2E+06	ND	1.5E+07	5.8E+04
Kd (partition coefficient for inorganics)	ml/g	ND	ND	ND	ND	8.2E+01	ND	ND
log Kow -- Octanol/Water Partition Coefficient	L/kg	6.1E+00	6.2E+00	7.1E+00	6.2E+00	ND	7.3E+00	4.8E+00
Diffusion Coeff. in Air	cm^2/s	4.3E-02	2.3E-02	4.1E-02	2.3E-02	ND	3.5E-02	3.9E-02
Diffusion Coefficient in Water	cm^2/s	9.0E-06	5.6E-06	4.9E-06	5.6E-06	ND	3.7E-06	7.0E-06
Degradation Rate -- high end of range	1/day	6.1E-03	9.6E-04	5.9E-04	3.9E-04	ND	ND	ND
Degradation Rate -- low end of range	1/day	6.5E-04	5.7E-04	5.3E-04	1.6E-04	ND	ND	ND
Uptake Factor for Plants	-	Use Kow	Use Kow	Use Kow	Use Kow	1.00E-02	Use Kow	Use Kow
Toxicity Parameters								
EPA Classification	-	B2	B2	D	B2	B1	B2	C
Slope Factor Oral	1/(mg/kg-d)	7.3E+00	7.3E-01	ND	7.3E-02	ND	1.4E-02	ND
Slope Factor Inhalation	1/(mg/kg-d)	3.1E+00	3.1E-01	ND	3.1E-02	8.4E+00	1.4E-02	ND
RfD Oral	mg/kg-d	ND	ND	ND	ND	2.0E-03	2.0E-02	2.0E-01
RfD Inhalation	mg/kg-d	ND	ND	ND	ND	5.7E-06	2.2E-02	ND
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.1	0.1	0.1	0.01	0.1	0.1
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	1.2E+00	1.2E+00	1.7E+00	1.1E+00	1.0E-03	3.3E-02	7.4E-02
Maximum Contaminant Levels in Groundwater								
MCL (Maximum Contaminant Level)	mg/l	2.0E-04	ND	ND	ND	ND	ND	ND

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Cadmium**	**Carbon Disulfide**	**Carbon Tetrachloride**	**Chloro benzene**	**Chloroform**	**Chromium (III)**	**Chromium (VI)**	**Chrysene**
CAS Number	-	7440-43-9	75-15-0	56-23-5	108-90-7	67-66-3	7440-47-2	7440-47-3	218-01-9
Molecular Weight	g/mol	112.4	76.1	153.8	112.6	119.4	52.0	52.0	228.3
Density	g/cm^3	ND	1.26	1.59	1.11	1.49	ND	ND	1.27
Vapor Pressure	mmHg	0.0E+00	3.6E+02	1.2E+02	1.2E+01	2.0E+02	0.0E+00	0.0E+00	6.2E-09
Solubility	mg/L	ND	1.19E+03	7.93E+02	4.72E+02	7.92E+03	ND	ND	1.60E-03
Henry's Law Constant (no NDs)	-	0.00E+00	5.92E-01	1.25E+00	1.52E-01	1.50E-01	0.00E+00	0.00E+00	3.88E-03
Koc (for organics -- ND for inorganics)	ml/g	ND	4.6E+01	1.7E+02	2.2E+01	4.0E+01	ND	ND	4.0E+05
Kd (partition coefficient for inorganics)	ml/g	3.7E+01	ND	ND	ND	ND	2.0E+05	2.3E+01	ND
log Kow -- Octanol/Water Partition Coefficient	L/kg	ND	2.1E+00	2.7E+00	2.9E+00	1.9E+00	ND	ND	5.7E+00
Diffusion Coeff. in Air	cm^2/s	ND	1.0E-01	7.8E-02	7.3E-02	1.0E-01	ND	ND	2.5E-02
Diffusion Coefficient in Water	cm^2/s	ND	1.0E-05	8.8E-06	8.7E-06	1.0E-05	ND	ND	6.2E-06
Degradation Rate -- high end of range	1/day	ND	ND	1.0E-01	5.1E-03	1.2E-02	ND	ND	9.3E-04
Degradation Rate -- low end of range	1/day	ND	ND	1.9E-03	2.0E-03	4.0E-04	ND	ND	3.0E-04
Uptake Factor for Plants	-	5.50E-01	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow
Toxicity Parameters									
EPA Classification	-	B1	ND	B2	D	B2	D	A	B2
Slope Factor Oral	1/(mg/kg-d)	ND	ND	1.3E-01	ND	6.1E-03	ND	ND	7.3E-03
Slope Factor Inhalation	1/(mg/kg-d)	6.3E+00	ND	5.3E-02	ND	8.1E-02	ND	2.9E+02	3.1E-03
RfD Oral	mg/kg-d	5.0E-04	1.0E-01	7.0E-04	2.0E-02	1.0E-02	1.5E+00	3.0E-03	ND
RfD Inhalation	mg/kg-d	ND	2.0E-01	7.0E-04	1.7E-02	8.6E-05	ND	ND	ND
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.001	0.1	0.1	0.1	0.1	0.01	0.01	0.1
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	1.0E-03	2.4E-02	2.2E-02	4.1E-02	8.9E-03	1.3E-03	1.3E-03	8.1E-01
Maximum Contaminant Levels in Groundwater									
MCL (Maximum Contaminant Level)	mg/l	5.0E-03	ND	5.0E-03	1.0E-01	1.0E-01	ND	ND	ND

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Copper**	**Cresol(m)**	**Cresol(o)**	**Cresol(p)**	**Cyanide**	**Dibenz(a,h) anthracene**	**Dichloro ethane (1,1)**	**Dichloro ethane (1,2) (EDC)**
CAS Number	-	7440-50-8	108-39-4	95-48-7	106-44-5	57-12-5	53-70-3	75-34-3	107-06-2
Molecular Weight	g/mol	63.5	108.1	108.1	108.1	0.0	278.4	99.0	99.0
Density	g/cm^3	ND	1.04	1.04	1.03	ND	1.28	1.17	1.17
Vapor Pressure	mmHg	0.0E+00	1.4E-01	3.0E-01	1.1E-01	0.0E+00	1.0E-10	2.3E+02	7.9E+01
Solubility	mg/L	ND	2.27E+04	2.60E+04	3.53E+04	ND	2.49E-03	5.06E+03	8.52E+03
Henry's Law Constant (no NDs)	-	0.00E+00	3.55E-05	4.92E-05	4.10E-05	0.00E+00	6.03E-07	2.30E-01	4.01E-02
Koc (for organics -- ND for inorganics)	ml/g	ND	8.7E+01	9.1E+01	8.1E+01	ND	3.8E+06	3.2E+01	1.7E+01
Kd (partition coefficient for inorganics)	ml/g	2.5E+00	ND	ND	ND	9.9E+00	ND	ND	ND
log Kow -- Octanol/Water Partition Coefficient	L/kg	ND	2.0E+00	2.0E+00	2.0E+00	ND	6.7E+00	1.8E+00	1.5E+00
Diffusion Coeff. in Air	cm^2/s	ND	7.4E-02	7.4E-02	7.4E-02	ND	2.0E-02	7.4E-02	1.0E-01
Diffusion Coefficient in Water	cm^2/s	ND	1.0E-05	8.3E-06	1.0E-05	ND	5.2E-06	1.1E-05	9.9E-06
Degradation Rate -- high end of range	1/day	ND	ND	ND	ND	ND	9.6E-04	1.1E-02	7.0E-03
Degradation Rate -- low end of range	1/day	ND	ND	ND	ND	ND	3.7E-04	1.9E-03	1.9E-03
Uptake Factor for Plants	-	4.00E-01	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow
Toxicity Parameters									
EPA Classification	-	D	C	C	C	D	B2	C	B2
Slope Factor Oral	1/(mg/kg-d)	ND	ND	ND	ND	ND	7.3E+00	ND	9.1E-02
Slope Factor Inhalation	1/(mg/kg-d)	ND	ND	ND	ND	ND	3.1E+00	ND	9.1E-02
RfD Oral	mg/kg-d	3.7E-02	5.0E-02	5.0E-02	5.0E-03	4.0E-02	ND	1.0E-01	3.0E-02
RfD Inhalation	mg/kg-d	ND	5.0E-02	5.0E-02	5.0E-03	ND	ND	1.4E-01	1.4E-03
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.01	0.1	0.1	0.1	0.01	0.1	0.1	0.1
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	1.0E-03	1.5E-02	1.6E-02	1.8E-02	1.0E-02	2.7E+00	8.9E-03	5.3E-03
Maximum Contaminant Levels in Groundwater									
MCL (Maximum Contaminant Level)	mg/l	1.3E+00	ND	ND	ND	ND	ND	ND	5.0E-03

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Dichloro ethylene (1,1)**	**Dichloro ethylene (cis 1,2)**	**Dichloro ethene (trans 1,2)**	**Dimethylbenza(a) anthracene (7,12)**	**Dimethyl phenol (2,4)**	**di-n-Butyl phthalate**	**di-n-Octyl phthalate**
CAS Number	-	75-35-4	156-59-2	156-60-5	57-97-6	105-67-9	84-74-2	117-84-0
Molecular Weight	g/mol	96.9	96.9	96.9	147	122.2	178.3	390.6
Density	g/cm^3	1.22	1.21	1.26	1.30	1.04	1.05	1.00
Vapor Pressure	mmHg	6.0E+02	2.0E+02	3.3E+02	5.6E-09	9.8E-02	7.3E-05	2.6E-06
Solubility	mg/L	2.25E+03	3.50E+03	6.30E+03	6.10E-02	7.87E+03	1.12E+01	2.90E-01
Henry's Law Constant (no NDs)	-	1.07E+00	1.67E-01	3.85E-01	1.28E-06	8.20E-05	3.85E-08	7.50E-09
Koc (for organics -- ND for inorganics)	ml/g	5.9E+01	3.6E+01	5.3E+01	4.8E+05	2.1E+02	8.3E+07	1.1E+05
Kd (partition coefficient for inorganics)	ml/g	ND	ND	ND	ND	ND	ND	ND
log Kow -- Octanol/Water Partition Coefficient	L/kg	2.1E+00	1.9E+00	2.1E+00	5.8E+00	2.4E+00	4.6E+00	9.2E+00
Diffusion Coeff. in Air	cm^2/s	9.0E-02	7.4E-02	7.1E-02	4.6E-02	5.8E-02	1.5E-02	3.7E-02
Diffusion Coefficient in Water	cm^2/s	1.0E-05	1.1E-05	1.2E-05	5.0E-06	8.7E-06	3.6E-06	4.0E-05
Degradation Rate -- high end of range	1/day	1.2E-02	ND	ND	ND	ND	ND	ND
Degradation Rate -- low end of range	1/day	5.0E-03	ND	ND	ND	ND	ND	ND
Uptake Factor for Plants	-	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow
Toxicity Parameters								
EPA Classification	-	C	C	C	ND	ND	D	ND
Slope Factor Oral	1/(mg/kg-d)	6.0E-01	ND	ND	ND	ND	ND	ND
Slope Factor Inhalation	1/(mg/kg-d)	1.8E-01	ND	ND	ND	ND	ND	ND
RfD Oral	mg/kg-d	9.0E-03	1.0E-02	2.0E-02	3.0E-02	2.0E-02	1.0E-01	2.0E-02
RfD Inhalation	mg/kg-d	9.0E-03	1.0E-02	2.0E-02	ND	2.0E-02	1.0E-01	2.0E-02
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	1.6E-02	1.0E-02	1.0E-02	1.2E+00	1.5E-02	3.3E-02	2.7E+01
Maximum Contaminant Levels in Groundwater								
MCL (Maximum Contaminant Level)	mg/l	7.0E-03	7.0E-02	1.0E-01	ND	ND	ND	ND

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Dinitro toluene (2,4)**	**Dioxane (1,4)**	**Ethyl benzene**	**Ethylene Dibromide**	**Fluoran thene**	**Fluorene**	**Indeno (1,2,3CD) pyrene**	**Lead**
CAS Number	-	121-14-2	123-91-1	100-41-4	106-93-4	206-44-0	86-73-7	193-39-5	7439-92-1
Molecular Weight	g/mol	182.1	88.1	106.2	187.9	202.3	166.2	276.3	0.0
Density	g/cm^3	1.31	1.03	0.87	2.18	1.25	1.20	1.35	ND
Vapor Pressure	mmHg	1.5E-04	3.8E+01	9.6E+00	1.1E+01	1.2E-08	8.4E-03	1.0E-10	0.0E+00
Solubility	mg/L	2.70E+02	1.10E-02	1.69E+02	4.30E+03	2.06E-01	1.98E+00	2.20E-05	ND
Henry's Law Constant (no NDs)	-	3.80E-06	1.10E-02	3.23E-01	2.89E-02	6.60E-04	2.61E-03	6.56E-05	0.00E+00
Koc (for organics -- ND for inorganics)	ml/g	9.6E+01	1.7E+01	3.6E+02	4.4E+01	1.1E+05	1.4E+04	3.5E+06	ND
Kd (partition coefficient for inorganics)	ml/g	ND	ND	ND	ND	ND	ND	ND	9.9E+00
log Kow -- Octanol/Water Partition Coefficient	L/kg	2.0E+00	-2.7E-01	3.1E+00	1.8E+00	5.1E+00	4.2E+00	6.7E+00	ND
Diffusion Coeff. in Air	cm^2/s	2.0E-01	2.3E-01	7.5E-02	5.0E-02	3.0E-02	3.6E-02	1.9E-02	ND
Diffusion Coefficient in Water	cm^2/s	7.1E-06	1.0E-05	7.8E-06	9.6E-06	6.4E-06	7.9E-06	5.7E-06	ND
Degradation Rate -- high end of range	1/day	ND	ND	1.0E-01	3.5E-02	2.5E-03	1.1E-02	5.8E-04	ND
Degradation Rate -- low end of range	1/day	ND	ND	3.0E-03	5.8E-03	7.9E-04	5.8E-03	4.8E-04	ND
Uptake Factor for Plants	-	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow
Toxicity Parameters									
EPA Classification	-	B2	B2	D	B2	D	D	B2	NA
Slope Factor Oral	1/(mg/kg-d)	6.8E-01	1.1E-02	ND	8.5E+01	ND	ND	7.3E-01	ND
Slope Factor Inhalation	1/(mg/kg-d)	6.8E-01	1.1E-02	ND	7.7E-01	ND	ND	3.1E-01	ND
RfD Oral	mg/kg-d	2.0E-03	ND	1.0E-01	ND	4.0E-02	4.0E-02	ND	3.6E-03
RfD Inhalation	mg/kg-d	2.0E-03	ND	2.9E-01	ND	4.0E-02	4.0E-02	ND	ND
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.01
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	3.8E-03	3.6E-04	7.4E-02	3.3E-03	3.6E-01	3.6E-01	1.9E+00	0.0E+00
Maximum Contaminant Levels in Groundwater									
MCL (Maximum Contaminant Level)	mg/l	ND	ND	7.0E-01	5.0E-05	ND	ND	ND	1.5E-02

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Mercury**	**Methanol**	**Methyl ethyl ketone**	**Methylene Chloride**	**Methyl napthalene (2)**	**MTBE**	**Naphthalene**	**Nickel**
CAS Number	-	7439-97-6	67-56-1	78-93-3	75-09-2	91-57-6	1634-04-4	91-20-3	7440-02-0
Molecular Weight	g/mol	200.6	32	72.1	84.93	142.2	88.17	128.2	58.7
Density	g/cm^3	ND	0.80	0.82	1.34	0.99	0.74	1.16	ND
Vapor Pressure	mmHg	1.3E-03	1.3E+02	9.5E+01	4.4E+02	8.3E-03	2.5E+02	8.5E-02	0.0E+00
Solubility	mg/L	ND	1.00E+06	2.12E+05	1.30E+04	2.46E+01	4.80E+04	3.10E+01	1.73E+05
Henry's Law Constant (no NDs)	-	4.67E-01	1.87E-04	2.33E-03	8.98E-02	2.12E-02	2.04E-02	1.98E-02	0.00E+00
Koc (for organics -- ND for inorganics)	ml/g	ND	0.0E+00	4.5E+00	1.2E+01	8.5E+03	1.2E+01	2.0E+03	ND
Kd (partition coefficient for inorganics)	ml/g	8.2E+01	ND	ND	ND	ND	ND	ND	8.8E+01
log Kow -- Octanol/Water Partition Coefficient	L/kg	ND	-7.7E-01	2.9E-01	1.3E+00	4.1E+00	1.3E+00	3.4E+00	ND
Diffusion Coeff. in Air	cm^2/s	3.1E-02	1.6E-01	8.1E-02	1.0E-01	5.8E-02	7.1E-02	5.9E-02	ND
Diffusion Coefficient in Water	cm^2/s	6.3E-06	1.6E-05	9.8E-06	1.2E-05	7.4E-06	9.0E-06	7.5E-06	ND
Degradation Rate -- high end of range	1/day	ND	ND	ND	5.0E-02	ND	1.2E-02	7.0E-01	ND
Degradation Rate -- low end of range	1/day	ND	ND	ND	1.2E-02	ND	1.9E-03	2.7E-02	ND
Uptake Factor for Plants	-	9.00E-01	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	4.00E-02
Toxicity Parameters									
EPA Classification	-	D	ND	D	B2	ND	ND	C	A
Slope Factor Oral	1/(mg/kg-d)	ND	ND	ND	7.5E-03	ND	ND	ND	ND
Slope Factor Inhalation	1/(mg/kg-d)	ND	ND	ND	1.6E-03	ND	ND	ND	8.4E-01
RfD Oral	mg/kg-d	3.0E-04	5.0E-01	6.0E-01	6.0E-02	4.0E-02	ND	2.0E-02	2.0E-02
RfD Inhalation	mg/kg-d	8.6E-05	5.0E-01	2.9E-01	8.6E-01	4.0E-02	8.6E-01	8.6E-04	ND
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.01
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	1.7E-03	3.5E-04	5.0E-03	4.5E-03	1.8E-01	3.1E-03	6.9E-02	1.0E-03
Maximum Contaminant Levels in Groundwater									
MCL (Maximum Contaminant Level)	mg/l	2.0E-03	ND	ND	5.0E-03	ND	2.0E-02	ND	1.0E-01

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Nitrobenzene**	**PCBs**	**Phenanthrene**	**Phenol**	**Pyrene**	**Pyridine**	**Selenium**	**Silver**
CAS Number	-	98-95-3	1336-36-3	85-01-8	108-95-2	129-00-0	110-86-1	7782-49-2	7440-22-4
Molecular Weight	g/mol	123.1	225.1	178.2	94.1	202.3	79.1	79.0	107.9
Density	g/cm^3	1.20	1.10	1.18	1.07	1.27	0.98	ND	ND
Vapor Pressure	mmHg	2.5E-01	8.0E-05	1.1E-04	3.5E-01	2.5E-06	2.0E+01	0.0E+00	0.0E+00
Solubility	mg/L	2.09E+03	4.20E-01	1.29E+00	8.28E+04	1.35E-01	1.00E+06	ND	ND
Henry's Law Constant (no NDs)	-	9.84E-04	1.11E-02	1.60E-03	1.63E-05	4.51E-04	4.51E-04	0.00E+00	0.00E+00
Koc (for organics -- ND for inorganics)	ml/g	6.5E+01	3.1E+05	2.3E+04	2.9E+01	1.1E+05	5.4E+01	ND	ND
Kd (partition coefficient for inorganics)	ml/g	ND	ND	ND	ND	ND	ND	4.3E+00	1.3E+01
log Kow -- Octanol/Water Partition Coefficient	L/kg	1.8E+00	5.7E+00	4.6E+00	1.5E+00	5.1E+00	6.5E-01	ND	ND
Diffusion Coeff. in Air	cm^2/s	7.6E-02	1.0E-01	5.2E-02	8.2E-02	2.7E-02	9.1E-02	ND	ND
Diffusion Coefficient in Water	cm^2/s	8.6E-05	1.0E-05	5.9E-06	9.1E-06	7.2E-06	7.6E-06	ND	ND
Degradation Rate -- high end of range	1/day	ND	ND	2.2E-02	ND	1.7E-03	ND	ND	ND
Degradation Rate -- low end of range	1/day	ND	ND	2.0E-03	ND	1.8E-04	ND	ND	ND
Uptake Factor for Plants	-	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	2.50E-02	4.00E-01
Toxicity Parameters									
EPA Classification	-	D	B2	D	D	D	ND	D	D
Slope Factor Oral	1/(mg/kg-d)	ND	2.0E+00	ND	ND	ND	ND	ND	ND
Slope Factor Inhalation	1/(mg/kg-d)	ND	2.0E+00	ND	ND	ND	ND	ND	ND
RfD Oral	mg/kg-d	5.0E-04	ND	ND	6.0E-01	3.0E-02	1.0E-03	5.0E-03	5.0E-03
RfD Inhalation	mg/kg-d	5.7E-04	ND	ND	6.0E-01	3.0E-02	1.0E-03	ND	ND
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.14	0.1	0.1	0.1	0.1	0.01	0.01
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	7.0E-03	1.3E+00	2.7E-01	5.5E-03	3.2E-01	1.8E-03	1.0E-03	6.0E-04
Maximum Contaminant Levels in Groundwater									
MCL (Maximum Contaminant Level)	mg/l	ND	5.0E-04	ND	ND	ND	ND	5.0E-02	1.0E-01

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**Styrene**	**Tetrachloro ethane (1,1,2,2)**	**Tetrachloro ethylene (PCE)**	**Tetraethyl Lead**	**Toluene**	**TPH Aliphatic C5-6**	**TPH Aliphatic C6-8**	**TPH Aliphatic C8-10**
CAS Number	-	100-42-5	79-34-5	127-18-4	78-00-2	108-88-3	NA	NA	NA
Molecular Weight	g/mol	104.2	167.9	165.8	323	92.1	81	100	130
Density	g/cm^3	0.90	1.60	1.63	1.66	0.87	0.64	0.68	0.72
Vapor Pressure	mmHg	6.4E+00	4.6E+00	1.9E+01	3.0E+01	2.8E+01	2.7E+02	4.8E+01	4.8E+00
Solubility	mg/L	3.10E+02	2.97E+03	2.00E+02	2.10E-01	5.26E+02	3.60E+01	5.40E+00	4.30E-01
Henry's Law Constant (no NDs)	-	1.13E-01	1.41E-02	7.54E-01	2.33E+01	2.72E-01	3.40E+01	5.10E+01	8.20E+01
Koc (for organics -- ND for inorganics)	ml/g	7.8E+02	9.3E+01	1.6E+02	4.9E+03	1.8E+02	7.9E+02	4.0E+03	3.2E+04
Kd (partition coefficient for inorganics)	ml/g	ND	ND	ND	ND	ND	ND	ND	ND
log Kow -- Octanol/Water Partition Coefficient	L/kg	2.9E+00	2.4E+00	2.7E+00	4.9E+00	2.8E+00	3.3E+00	4.0E+00	4.8E+00
Diffusion Coeff. in Air	cm^2/s	7.1E-02	7.1E-02	7.2E-02	5.7E-02	8.7E-02	1.0E-01	1.0E-01	1.0E-01
Diffusion Coefficient in Water	cm^2/s	8.0E-06	7.9E-06	8.2E-06	6.4E-06	8.6E-06	1.0E-05	1.0E-05	1.0E-05
Degradation Rate -- high end of range	1/day	2.5E-02	1.6E+00	1.9E-03	ND	1.0E-01	ND	ND	ND
Degradation Rate -- low end of range	1/day	3.0E-03	1.5E-02	9.6E-04	ND	2.5E-02	ND	ND	ND
Uptake Factor for Plants	-	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow
Toxicity Parameters									
EPA Classification	-	ND	C	B2	ND	D	D	D	D
Slope Factor Oral	1/(mg/kg-d)	ND	2.0E-01	5.2E-02	ND	ND	ND	ND	ND
Slope Factor Inhalation	1/(mg/kg-d)	ND	2.0E-01	2.0E-03	ND	ND	ND	ND	ND
RfD Oral	mg/kg-d	2.0E-01	6.0E-02	1.0E-02	1.0E-07	2.0E-01	5.0E+00	5.0E+00	1.0E-01
RfD Inhalation	mg/kg-d	2.9E-01	6.0E-02	1.1E-01	ND	1.1E-01	5.0E+00	5.0E+00	2.7E-01
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	5.5E-02	9.0E-03	4.8E-02	3.6E-02	4.5E-02	1.4E-01	3.0E-01	7.5E-01
Maximum Contaminant Levels in Groundwater									
MCL (Maximum Contaminant Level)	mg/l	1.0E-01	ND	5.0E-03	1.5E-02	1.0E+00	ND	ND	ND

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**TPH Aliphatic C10-12**	**TPH Aliphatic C12-16**	**TPH Aliphatic C16-35**	**TPH Aromatic C5-7**	**TPH Aromatic C7-8**	**TPH Aromatic C8-10**	**TPH Aromatic C10-12**	**TPH Aromatic C12-16**	**TPH Aromatic C16-21**
CAS Number	-	NA	NA	NA	NA	NA	NA	NA	NA	NA
Molecular Weight	g/mol	160	200	270	78	92	120	130	150	190
Density	g/cm^3	0.74	0.76	0.79	0.88	0.87	0.88	0.88	1.00	1.10
Vapor Pressure	mmHg	4.9E-01	3.6E-02	5.8E-03	9.9E+01	2.9E+01	4.8E+00	4.8E-01	3.6E-02	5.8E-03
Solubility	mg/L	3.40E-02	7.60E-04	1.30E-06	1.80E+03	5.20E+02	6.50E+01	2.50E+01	5.80E+00	5.10E-01
Henry's Law Constant (no NDs)	-	1.30E+02	5.40E+02	6.40E+03	2.30E-01	2.70E-01	4.90E-01	1.40E-01	5.40E-02	1.30E-02
Koc (for organics -- ND for inorganics)	ml/g	2.5E+05	5.0E+06	1.0E+09	7.9E+01	2.5E+02	1.6E+03	2.5E+03	5.0E+03	1.6E+04
Kd (partition coefficient for inorganics)	ml/g	ND	ND	ND	ND	ND	ND	ND	ND	ND
log Kow -- Octanol/Water Partition Coefficient	L/kg	5.6E+00	6.8E+00	8.9E+00	2.1E+00	2.5E+00	3.1E+00	3.5E+00	3.9E+00	4.7E+00
Diffusion Coeff. in Air	cm^2/s	1.0E-01	1.0E-01	1.0E-01	1.0E-01	1.0E-01	1.0E-01	1.0E-01	1.0E-01	1.0E-01
Diffusion Coefficient in Water	cm^2/s	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05	1.0E-05
Degradation Rate -- high end of range	1/day	ND	ND	ND	ND	ND	ND	ND	ND	ND
Degradation Rate -- low end of range	1/day	ND	ND	ND	ND	ND	ND	ND	ND	ND
Uptake Factor for Plants	-	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow	Use Kow
Toxicity Parameters										
EPA Classification	-	D	D	D	D	D	D	D	D	D
Slope Factor Oral	1/(mg/kg-d)	ND	ND	ND	ND	ND	ND	ND	ND	ND
Slope Factor Inhalation	1/(mg/kg-d)	ND	ND	ND	ND	ND	ND	ND	ND	ND
RfD Oral	mg/kg-d	1.0E-01	1.0E-01	2.0E+00	2.0E-01	2.0E-01	4.0E-02	4.0E-02	4.0E-02	3.0E-02
RfD Inhalation	mg/kg-d	2.7E-01	2.7E-01	ND	1.1E-01	1.1E-01	5.5E-02	5.5E-02	5.5E-02	ND
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	1.9E+00	8.2E+00	9.2E+01	1.8E-02	2.9E-02	6.0E-02	8.7E-02	1.4E-01	3.0E-01
Maximum Contaminant Levels in Groundwater										
MCL (Maximum Contaminant Level)	mg/l	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table 11-1. Chemical Properties Database in RISC

Chemical Parameters	**Units**	**TPH Aromatic C21-35**	**Trichloro ethane (1,1,1)**	**Trichloro ethane (1,1,2)**	**Trichloro ethylene (TCE)**	**Vanadium**	**Vinyl Chloride**	**Xylenes**	**Zinc**
CAS Number	-	NA	71-55-6	79-00-5	79-01-6	7440-62-2	75-01-4	1330-20-7	7440-66-6
Molecular Weight	g/mol	240	133.4	133.4	131.4	50.9	62.5	106.2	65.38
Density	g/cm^3	1.20	1.35	1.35	1.46	ND	0.91	0.87	ND
Vapor Pressure	mmHg	3.3E-06	1.2E+02	2.3E+01	6.9E+01	0.0E+00	3.0E+03	8.8E+00	0.0E+00
Solubility	mg/L	6.60E-03	1.33E+03	4.42E+03	1.10E+03	ND	2.76E+03	1.98E+02	ND
Henry's Law Constant (no NDs)	-	6.80E-04	7.05E-01	3.74E-02	4.22E-01	0.00E+00	1.11E+00	2.90E-01	0.00E+00
Koc (for organics -- ND for inorganics)	ml/g	1.3E+05	1.1E+02	5.0E+01	1.7E+02	ND	1.9E+01	2.4E+02	ND
Kd (partition coefficient for inorganics)	ml/g	ND	ND	ND	ND	1.0E+03	ND	ND	7.5E+01
log Kow -- Octanol/Water Partition Coefficient	L/kg	6.1E+00	2.5E+00	2.1E+00	2.7E+00	0.0E+00	1.5E+00	3.3E+00	0.0E+00
Diffusion Coeff. in Air	cm^2/s	1.0E-01	7.8E-02	7.8E-02	7.9E-02	ND	1.1E-01	7.2E-02	ND
Diffusion Coefficient in Water	cm^2/s	1.0E-05	8.8E-06	8.8E-06	9.1E-06	ND	1.2E-06	8.5E-06	ND
Degradation Rate -- high end of range	1/day	ND	5.0E-03	5.1E-03	2.2E-03	ND	1.2E-02	5.0E-02	ND
Degradation Rate -- low end of range	1/day	ND	1.3E-03	9.5E-04	4.0E-04	ND	2.4E-04	1.9E-03	ND
Uptake Factor for Plants	-	Use Kow	Use Kow	Use Kow	Use Kow	5.50E-03	Use Kow	Use Kow	1.50E+00
Toxicity Parameters									
EPA Classification	-	D	D	C	B2	ND	A	D	D
Slope Factor Oral	1/(mg/kg-d)	ND	ND	5.7E-02	1.1E-02	ND	1.5E+00	ND	ND
Slope Factor Inhalation	1/(mg/kg-d)	ND	ND	5.6E-02	6.0E-03	ND	3.1E-02	ND	ND
RfD Oral	mg/kg-d	1.0E+00	3.5E-02	4.0E-03	6.0E-03	7.0E-03	3.0E-03	2.0E+00	3.0E-01
RfD Inhalation	mg/kg-d	ND	2.9E-01	4.0E-03	6.0E-03	ND	2.9E-02	2.0E-01	ND
Absorption Adjustment Factor: Oral-Soil	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Oral-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Dermal-Soil	-	0.1	0.1	0.1	0.1	0.01	0.1	0.1	0.01
Absorption Adjustment Factor: Dermal-Water	-	1	1	1	1	1	1	1	1
Absorption Adjustment Factor: Inhalation	-	1	1	1	1	1	1	1	1
Skin Permeability Coefficient	cm/hr	1.5E+00	1.7E-02	8.4E-03	2.3E-01	1.0E-03	7.3E-03	8.0E-02	6.0E-04
Maximum Contaminant Levels in Groundwater									
MCL (Maximum Contaminant Level)	mg/l	ND	2.0E-01	5.0E-03	5.0E-03	ND	2.0E-03	1.0E+01	ND

Chapter 12.0

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USEFUL WEB PAGES

U.S. EPA Risk Based Decision Management home page:
http://www.epa.gov/swerust1/rbdm/rbdmlnks.htm

U.S. EPA New Exposure Factors Handbook:
http://www.epa.gov/ncea/exposfac.htm

U.S. EPA Integrated Risk Information System (IRIS):
http://www.epa.gov/iris/

U.S. EPA Region 9 Preliminary Remediation Goals (PRGs) [source of default values for slope factors, reference doses, and dermal absorption adjustment factors]:
http://www.epa.gov/region09/waste/sfund/prg/intro.htm

Association for the Environmental Health of Soils:
http://www.aehs.com

TPH Criteria Working Group document on calculating site-specific TPH risk-based screening levels:
www.aehs.com/publications/catalog/contents/Volume5.pdf

Texas Risk Reduction Rules
http://www.tnrcc.state.tx.us/oprd/rules/indxpdf5.html

Guidance documents for calculating clean-up levels for TPH mixtures search from (document number #366 or RG-366/TRRP-27):
http://www.tnrcc.state.tx.us/permitting/trrp.htm

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Vadose Zone Model

A.1 MODEL DESCRIPTION

The Vadose Zone model in RISC simulates contaminant transport through unsaturated soil. The transport equations are solved using the analytical solutions of the one-dimensional advective-dispersive solute transport equation (van Genuchten and Alves, 1982). The model considers the following fate and transport processes: (i) a well-mixed finite-mass source zone, (ii) pseudo steady-state volatilization and diffusive vapor transport from the source to ground surface, (iii) leaching from the source zone, (iv) advective dissolved-phase transport, (v) dissolved-phase dispersion, (vi) adsorption, and vii) first-order decay in the leachate.

This model is similar to the vadose zone model presented by Unlü et al. (1992) with the exception of several significant differences that are discussed. The most significant change is that the Vadose Zone transport model in RISC allows for the presence of a second soil layer located between the source zone and the ground surface; this layer may have soil properties different from the rest of the vadose zone which can dramatically affect vapor emissions to the surface.

The purpose of the Vadose Zone model is to predict (1) loading to groundwater and (2) volatilization losses. The groundwater loading term may be used as a source input to the saturated zone model (Appendix B). The volatilization losses may be used as a source for the box air model to calculate concentrations in outdoor air (Appendix F). Figure A-1 shows the processes simulated by the Vadose Zone model.

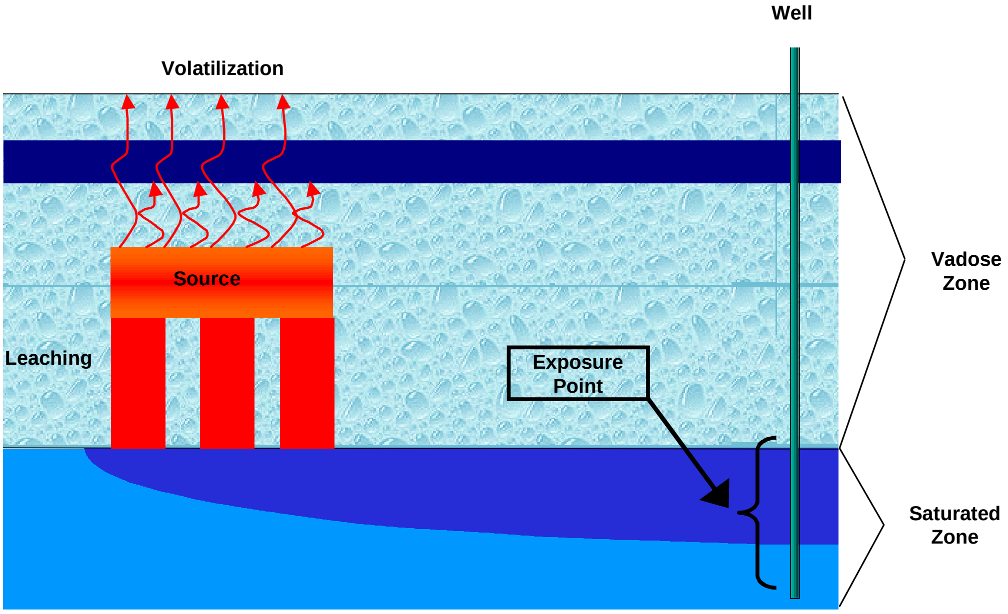

FIGURE A-1. Schematic of the Vadose Zone Model.

This appendix describes the equations used to predict volatile losses from a vadose zone source, leaching/mass loading rates from the source to groundwater and concentration distributions in the vadose zone. Appendix B describes the model used for the saturated zone (including groundwater transport).

A.2 APPLICATIONS OF THIS MODEL

This is a partial list of the main applications and limitations of the model:

- This model estimates the mass loading to groundwater from a vadose zone source. The model accounts for source depletion due to volatilization and leaching. The volatilization flux is only used to estimate losses from the source; it is not linked with an indoor or outdoor air model.
- This model does not simulate the movement of NAPL (free phase product). It is a dissolved phase-only model. Volatilization losses from the source are accounted for, however, the vapor phase concentrations with depth are not estimated. The volatile losses are assumed to be instantaneous and irreversible.

- Degradation is considered in the dissolved phase for the region between the source and the water table.
- The vadose zone model is automatically linked with the dissolved phase model in RISC so that concentrations in groundwater may be estimated.
- The model accounts for the presence of NAPL by limiting the dissolved phase concentration in the source region to the chemicals' effective solubility limit. This is important for two reasons:
    1. Otherwise the leachate and groundwater concentrations may be greatly over-estimated.
    2. Limiting the leachate concentrations to effective solubility limits may cause the source to deplete at a slower rate, thereby increasing the length of time for loading to groundwater. Depending on the problem being simulated, this approach may be more conservative than ignoring solubility limitations because it increases the exposure duration and hence the estimate of long-term cancer risk.

- The source is assumed to be located in the vadose zone. The region in the vadose zone below the source and the groundwater aquifer itself is assumed to be "clean" at the start of the simulation. This means that the vertical extent of the contamination in the vadose zone must be known. If the groundwater is already contaminated there are several ways to model the situation. Here are two ideas:
    1. Assume that the start of the simulation coincides with the date that the spill occurred ("back it up in time"). Run the model through the present day using the current site information to calibrate the model (e.g. make the model predict the current distribution of contaminants in the soil and groundwater).
    2. Skip the vadose zone portion and model the site with one of the groundwater models. If there is still a large amount of contamination in the vadose zone but the system appears to be at steady-state (i.e. the groundwater concentrations are not increasing with time) then use the dissolved phase model with a constant source.

- It is important to choose the source concentration and size of the source carefully. The best approach is to estimate (roughly) the amount of mass thought to be in the vadose zone. The average concentration multiplied by the source size should not exceed the estimated mass. This seems obvious, however, it is very easy to use an unreasonably large source mass especially if maximum concentrations and the maximum extent of detection are used simultaneously.

- The size of the source in the vadose zone is "mapped" onto the water table and becomes the footprint of the groundwater source size. If the receptor well is close to the source region, it may be more conservative to use a smaller source size and a larger source concentration than to average the concentrations across a large source region. More concentrated (but smaller) sources in the groundwater yield higher concentrations along the centerline of the plume when the receptor point is close to the source region.

A.3 FATE AND TRANSPORT PROCESSES

RISC's vadose zone transport model uses a "compartmental" approach; in other words, different models are used to describe the source zone, the vadose zone above the source, and the vadose zone between the source and groundwater.

The source zone is described as being a well-mixed finite source that depletes with time, while the vadose zone above the source is treated as being one-dimensional and at pseudo-steady state.

Beneath the source zone, solute transport of leachate occurs via advection and dispersion, and mass loss may occur through a first-order degradation reaction. The one-dimensional transport equation (including adsorption) in this zone is given by:

$$R\frac{\partial C_w}{\partial t} = D_x\frac{\partial^2 C_w}{\partial x^2} - \bar{v}\frac{\partial C_w}{\partial x} - \mu C_w \tag{A-1}$$

where

C_w = dissolved phase concentration of chemical [mg/L]

D_x = dispersion coefficient in the unsaturated zone [cm^2/d]

$\bar{v}$ = seepage velocity (or interstitial velocity) [cm/d]

μ = first-order decay coefficient for chemical [1/d]

x = distance below the source (measured positively downward) [cm]

t = time [d]

R = retardation factor (defined in Equation A-31) [-]

The x-axis is assumed to be aligned with the direction of fluid flow; in the vadose zone that direction is vertically downward. The model considers dispersion in the downward direction only (longitudinal dispersion). The advection-dispersion equation is used to solve for aqueous-phase concentration with depth below the source. This concentration at the water table will be used with the infiltration rate to estimate mass loading to groundwater.

A note on nomenclature: In this appendix the variable, C (C_w, C_v, or C_T), will always refer to the concentration of the individual chemical being modeled (not the TPH mixture). If the concentration of TPH is being referenced, the variable C_{TPH} will be used. The same applies to all chemical properties. For example, D_{eff} refers to the chemical-specific diffusion coefficient, MW refers to the chemical-specific molecular weight, and MW_{TPH} refers to the molecular weight of the TPH mixture.

A.3.1 Initial and Boundary Conditions

Below the source it is assumed that concentrations are zero at time = 0:

$$C_w(x, 0) = 0 \tag{A-2}$$

The leachate concentration leaving the source zone is assumed to decay exponentially with time

$$C_w(0,t) = C_{w_0} e^{-\beta t} \tag{A-3}$$

where

C_{wo} = dissolved phase concentration of chemical in the source at the beginning of the simulation [mg/L]

β, = source depletion term [-]

The source depletion term, β, is described in equations A-19 and A-23. At a "long distance" below the source the concentration gradient is always zero.

$$\frac{\partial C_w}{\partial x}(\infty, t) = 0 \qquad \textbf{(A-4)}$$

The solution for the advection-dispersion equation (A-1) with the above boundary conditions is given by van Genuchten and Alves (1982)

$$C_w(x,t) = C_0 e^{-\beta t} B(x,t) \qquad \textbf{(A-5)}$$

where

$$B(x,t) = \frac{1}{2}\exp\left[\frac{(\bar{v}-w)x}{2D_x}\right] erfc\left[\frac{Rx - wt}{2\sqrt{D_x Rt}}\right] + \frac{1}{2}\exp\left[\frac{(\bar{v}+w)x}{2D_x}\right] erfc\left[\frac{Rx + wt}{2\sqrt{D_x Rt}}\right]$$

(A-6)

and

$$w = \bar{v}\sqrt{1 + \frac{4D_x}{\bar{v}^2}\left[\mu - R\beta\right]} \qquad \textbf{(A-7)}$$

where

$C_w(x,t)$ = dissolved phase concentration of chemical at distance x (in cm) below the source and time (in days) [mg/L]

β = source zone depletion coefficient (loss term) defined in equations A-19 and A-23 [-]

In order to solve the above set of equations, the first-order source decay rate must be determined.

A.4 SOURCE TERM

Depletion of the source is assumed to occur due to volatilization and leaching losses. Note that the source is not assumed to undergo microbial decay, or biodegradation, on the assumption that high soil concentrations are toxic to the microorganisms. In terms of a molar balance this can be written as

$$\frac{dm}{dt} = -\frac{J_w}{MW} - \frac{J_v}{MW} \tag{A-8}$$

where

m = number of moles of chemical per unit area in the hydrocarbon source [moles/cm^2]

MW = molecular weight of chemical [g/mol]

J_w = rate of mass depletion per area due to percolating water [g/cm^2/d]

J_v = rate of mass depletion per area due to volatilization [g/cm^2/d]

t = time [d]

A.4.1 Aqueous Losses

The leaching loss is assumed to be purely advective (due to water percolating through the source)

$$J_w = qC_{ws}\left(\frac{L}{1000cm^3}\right)\cdot\left(\frac{g}{1000mg}\right) \tag{A-9}$$

where

J_w = rate of mass depletion per area due to percolating water [g/cm^2/d]

q = net recharge or infiltration rate [cm/d]

C_{ws} = dissolved phase concentration in the source [mg/L]

In the RISC model, the dissolved phase concentration, C_{ws}, is checked for solubility limitations and therefore is calculated differently depending on whether or not residual phase hydrocarbon (NAPL) is present (see Sections A.4.5 through A.4.7). (Unlü et al., 1992, assumes that the source always contains immiscible phase hydrocarbons.)

A.4.2 Volatilization Losses (Incorporating Lens)

The diffusive vapor loss is estimated using Fick's Law, assuming a linear concentration drop from the source area to the soil surface. Source zone volatilization losses are calculated using a pseudo-steady state vapor flux model based on Fick’s Law. In this approach, the steady-state solution for vapor transport is coupled with a source zone concentration that is changing with time. It is assumed that vapor transport reaches steady conditions much faster than the rate at which the source zone concentration changes with time. It is also assumed that vapor concentrations at ground surface are much less than those at the source zone. The mass depletion rate of the source due to volatilization (the volatile losses) is calculated from:

$$J_v = D_{eff} \frac{C_{vs}}{L_d}\left(\frac{86400s}{d}\right) \tag{A-10}$$

where

J_v = rate of mass depletion per area due to volatilization $[\mathrm{g/cm^2/d}]$

D_{eff} = effective diffusion coefficient in soil $[\mathrm{cm^2/s}]$

C_{vs} = vapor-phase concentration of chemical in the source area [g chemical/$\mathrm{cm^3}$ vapor]

L_d = diffusion path length [cm]

Equation A-10 is Fick's Law applied to the concentration gradient from the source to the ground surface. The concentration of chemical in vapor at the soil surface is assumed to be equal to zero (or very small compared to the source vapor phase concentration). The diffusion path length is assumed to be equal to the distance from the soil surface to the center of the source.

The vapor concentration in the source zone is calculated from Henry's Law:

$$C_{vs} = K_H C_{ws} \left(\frac{L}{1000cm^3} \right) \left(\frac{g}{1000mg} \right) \qquad \textbf{(A-11)}$$

where

K_H = Henry’s Law Constant for chemical [(mg/l vapor)/(mg/l water)]

A.4.3 Effective Diffusion Coefficients

The effective diffusion coefficient in vadose zone soil and the lens soil is estimated using the Millington-Quirk relationships:

$$D_{eff\ v} = D_{air} \left(\frac{\theta_{a_v}^{\ 10/3}}{\theta_{T\ v}^{\ 2}} \right) + D_{water} \frac{1}{K_H} \left(\frac{\theta_{W\ v}^{\ 10/3}}{\theta_{T\ v}^{\ 2}} \right) \qquad \textbf{(A-12a)}$$

$$D_{eff\ lens} = D_{air} \left(\frac{\theta_{a\ lens}^{\ 10/3}}{\theta_{T\ lens}^{\ 2}} \right) + D_{water} \frac{1}{K_H} \left(\frac{\theta_{W\ lens}^{\ 10/3}}{\theta_{T\ lens}^{\ 2}} \right) \qquad \textbf{(A-12b)}$$

where

$D_{eff\ v}$ = effective diffusion coefficient for the vadose zone above the source (not including the lens) [cm^2/s]

$D_{eff\ lens}$ = effective diffusion coefficient for the lens [cm^2/s]

D_{air} = molecular diffusion coefficient for chemical in air [cm^2/s]

D_{water} = molecular diffusion coefficient for chemical in water [cm^2/s]

θ_{a_v} = air-filled porosity in the vadose zone [cm^3 air/cm^3 soil]

θ_{w_v} = water-filled porosity in the vadose zone [cm^3 water/cm^3 soil]

$\theta_{T\ v}$ = total porosity in the vadose zone [cm^3 pores/cm^3 soil]

$\theta_{a\ lens}$ = air-filled porosity in the lens [cm^3 air/cm^3 soil]

$\theta_{w\,lens}$ = water-filled porosity in the lens [cm^3 water/cm^3 soil]

$\theta_{T\,lens}$ = total porosity in the lens [cm^3 pores/cm^3 soil]

K_H = Henry's Law Constant for chemical [(mg/l vapor)/(mg/l water)]

Note, the above porosity terms used by the diffusion equations should be total porosity rather than effective porosity. The total effective diffusion coefficient for the vadose zone and lens combined is estimated as the depth-weighted average (Johnson and Ettinger, 1995):

$$D_{eff} = \frac{\left(h_v + h_{lens}\right)}{\dfrac{h_{lens}}{D_{eff\ lens}} + \dfrac{h_v}{D_{eff\ v}}} \qquad \textbf{(A-13)}$$

where

D_{eff} = depth-weighted average effective diffusion coefficient for the vadose zone in between the source and the soil surface [cm^2/s]

h_v = thickness of the vadose zone above the source (minus the lens thickness) [cm]

h_{lens} = thickness of the lens [cm]

As a consequence of the modeling assumptions, one can actually account for more than one lens above the source zone, as long as each lens has the same material properties (total porosity, moisture content, etc.). If this is the case, then the user simply sets h_{lens} equal to the combined thickness of all the lenses and h_v is the remaining thickness of the vadose zone.

A.4.4 Overall Source Depletion Rate

Combining equations A-8 through A-11 yields:

$$\frac{dm}{dt} = -\beta m = -\left[\bar{v}\,\theta_w + \frac{K_H D_{eff}}{L_d}\right] C_w \qquad \textbf{(A-14)}$$

where β is a loss term accounting for both dissolution and volatile losses. The loss term is calculated differently depending on whether or not residual phase is present.

A.4.5 Calculating Whether or Not Residual Phase Hydrocarbon is Present

To determine if residual phase hydrocarbon is present, the following condition for multiple chemicals must be met:

$$1 > \sum_{i=1}^{N} \frac{C_{T_i} \rho_b}{S_i \left(\rho_b K_{oc_i} F_{oc} + \theta_w + \theta_a K_{H_i}\right)} \qquad \textbf{(A-15)}$$

where

N = total number of chemicals in mixture

$C_{T\,i}$ = total concentration of chemical *i* in soil [mg/kg]

S_i = liquid phase solubility for chemical *i* [mg/l or kg/m^3]

ρ_b = soil bulk density of the source area [g/cm^3]

F_{oc} = fraction organic carbon in soil [g oc/g soil]

$K_{oc\,i}$ = organic carbon partition coefficient for chemical *i* [ml/g]

$K_{H\,i}$ = Henry's Law Constant for chemical *i* [(mg/l vapor)/(mg/l water)]

This partitioning equation assumes that the total soil concentration for each chemical, $C_{T\,i}$, can be accounted for by summing the mass in the solid, liquid, and vapor phases (i.e. no residual is present). However, equation A-15 requires that all of the chemicals in the mixture are accounted for in the sum. In risk assessments, more often the number of chemicals of concern (and characterized with respect to their concentration) is a small subset of the total number of chemicals present in the mixture. The vadose zone model checks the following equation for each chemical used in the model

$$C_w = \frac{C_T \rho_b}{\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H} \qquad \textbf{(A-16)}$$

Again, it is assumed that C_T can be accounted for by summing the mass in the solid, liquid, and vapor phases (i.e. no residual is present). If the liquid phase concentration, C_W, calculated with equation A-15a exceeds the effective solubility of the compound, then it is assumed that residual phase is present (and equation A-15a does not apply).

A.4.6 Source -- When Residual Phase Hydrocarbon is Present

If there is residual phase hydrocarbon present in the source, the aqueous concentration, C_w, will be calculated from

$$C_w = xS \tag{A-17}$$

where

S = aqueous solubility of pure component [mg/l or kg/m^3]

x = mole fraction of component in the hydrocarbon mixture [mol/mol]

The mole fraction is calculated from

$$x = \frac{m}{m_{TPH}} \tag{A-18}$$

$$x = \frac{F_i MW_{TPH}}{MW_i F_{TPH}} \tag{A-19}$$

where

m = total moles of component [mol] $\left(\frac{\rho_b L_w F_i}{MW_i} A\right)$

m_{TPH} = total moles of hydrocarbon mixture [mol] $\left(\frac{\rho_b L_w F_{TPH}}{MW_{TPH}} \mathrm{A}\right)$

L_w = thickness of the source area [cm]

A = area (plan view) of the source [cm^2]

MW_{TPH} = average molecular weight of hydrocarbon [g/mol]

MWi = average molecular weight of component *i* [g/mol]

F_{TPH} = mass fraction (concentration) of hydrocarbon mixture in the soil source [TPH concentration) [g/g]

F_i = mass fraction (concentration) of component *i* in the soil source [component concentration) [g/g]

As long as there is immiscible phase present, the aqueous phase concentration is given by Equation A-16. Once immiscible phase has been depleted, then the remaining amount of each compound is depleted from the source according with the decay rate given in Equation A-22. In the RISC model, however, it is assumed that if immiscible phase is present initially, then it is present for all time, Thus the approximation developed below is for the case of a more soluble compound leaching from a less soluble mixture, (e.g., benzene from a petroleum fuel mixture).

The source zone depletion coefficient (loss term), β, for the residual case is given by

$$\beta = \frac{qMW_{TPH}S}{\rho_b L_w F_{TPH} MW} + \frac{D_{eff} K_H MW_{TPH} S}{\rho_b L_d L_w F_{TPH} MW} = \beta_w + \beta_v \qquad \textbf{(A-20)}$$

The source zone depletion coefficient is the sum of the leachate losses (β_w) and the vapor losses (β_v). If it is assumed that F_{TPH} is constant (this assumption is only approximate since the source does deplete slowly over time) equation A-8 may be solved analytically to obtain

$$m = m_0 \exp(-\beta t) \qquad \textbf{(A-21)}$$

where

m_0 = initial moles of chemical per area [mol/cm^2]

The aqueous concentration decreases similarly

$$C_w = C_{w0} \exp(-\beta t) \qquad \textbf{(A-22)}$$

where

C_{w0} = initial aqueous concentration of species defined in equation A-16 [mg/l]

Unlü et al. (1992) assumes there is always residual phase hydrocarbon present and uses equation A-19 to estimate losses from the source. This approach is realistic for the types of waste zones that Unlü et al. equations were developed for -- waste sludge pits with high levels of hydrocarbons. However, RISC also allows the user to estimate the behavior of sources for which immiscible phase is not initially present (e.g., equation A-15a is satisfied).

A.4.7 Source -- When Residual Phase Hydrocarbon is Not Present

When an immiscible phase is not present it is assumed that the concentrations of the chemical in each phase are in equilibrium. The equilibrium partitioning equation is:

$$C_{ws} = \frac{C_T \rho_b}{\left(\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H\right)} \qquad \textbf{(A-23)}$$

which when inserted into Equation A-14 yields:

$$\beta = \frac{q}{(\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H) L_w} + \frac{D_{eff} K_H}{(\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H) L_d L_w} = \beta_w + \beta_v \qquad \textbf{(A-24)}$$

where all the variables are as defined previously.

A.5 LEACHING AND PERCOLATION RATE

Following Unlü et al. (1992), the RISC Vadose Zone model uses a unit hydraulic gradient approximation, estimating the unsaturated hydraulic conductivity with the Brooks and Corey (1964) model. The unit gradient approach assumes that the pressure (suction) head in the soil profile is constant, as is the moisture content. This is a major simplification of the real processes that control flow in the unsaturated zone. However, the goal in modeling the concentration is to estimate average conditions over long time periods (for purposes of risk assessment: 7 to 30 years). For this objective, the unit gradient approach has been shown to work reasonably well (Unlü et al., 1992).

A.5.1 Unit Gradient Approach

For more information on this subject the reader is referred to the two papers mentioned above as well as Carsel and Parrish (1988). Briefly, Darcy's equation for the unit gradient case may be written as:

$$q = k_r K_{su} \tag{A-25}$$

where

q = infiltration rate or net recharge rate [cm/d]

k_r = relative permeability [unitless]

K_{su} = hydraulic conductivity of the unsaturated zone if it were fully saturated [cm/d]

When using RISC, the user is asked to input the infiltration rate, q, and the unsaturated zone's hydraulic conductivity (K_{su}). This term, K_{su}, is the hydraulic conductivity of the unsaturated zone if it were assumed to be fully saturated, i.e. no air-filled porosity. In many applications of RISC, K_{su} is assumed equal to the hydraulic conductivity of the soil below the water table. If the value entered for the infiltration rate exceeds K_{su}, then q is set to K_{su} assuming that the excess flow will be diverted as runoff.

Having values for q and K_{su}, Equation A-25 is used to solve for the relative permeability, k_r:

$$k_r = \frac{K_{su}}{q} \tag{A-26}$$

where the terms are as defined for Equation A-24.

A.5.2 Estimating the Unsaturated Zone Hydraulic Conductivity

In the unsaturated zone, the hydraulic conductivity varies as a function of the moisture content. It is assumed that this relationship can be described by the Brooks and Corey (1964) model

$$k_r = \left[\frac{\theta_w - \theta_r}{\theta_T - \theta_r}\right]^{\gamma} \tag{A-27}$$

where

θ_T = total porosity in unsaturated zone [-]

θ_w = volumetric water content or water-filled porosity [cm^3 water/cm^3 soil]

θ_r = irreducible water content [cm^3 water/cm^3 soil]

γ = pore size distribution parameter [-]

The pore size distribution parameter is estimated from the van Genuchten *"n"* parameter using the following relationship (Lenhard et al., 1989)

$$\gamma = 3 + \frac{2}{(n-1)(1-0.5^{\frac{n}{(n-1)}})} \tag{A-28}$$

The model requires the user to enter *n*. Carsel and Parrish (1988) have a large database of van Genuchten's *"n"* for various soil types. This database is also available in the RISC software.

A.5.3 Estimating Moisture Content and Seepage Velocity

The water-filled porosity, θ_w, is calculated using Equation A-27 since values of all the other terms are either specified or previously derived. The calculated water-filled porosity is then used to estimate the seepage velocity, $\bar{v}$:

$$\bar{v} = \frac{q}{\theta_w} \qquad \textbf{(A-29)}$$

where

$\bar{v}$ = seepage velocity (actual water flowrate through vadose zone) [cm/d]

q = infiltration rate (recharge rate to groundwater) [cm/d]

θ_w = volumetric water content or water-filled porosity [cm^3 water/cm^3 soil]

The seepage velocity, $\bar{v}$, is the average rate of flow that the model uses for the water percolating through the vadose zone.

The water content for the lens may differ from the vadose zone and is also calculated from the same equations as presented above using the lens properties. The values of the estimated moisture contents are presented in the RISC model output. The moisture content is not calculated by the volatilization models (Appendices D, E, J and K) since it is assumed that for soils under a house or building, the infiltration rate is close to zero. In these models the user is requested to specify the average moisture content in the vadose zone. If the vadose zone is subject to infiltration, the above algorithm may be run using the vadose zone model to estimate likely ranges of moisture content. The moisture content can then be entered in the air models.

A.6 UNSATURATED ZONE TRANSPORT

Equations A-5 through A-7 are used to calculate the dissolved phase concentrations in the unsaturated zone from the bottom of the source zone to the groundwater aquifer.

A.6.1 Mass Loading To Groundwater

The mass flux of contaminant at the water table is calculated using Equation A-5 solved at the water table multiplied by the infiltration rate:

$$Q(L_u,t) = q\ C(L_u,t) \cdot \left(\frac{L}{1000cm^2} \right) \qquad \textbf{(A-30)}$$

where

$Q(L_u,t)$ = mass flux at the water table as a function of time [g/cm^2/d]

$C(L_u,t)$ = dissolved phase concentration of contaminant at the water table as a function of time [mg/L]

L_u = the distance from the source to the water table [cm]

q = net infiltration rate [cm/d]

The mass flux, Q, is used as the time-varying source for the saturated zone model described in Appendix B.

A.6.2 Retardation

The retardation factor for the unsaturated zone, R, is estimated using

$$R = 1 + \frac{\rho_b F_{oc} K_{oc}}{\theta_w} \qquad \textbf{(A-31)}$$

where

F_{oc} = fraction organic carbon in dry soil [g/g]

K_{oc} = organic carbon normalized partition coefficient [ml/g]

This retardation equation is assumed to be valid when $F_{oc} > 0.001$. [Below values of 0.001 the retardation is estimated to be equal to 1 -- essentially non-retarded.)

A.6.3 Degradation

Degradation is assumed to be a first-order reaction occurring only in the aqueous phase as the leachate is carried from the source to the water table.

A.6.4 Dispersion

The dispersion coefficient is assumed to be a linear function of the seepage velocity, $\bar{v}$, (defined in Equation A-27)

$$D = \alpha_L \left(\bar{v} \cdot \frac{m}{100cm} \right) \tag{A-32}$$

where

α_L = longitudinal dispersivity [m]

The longitudinal dispersivity is calculated using data from Gelhar et al. (1985) as a function of the vertical distance from the source:

$$\ln \alpha_L = -4.933 + 3.811 \ln x_m \qquad x_m \leq 2m \tag{A-33a}$$

$$\ln \alpha_L = -2.727 + 0.584 \ln x_m \qquad x_m \geq 2m \tag{A-33b}$$

where

x_m = distance from the source to the observation location [m]

A.7 DATA REQUIREMENTS

The data required to run the Vadose Zone model are shown in Table A-1.

Table A-1. Data Requirements for the Vadose Zone Model

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
MEDIA-SPECIFIC PARAMETERS			
Porosity	cm^3/cm^3	0.01	0.5
Irreducible Water Content	cm^3/cm^3	0	porosity
Fraction Organic Carbon	g oc/g soil	0.001	0.05
Hydraulic Conductivity	m/day	1.00E-07	100
Soil Bulk Density	fraction	1.4	2.2
van Genuchten Parameter	dimensionless	~1	~3
Unsaturated Zone Thickness	m	site-specific	site-specific
SOURCE PARAMETERS			
Length of Source (x-direction)	m	site-specific	site-specific
Width of Source (y-direction)	m	site-specific	site-specific
Thickness of Source (z-direction)	m	site-specific	site-specific
TPH DATA			
Molecular Weight of TPH	g/mol	80	120
Concentration of TPH	mg/kg	site-specific	site-specific
CHEMICAL SPECIFIC DATA (individual chemical component)			
Molecular Weight	g/mol	chem-specific	chem-specific
Source Concentration	mg/kg	site-specific	site-specific
Solubility	mg/l	chem-specific	chem-specific
Diffusion Coefficient in Air	cm^2/s	chem-specific	chem-specific
Diffusion Coefficient in Water	cm^2/s	chem-specific	chem-specific
K_{oc}	ml/g	chem-specific	chem-specific
Degradation Rate	1/d	site-specific	site-specific
Henry's Law Constant	(mg/l)/(mg/l)	chem-specific	chem-specific

A.8 ASSUMPTIONS AND LIMITATIONS OF THE VADOSE ZONE MODEL

1. The Vadose Zone model simulates the transport of dissolved phase contaminants downward, and vapor phase contaminants upward. It does not simulate the movement of non-aqueous phase liquids (NAPLs).

2. The Vadose Zone model is a one-dimensional model (from the source to the water table) and accounts for volatile and leachability losses from the source.

3. The vadose zone is considered to be homogeneous and uniform below the source (a lens may be modeled above the source). The hydraulic conductivity is calculated as a function of moisture content, however, this derived moisture content is assumed to be constant for the entire depth of the soil column.

4. The contaminant source has a uniform concentration across the user-specified source volume.

5. Water table fluctuations are not considered. The depth to the aquifer is considered fixed.

A.9 REFERENCES

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Appendix B

Dissolved-Phase Transport Model

B.1 MODEL DESCRIPTION

The groundwater model in RISC simulates dissolved phase contaminant transport in the groundwater aquifer. This model can be used (i) to predict the concentration in groundwater at a "receptor well", or, (ii) to predict the concentration in groundwater as a source for volatile emissions into a building (see Appendix E). It is appropriate to use this model either when soils data is lacking, or when the groundwater at the source is already impacted and it is not necessary to model the soil-to-groundwater pathway. To run the model, the user defines the source by specifying a dissolved-phase source concentration, the pulse length (which simulates how long the source is active), and the volume of the source. Figure B-1 shows a schematic of the dissolved phase groundwater model and the processes simulated.

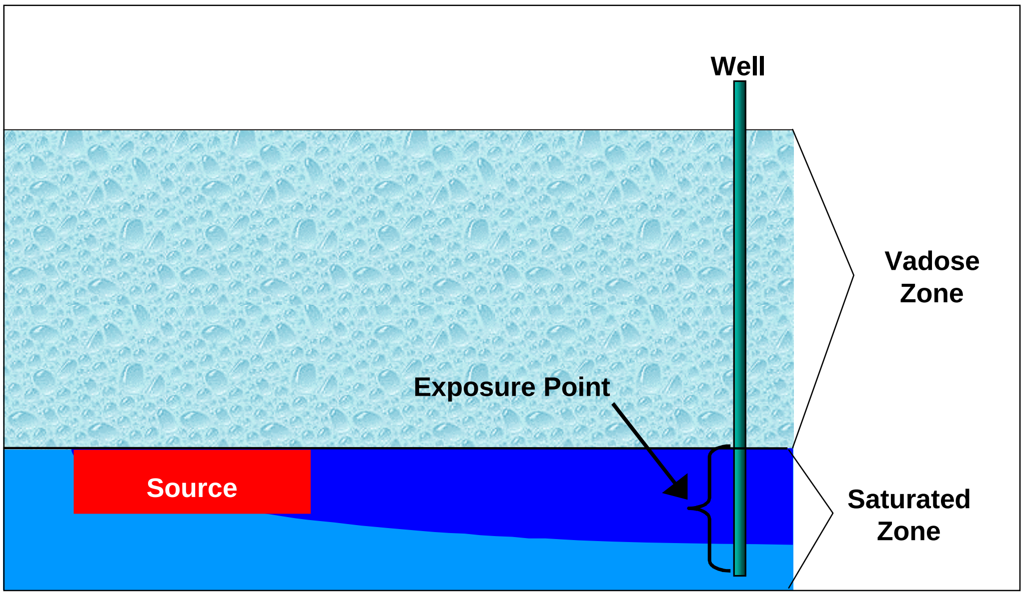

FIGURE B-1. Saturated Zone Model with Source in Groundwater

B.2 TRANSPORT EQUATIONS AND PROCESSES

The model considers the following fate and transport processes:

- one-dimensional flow
- three-dimensional dispersion
- retardation (adsorption)
- degradation.

This model is identical to the AT123D code (Yeh, 1981) with the exception of allowing the user to input a source concentration rather than a mass loading. (The model in RISC automatically calculates the mass loading from the source concentration input.) The three-dimensional dispersion equation for a uniform flow field is given by:

$$R\frac{\partial C_w}{\partial t} = D_x\frac{\partial^2 C_w}{\partial x^2} + D_y\frac{\partial^2 C_w}{\partial y^2} + D_z\frac{\partial^2 C_w}{\partial z^2} - \bar{v}\frac{\partial C_w}{\partial x} - \mu C_w + \frac{\dot{M}}{\theta} \qquad \textbf{(B-1)}$$

where

C_w = concentration of component in the aqueous phase ([g/l or g/m^3]

x = distance in the direction of groundwater flow [m]

y = cross-gradient distance (from centerline of plume) [m]

z = vertical distance positive downwards from water table [m]

D_x = dispersion coefficient in the direction of groundwater flow [m^2/d]

D_y = transverse dispersion coefficient [m^2/d]

D_z = vertical dispersion coefficient [m^2/d]

$\bar{v}$ = seepage velocity [m/d]

μ = first-order decay coefficient for chemical [1/d]

t = time [d]

R = retardation factor [-]

$\dot{M}$ = source term [mass flux) for chemical [g/d/m^3]

θ = porosity (effective) of the saturated zone [cm^3/cm^3]

The source term, $\dot{M}$, is non-zero over a finite rectangular area at the water table and zero elsewhere. When the model is run, the user must specify the length, width and thickness of the source. The length of the source is in the direction of groundwater flow.

The aquifer is considered to be infinite in depth and width. The source term may be a constant concentration specified for a certain duration ("pulse") or it may vary with time. The length of the pulse is tantamount to specifying how long the source is active (i.e., the duration between the spill event and the point in time when either the source is removed or is naturally depleted).

B.2.1 Initial and Boundary Conditions

At the beginning of the simulation, the aquifer is assumed to have a concentration of zero everywhere. The mass loading is assumed to occur uniformly over the volume of the source. The model simulates dissolved phase transport only so the contaminant mass is assumed to be instantly dissolved and mixed uniformly over the source volume. The concentration at a great distance away from the source is assumed to be zero for all times. The advection-dispersion equation (B-1) is solved using Green's functions for the conditions described (Galya, 1987).

B.2.2 Retardation Coefficient

Retardation describes a contaminants movement relative to the bulk movement of groundwater flow. The retardation factor, R, is estimated using

$$R = 1 + \frac{\rho_b F_{oc} K_{oc}}{\theta} \qquad \text{for organic chemicals} \qquad \textbf{(B-2a)}$$

$$R = 1 + \frac{\rho_b K_d}{\theta} \qquad \text{for inorganic chemicals} \qquad \textbf{(B-2b)}$$

where

F_{oc} = fraction organic carbon in dry soil [g oc/g soil]

K_{oc} = organic carbon normalized partition coefficient [ml/g or m^3/kg]

K_d = inorganic distribution coefficient [ml/g]

ρ_b = soil bulk density of the saturated zone [g/cm^3]

θ = porosity (effective) of the saturated zone [cm^3/cm^3]

If a non-zero value for K_d is entered in the RISC chemical database, the code uses equation B-2b. For organic chemicals that do not have K_d values the code assumes that the only process causing retardation is the sorption of the chemical due to the presence of organic carbon in the aquifer. In this situation, the quantity $K_{oc}*F_{oc}$ is used to estimate the distribution coefficient (K_d). In reality there may be several processes (such as the presence of silts and clays) contributing to the retardation (or sorption) of the chemical. The equations in RISC (and most fate and transport models) assume that the retardation can be completely predicted using the relationship in Equation B-2a. This will usually under-predict the amount of sorption (and hence retardation) that is actually occurring. Usually this will be conservative for purposes of estimating risk. If it appears that there may be much more retardation occurring than what the site-specific measured value of F_{oc} would indicate (usually the case for low F_{oc} soils), the actual partitioning may be measured in a lab and then the measured K_d value could be entered for the chemical being modeled.

This retardation equation assumes that sorption and desorption processes are instantaneous and fully reversible. See Chapter 11 (the chemical database) for equations for estimating K_{oc} from other chemical parameters.

B.2.3 Dispersion Coefficients

The dispersion coefficients in equation B-1 are calculated using the following relationships

$$D_x = \frac{\alpha_x V}{\theta},\ D_y = \frac{\alpha_y V}{\theta},\ D_z = \frac{\alpha_z V}{\theta} \qquad \textbf{(B-3)}$$

where

α_x , α_y, α_z = dispersivity in x, y, and z directions [m] (longitudinal, transverse and vertical dispersivities)

V = Darcy velocity [m/d]

The Darcy velocity is defined as follows

$$V = K\,i \qquad \textbf{(B-4)}$$

where

K = saturated zone conductivity [m/d]

i = hydraulic gradient [m/m]

The seepage groundwater flow velocity, $\bar{v}$, is calculated from the Darcy velocity

$$\bar{v} = \frac{V}{\theta} \qquad \textbf{(B-5)}$$

where the variables are as defined previously.

The dispersivities can be calculated by the model or the user may enter values. If the code calculates the dispersivities, the longitudinal dispersivity (α_x) is calculated from

$$\ln \alpha_x = -3.795 + 1.774 \ln x - 0.093\ (\ln x)^2 \qquad \textbf{(B-6)}$$

where x is the distance downgradient *(m)* from the source to the receptor well (Gelhar et al., 1985). Equation B-6 is different from the equation used to calculate dispersivity in the Vadose Zone model (equation A-32) where the dispersivity in the vertical direction (the direction of groundwater flow) is being calculated. In equation B-5, the dispersivity is calculated in the horizontal direction. Both these equations are based on empirical data and not derived from mathematical "first principles".

From an American Petroleum Institute's report (1987), the transverse and vertical dispersivities are assumed to be related to the longitudinal dispersivity as follows:

$$\alpha_y = \frac{\alpha_x}{\tau_1}, \qquad \alpha_z = \frac{\alpha_y}{\tau_2} \qquad \textbf{(B-7)}$$

where τ_1 and τ_2 are assumed to have a mean value of 3 and 87, respectively, based on field data. If the user chooses to have RISC calculate the dispersivities, then the values of τ_1 and τ_2 are assumed to be equal to 3 and 87 respectively.

B.3 ESTIMATING THE CONCENTRATION IN THE WELL

The concentration in the well is estimated by vertically averaging the estimated concentrations over the "screened interval" of the well. The user specifies the distance downgradient from the downgradient edge of the source to the exposure point location (possibly a well screen). A distance off the centerline may also be entered. To estimate the concentration on the centerline of the plume, this value should be left at zero. The code will always predict the highest concentrations to be along the centerline of the plume because it assumes a uniform flow field. The depth to the top and bottom of the well screen measured from the water table (not ground surface) must be specified. The code will calculate concentrations in the groundwater at the top and bottom of the well screen at a minimum. The user may increase the number of points used to average the concentration across the well screen. A minimum of two averaging points must be specified in the input, i.e. the output will be an average of the concentrations at the top and bottom of the well screen. If more than two points are used, the averaging points are assumed to be located at equal intervals (= n-1 intervals, where n = number of points) with one point at the top of the well screen and one at the bottom. The concentrations at the top and bottom of the well screen are weighted at 1/2 the value of the concentrations at the other points. The maximum number of averaging points is ten. Figure B-2 shows a schematic with three averaging points as an example.

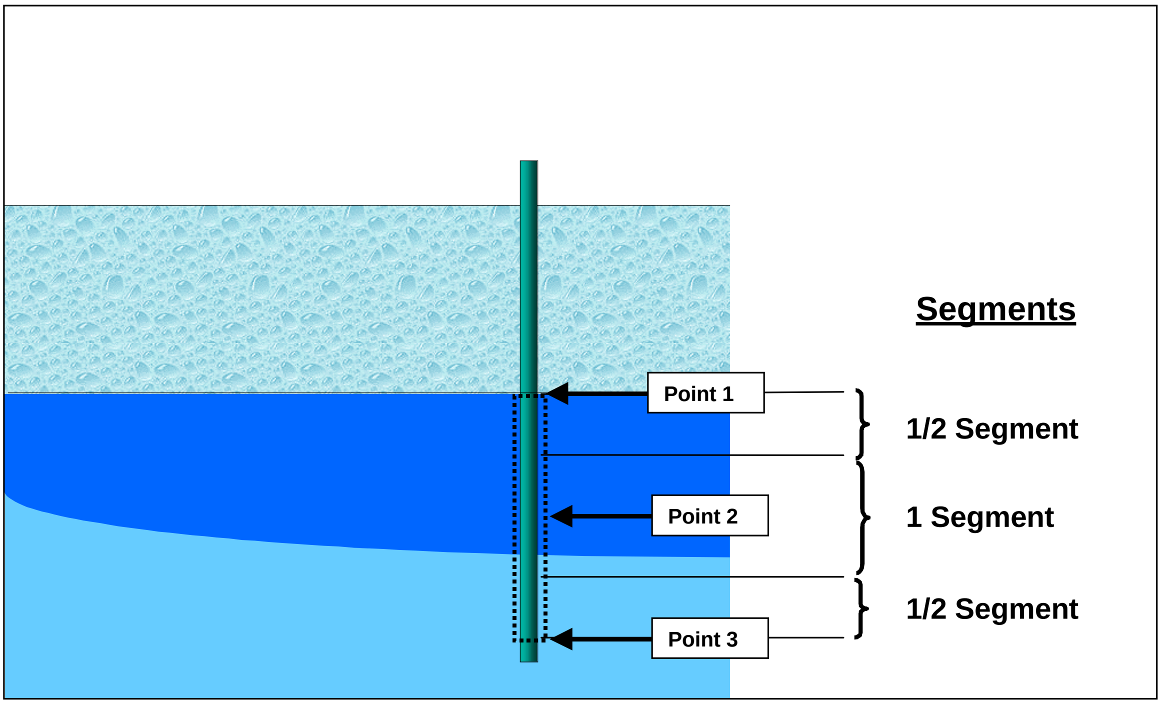

Figure B-2. Vertically Averaging the Concentration Over the Length of the Well Screen (showing 3 averaging points)

For the case shown in Figure B-2 the average concentration would be calculated from the following equation

$$C_{ave} = \frac{\frac{1}{2}C_1 + C_2 + \frac{1}{2}C_3}{2} \qquad \textbf{(B-8)}$$

where

C_j = concentration at point j, (where j = 1, 2, or 3) [mg/l]

2 = the number of segments for averaging

B.4 SOURCE TERM

The source term used by the model is estimated by the code from the source concentration input by the user. The input concentration is assumed to be a dissolved-phase concentration that applies over the entire source volume and is constant for the duration of the release, i.e. the length of the pulse. The way in which the transport equation defined in B-1 is solved, however, requires a mass loading rate as the source term and not a concentration. The RISC code calculates the mass loading rate as follows:

$$\dot{M} = A \cdot V \cdot C_{gw} \cdot \left(\frac{1000l}{m^3} \right) \tag{B-9}$$

where

$\dot{M}$ = mass loading rate [mg/day]

A = cross-sectional area of the source perpendicular to groundwater flow (=y*z dimensions) [m^2]

V = groundwater flux (Darcy velocity) [m/day]

C_{gw} = concentration in groundwater at the source [mg/l]

B.4.1 Using the Groundwater Model With a Source Containing Non-Mobile Residual Hydrocarbons

There are several ways to use RISC to model the plume emanating from a residual source. The first option is to use the dissolved phase groundwater model with a constant source term. This approach is described below. The second option is to use the saturated soil model described in Appendix C. The saturated soil model is appropriate if the volume of the source and the concentrations of the chemicals in the source are known. The saturated soil model uses a depleting source term and therefore accounts for mass balance.

The dissolved phase groundwater model can be used with some conservative assumptions to predict concentrations downgradient of a source that has residual hydrocarbon present. This model is appropriate when the volume of and/or concentrations in the source are not known. This is a fairly common situation when the product has reached the water table as a separate phase. Residual non-mobile hydrocarbon is not free to move on top of the groundwater as a separate phase. The groundwater model cannot simulate the movement of free phase residual; rather it simulates the dissolved phase plume that may originate from a residual source. Figure B-3 shows a simplified schematic.

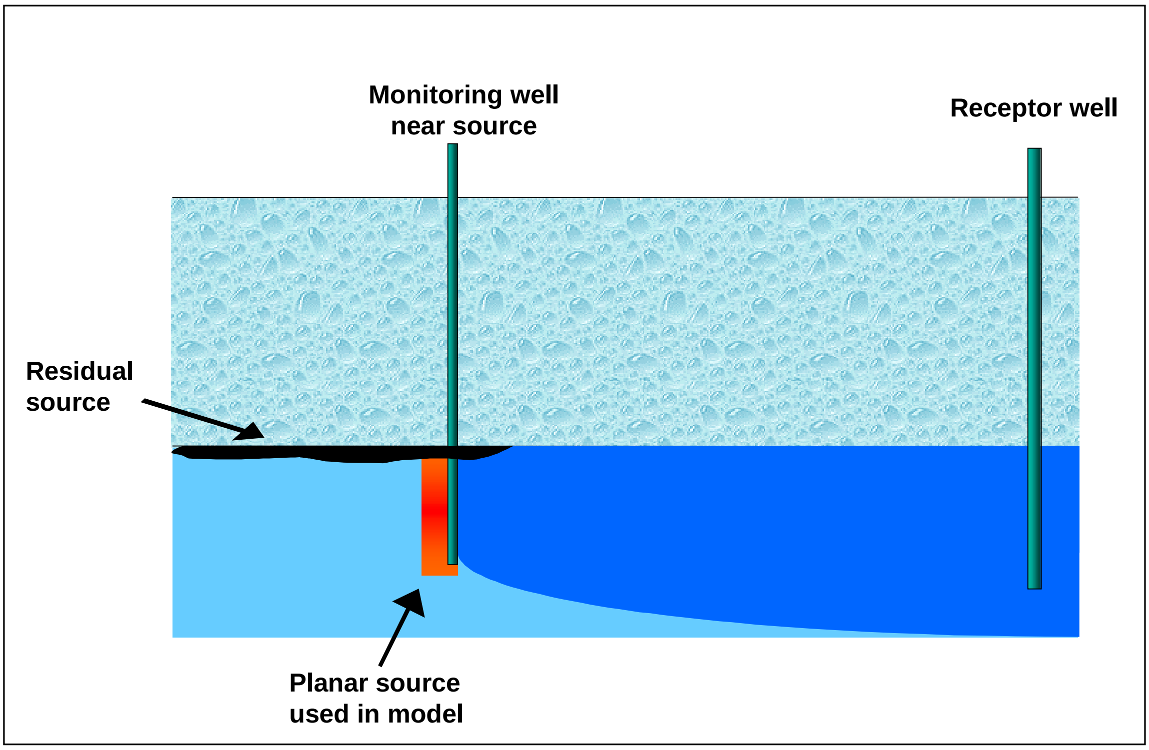

Figure B-3. Schematic of Groundwater Model With a Residual Source

In Figure B-3, the source is assumed to be in the shape of a vertical plane perpendicular to the direction of groundwater flow. Using a vertical plane is similar to the geometry assumed in the Domenico groundwater model (Domenico, 1987). The width and depth of the vertical planar source should be estimated based on site data. Usually the size of the source will not be known so estimating a conservative value may be appropriate.

B.4.2 Using the Model Without Concentration Data in the Source

If there are no measurements of dissolved phase concentrations near or just downgradient of the source, the source concentrations can be assumed to equal the chemical's effective solubility. For this case, all of the groundwater passing through the source area is assumed to be equal to the constituent's effective solubility. Since there are residual levels of contaminants in the source it might be reasonable (and conservative) to assume that the source is constant (non-depleting) over the simulation time.

As an example, if the product spilled is fresh gasoline, the mass fraction of benzene in the product can be estimated based on published product data or based on measured data from similar sites. If the mass fraction of benzene is assumed to be 0.03 in the product (fairly conservative, i.e. high, for gasoline), the effective solubility can be roughly calculated from the following equation:

$$C_w = xS \tag{B-10}$$

where

C_w = dissolved concentration of chemical adjacent to residual product [mg/l]

S = aqueous solubility of pure component [mg/l]

x = mole fraction of component in the hydrocarbon mixture [mol/mol]

This equation is also discussed in Appendix A (equation A-16). Of course, it is not easy to estimate the mole fraction of the chemical. For chemicals and product mixtures that have similar molecular weights, the mole fraction can be replaced by the mass fraction. This example assumes that benzene is 3% by mass of the product. The pure chemical solubility for benzene is 1750 mg/l, therefore the effective solubility can be estimated as = 0.03*1750 mg/l (solubility of benzene) = 52.5 mg/l. This is the concentration that would be specified for the source concentration.

B.4.3 Using the Model With Measured Concentration Data

If there is a monitoring well in the source or just down gradient, this information can be used to estimate the model source depth and the source concentrations. If the monitoring well has a screen length of 2 meters and has benzene concentrations around 5 mg/l then the source depth would be assumed to be 2 meters and the source concentration would equal the measured value. Note, in many situations the residual can be located in the top few inches of the aquifer (at the water table) but the concentrations measured in the monitoring well average the concentration over the well screen length. If the source is assumed to be only a few inches thick, then the source concentrations should be increased to account for the higher concentrations at the top of the aquifer.

B.5 DATA REQUIREMENTS

The data required to run the saturated zone model in RISC are listed in Table B-1.

Table B-1. Data Requirements for the Saturated Zone Model

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
MEDIA-SPECIFIC PARAMETERS			
Porosity	fraction	0.01	0.5
Fraction Organic Carbon	fraction	0.001	0.05
Hydraulic Conductivity	m/day	1.00E-07	100
Soil Bulk Density	fraction	1.4	2.2
Hydraulic Gradient	m/m	>0	0.05
Longitudinal Dispersivity (Note: May be code calculated)	m	site-specific	site-specific
Transverse Dispersivity (Note: May be code calculated)	m	site-specific	site-specific
Vertical Dispersivity (Note: May be code calculated)	m	site-specific	site-specific
WELL LOCATION			
Distance Downgradient	m	site-specific	site-specific
Distance Cross-Gradient	m	site-specific	site-specific
Depth to Top of Well Screen	m	site-specific	site-specific
Depth to Bottom of Well Screen	m	site-specific	site-specific
Number of averaging segments	-	1	10
DISSOLVED PHASE SOURCE			
Thickness of Source Area	m	site-specific	site-specific
Length of Source Area (in direction of GW flow)	m	site-specific	site-specific
Width of Source Area (perpendicular to GW flow)	m	site-specific	site-specific
CHEMICAL-SPECIFIC DATA (individual chemical component)			
Source Concentration	mg/l	site-specific	site-specific
Diffusion Coefficient in Water	cm^2/s	chem-specific	chem-specific
K_{oc}	ml/g	chem-specific	chem-specific
Degradation Rate	1/d	site-specific	site-specific

B.6 ASSUMPTIONS AND LIMITATIONS OF THE DISSOLVED PHASE TRANSPORT MODEL

1. The model simulates the transport of dissolved phase contaminants only. It does not simulate the movement of non-aqueous phase liquids (NAPLs).
2. The concentrations estimated by the model represent concentrations in the groundwater aquifer and not concentrations in a pumping well. The concentrations in a pumping well would probably be lower than the concentrations predicted in the aquifer due to dilution effects.
3. The aquifer is considered to be homogeneous and uniform, as well as being infinite in thickness and width.
4. Water table fluctuations are assumed to have no influence on the flow field of the aquifer.

B.7 REFERENCES

American Petroleum Institute. Oil and Gas Industry Exploration and Production Wastes, API Document No. 471-01-09. Washington, D.C.: API, 1987.

Galya, D.P. "A horizontal plan source model for ground-water transport." Ground Water 25 (1987):733-739.

Gelhar, L.W., Mantoglou, A., Welty, C. and Rehfeldt, K.R., 1985. A review of field-scale physical solute transport processes in saturated and unsaturated porous media. Electrical Power Research Institute (EPRI) Palo Alto, CA EA-4190, Res. Proj. 2485-5.

Yeh, G.T., 1981. AT123D: Analytical Transient One-,Two-, and Three-dimensional Simulation of Waste Transport in the Aquifer System. Oak Ridge National Laboratory. Oak Ridge, TN.

Appendix
C

Saturated Soil Model

C.1 MODEL DESCRIPTON

The saturated soil model in RISC simulates dissolved chemical transport from a soil source zone at or near the water table. The source's position, relative to the aquifer, may change during the year due to groundwater table fluctuations. Thus, it may be located entirely within the aquifer during part of the year, and located partially above the aquifer during the rest of the year. The location relative to the water table is important as the two different processes of rainwater infiltration and groundwater flow through the source are necessary to introduce contamination into the aquifer. The source term in this model is specified with a total soil concentration (mg/kg) whereas the source in the dissolved phase groundwater model (Appendix B) is specified as a dissolved phase concentration (mg/l).

This is a compartmental model, consisting of a source zone leaching model and a dissolved chemical groundwater transport model. The groundwater transport model is identical to the model described in Appendix B. This appendix focuses on presenting the source leaching model. Similar to the dissolved phase groundwater model, the saturated source model can be used (i) to predict the concentration in groundwater at a "receptor well", or, (ii) to predict the concentration in groundwater as a source for volatile emissions into a building (see Appendix E). The saturated soil model is not linked with a vadose zone model.

> In the saturated source model the source concentration is defined as a total soil concentration. This soil concentration may be above the residual limit. In the dissolved phase transport model (Appendix B), the input concentration must be a dissolved phase concentration.

Figure C-1 shows the schematic of the saturated soil (groundwater) model.

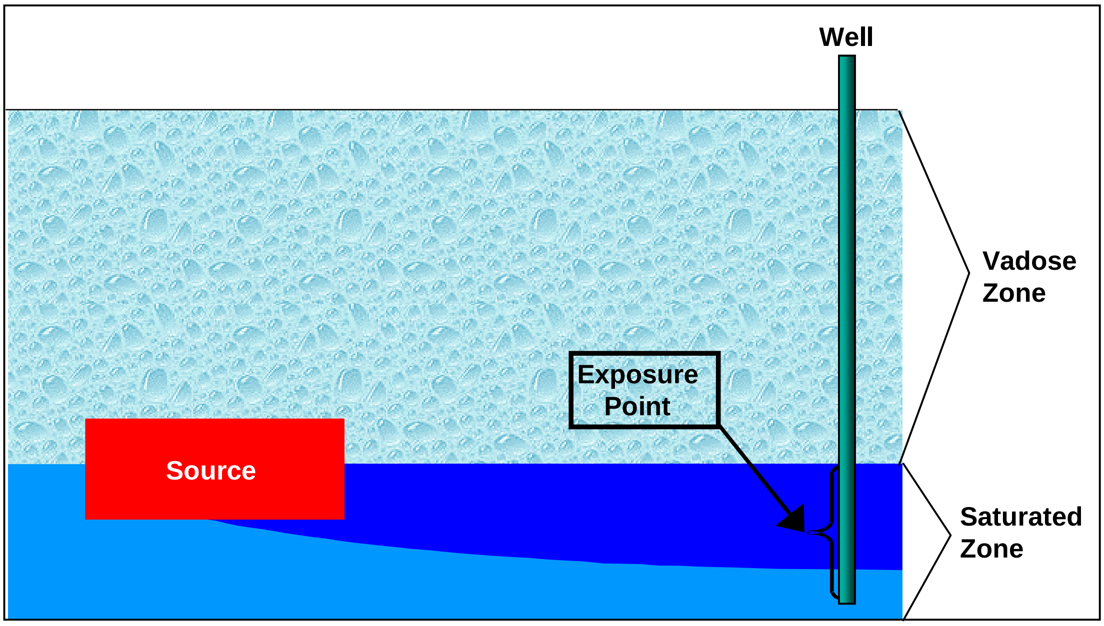

FIGURE C-1. Saturated Soil Model with Source in and above the Water Table

C.2 TRANSPORT EQUATIONS AND PROCESSES

The saturated soil model consists of a source model and a dissolved phase groundwater model. The source model is used to estimate the mass loading rate (that serves as a source for the dissolved phase model) based on the concentrations of the individual constituent in soil and the concentration of TPH (if used to indicate presence of a mixture).

The mass of chemical contained in the portion of the source above the water table (if any) is assumed to be leached due to infiltration. The mass in the portion of the source below the water table (if any) is assumed to be leached horizontally with the groundwater flow. These leaching rates are calculated from the effective solubility or from equilibrium partitioning. That is, the equilibrium dissolved phase concentration is estimated and is assumed to be constant until the source is gone. If the water table shifts during the year, the loading rates from the submerged portion of the source and the unsaturated portion also shift accordingly. If the water table doesn't fluctuate, the mass loading rate is assumed to be constant until the source is depleted. The source model accounts for mass balance as the source "shuts off" after the mass of the constituent has been depleted.

C.3 SOURCE MODEL

The source is defined by a specifying a total soil concentration for each chemical modeled and the total source volume. The source may be just above the water table, partially submerged, or completely submerged. The water table may be considered to fluctuate during part of the year. Mass loading is due to: (1) groundwater flow through the source zone that is submerged, and (2) rainwater infiltration through the source zone that is above the water table.

The total initial mass of contaminant is calculated as follows:

$$Mass = \frac{C_T \rho_b \; H \; W \; L \; \left(1E6\, cm^3 / m^3\right)}{\left(1000\, g / kg\right)} \qquad \textbf{(C-1)}$$

where

$Mass$ = total initial mass in saturated source [mg]

C_T = total concentration in soil [mg/kg]

ρ_b = soil bulk density [g/cm^3]

H = height of source [m]

W = width of source [m]

L = length of source [m]

The total initial mass is depleted when the groundwater carries away the contaminant in the dissolved phase. The depletion (and hence source term for the groundwater model) is calculated by estimating the dissolved phase contaminant concentration in the source volume and assuming that this concentration leaves the source with the bulk groundwater flow.

In order to estimate the dissolved phase concentration, it must be determined whether or not residual phase hydrocarbon (NAPL) is present. If residual phase hydrocarbons are present, the dissolved phase source concentration for each chemical is assumed to be equal to its effective solubility. This is the same approach used in the Vadose Zone model (discussed in Appendix A).

To determine if residual phase hydrocarbon is present, the following condition for multiple chemicals must be met

$$1 > \sum_{all\ chemicals} \frac{C_T \rho_b}{S_i \left(\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H \right)} \qquad \textbf{(C-2)}$$

where

C_T = total concentration of chemical in soil [mg/kg]

S_i = dissolved phase solubility for chemical *i* [mg/l]

ρ_b = soil bulk density of the source area [g/cm^3]

F_{oc} = fraction organic carbon in soil [g oc/g soil]

K_{oc} = chemical-specific organic carbon partition coefficient [ml/g or m^3/kg]

K_H = Henry’s Law constant [(mg/l)/(mg/l)]

θ_a = air-filled porosity of vadose zone [cm^3 of air/cm^3 total soil volume]

θ_w = water-filled porosity of vadose zone [cm^3 of water/cm^3 total soil volume]

This partitioning equation assumes that the total soil concentration, C_T, can be accounted for by summing the mass in the solid, liquid, and vapor phases (i.e. no residual is present). However, Equation C-2 requires that all of the chemicals in the mixture are accounted for in the sum. In risk assessments, the number of chemicals of concern is often a small subset of the total number of chemicals present in the mixture. The saturated soil model checks the following equation for each chemical used in the model:

$$C_w = \frac{C_T \rho_b}{\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H} \qquad \textbf{(C-2a)}$$

Again, it is assumed that C_T can be accounted for by summing the mass in the solid, liquid, and vapor phases (i.e. no residual is present). If the liquid phase concentration, C_W, calculated with equation C-2a exceeds the effective solubility of the compound, then it is assumed that residual phase is present (and equation C-2a does not apply).

The effective solubility is calculated from the following equation:

$$S_{eff_i} = \left(\frac{C_{T_i}}{C_{TPH}} \right) \left(\frac{MW_{TPH}}{MW_i} \right) S_i \qquad \textbf{(C-3)}$$

where

$S_{eff\,i}$ = effective solubility for chemical *i* [mg/l]

$C_{T\,i}$ = total concentration of chemical *i* in soil [mg/kg]

MW_{TPH} = average molecular weight of hydrocarbon [g/mol]

MW_i = average molecular weight of component *i* [g/mol]

C_{TPH} = concentration of total petroleum hydrocarbons in soil [mg/kg]

C.4 DATA REQUIREMENTS

The data required to run the saturated zone model in RISC are listed in Table C-1.

Table C-1. Data Requirements for the Saturated Soil Model

(Page 1 of 2)

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
MEDIA-SPECIFIC PARAMETERS			
Porosity	fraction	0.01	0.5
Fraction Organic Carbon	fraction	0.001	0.05
Hydraulic Conductivity	m/day	1.00E-07	100
Soil Bulk Density	fraction	1.4	2.2
Hydraulic Gradient	m/m	>0	0.05
Longitudinal Dispersivity (Note: May be code calculated)	m	site-specific	site-specific
Transverse Dispersivity (Note: May be code calculated)	m	site-specific	site-specific
Vertical Dispersivity (Note: May be code calculated)	m	site-specific	site-specific

Table C-1. Data Requirements for the Saturated Soil Model

(Page 2 of 2)

WELL LOCATION			
Distance Downgradient	m	site-specific	site-specific
Distance Cross-Gradient	m	site-specific	site-specific
Depth to Top of Well Screen	m	site-specific	site-specific
Depth to Bottom of Well Screen	m	site-specific	site-specific
Number of averaging segments	-	1	10
SATURATED SOIL SOURCE			
Total Thickness of Source (above and below water table)	m	site-specific	site-specific
Length of Source Area	m	site-specific	site-specific
Width of Source Area	m	site-specific	site-specific
Minimum Saturated Thickness of the Source	m	site-specific	site-specific
Thickness of Water Table Fluctuations	m	site-specific	site-specific
Fraction of Year at High Elevation	fraction	0	1
Infiltration rate in the Vadose Zone	m/d	>0	site-specific
TPH DATA			
Molecular Weight of TPH	g/mol	80	120
Concentration of TPH	mg/kg	site-specific	site-specific
Chemical Specific Data (individual chemical component)			
Molecular Weight	g/mol	80	120
Total Concentration in Soil	mg/kg	site-specific	site-specific
Solubility	mg/l	chem-specific	chem-specific
Diffusion Coefficient in Air	cm^2/s	chem-specific	chem-specific
Diffusion Coefficient in Water	cm^2/s	chem-specific	chem-specific
Koc	ml/g	chem-specific	chem-specific
Degradation Rate	1/d	site-specific	site-specific
Henry's Law Constant	dimensionless	chem-specific	chem-specific

C.5 ASSUMPTIONS AND LIMITATIONS OF THE SATURATED SOIL MODEL

1. The Saturated Soil model simulates the transport of dissolved phase contaminants only. It does not simulate the movement of non-aqueous phase liquids (NAPLs).
2. The concentrations estimated by the model represent concentrations in the groundwater aquifer and not concentrations in a pumping well. The concentrations in a pumping well would probably be lower than the concentrations predicted in the aquifer due to dilution effects.
3. The aquifer is considered to be homogeneous and uniform.
4. Water table fluctuations are used to calculate the relative contribution from infiltration and groundwater advection to source mass loss. The water table fluctuations are assumed to have no influence on the flow field of the aquifer.

C.6 REFERENCES

American Petroleum Institute. Oil and Gas Industry Exploration and Production Wastes, API Document No. 471-01-09. Washington, D.C.: API, 1987.

Galya, D.P. "A horizontal plan source model for ground-water transport." Ground Water 25 (1987):733-739.

Gelhar, L.W., Mantoglou, A., Welty, C. and Rehfeldt, K.R., 1985. A review of field-scale physical solute transport processes in saturated and unsaturated porous media. Electrical Power Research Institute (EPRI) Palo Alto, CA EA-4190, Res. Proj. 2485-5.

Yeh, G.T., 1981. AT123D: Analytical Transient One-,Two-, and Three-dimensional Simulation of Waste Transport in the Aquifer System. Oak Ridge National Laboratory. Oak Ridge, TN.

Appendix
D

Vapor Transport From Soil Into Buildings Without Biodegradation

D.1 MODEL DESCRIPTION

The vapor transport model for soil estimates emissions into a building from a soil source located either below or laterally adjacent to the building. This model is based on the paper entitled "Heuristic Model for Predicting the Intrusion Rate of Contaminant Vapors into Buildings" by Johnson and Ettinger (1991). This vapor transport model combines a model for both diffusive and advective transport through the soil with a simple model of transport through a building foundation.

Figure D-1 illustrates the problem geometry. Advection is caused by a slightly reduced pressure (versus atmospheric pressure) inside a building due to temperature differences, wind, barometric pressure fluctuations or a slight vacuum created by a basement heating system during operation. The pressure gradient is entered as an input parameter.

This is the basically the same model as the one used in the Tier 1 spreadsheet to calculate risk-based screening levels in soil that are protective of indoor inhalation. The enhancements made by the RISC software are twofold: (1) multiple soil horizons may be considered by using the lens and (2) the model calculates the effective solubility and limits the soil gas concentration at the source if residual levels are exceeded. This second option is an important consideration for chemicals that are part of mixtures such as petroleum hydrocarbons in fuel. The example equations presented in the ASTM RBCA guidance are identical to the Johnson and Ettinger model if the building under-pressurization is equal to zero (no advection).

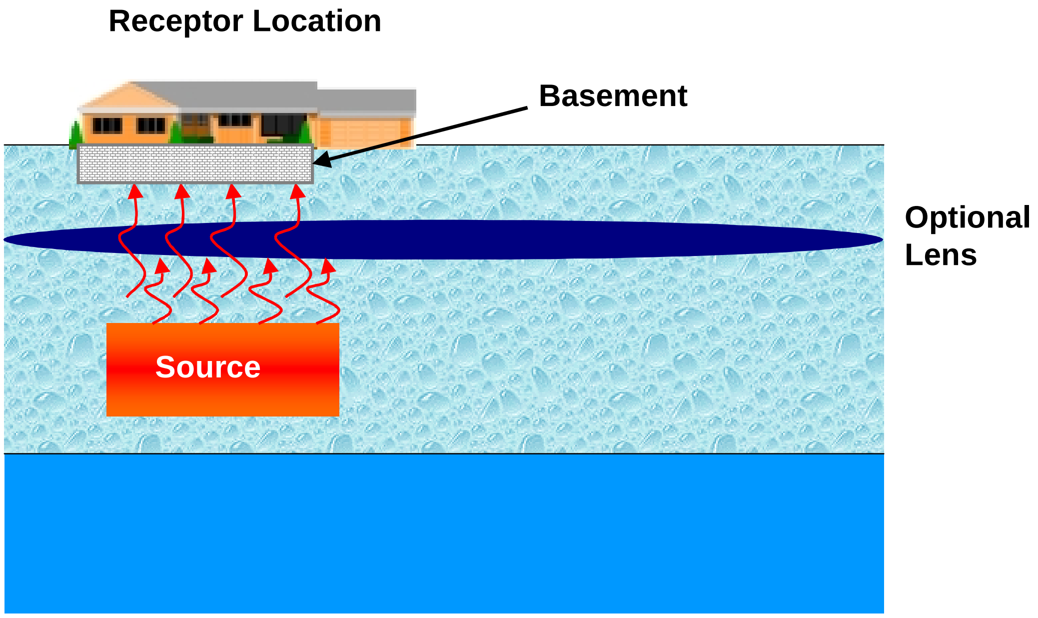

Figure D-1. Schematic of the Vapor Transport Model (from Soil into Buildings).

D.2 APPLICATIONS OF THIS MODEL

This is a partial list of the main applications of the model:

- This is a steady-state model. The source concentration is constant and the size does not deplete with time (i.e. an infinite source). This assumption is valid if the source is large compared to the mass flux rate into the building.
- This model is not linked with any other fate and transport model in RISC. The soil leaching to groundwater model is assumed to have a separate (depleting) source.
- Biodegradation of the chemical vapors is not considered. This is appropriate for chemicals that do not degrade readily, for very short diffusion distances, and/or for screening level calculations. BTEX constituents can have very high degradation rates (higher than in groundwater) under certain conditions. In this case it may be appropriate to use one of the other two vapor transport models in RISC that incorporate degradation.
- The source is located in the vadose zone. For sources located in the saturated zone the volatilization from groundwater model would be more appropriate.
- The likelihood of the building under-pressurization affecting the vapor transport should be evaluated. Often, the reason that advective transport

becomes important is the case where part of the building is sub-grade (e.g. basement) and the path of least resistance from the source is in the direction of the basement. This situation can occur for a laterally offset source if the preferential vapor flow pathways are horizontal (e.g. there are lower permeability units between the source and the ground surface). If the building is not large and does not have a sub-grade basement it is unlikely that the building under-pressurization is affecting the advection processes from an offset soil vapor source. The path of least resistance may be directly out through the ground surface.

- A building on a slab foundation can have advective effects if under-pressurization is present, the source is directly below and close to the foundation, and no partial low permeability lens is available to direct the vapors laterally away from the foundation. But a pier and beam house (where a crawl space is located under the house) would not be subject to advection (and may in fact have only limited diffusion as well if it is vented).

Appendix K.1.2 discusses vertical soil gas profile types and the applicability of the models in RISC to model different soil gas profiles.

D.3 TRANSPORT EQUATIONS AND PROCESSES

The Johnson-Ettinger model assumes that away from the structure, (i.e. out of the influence of pressure-driven flow), the contaminant transport is diffusive only and can be described using Fick's Law:

$$E = \frac{A_B \left(C_{vs} - C_{vf}\right) D_{eff}}{L_T} \qquad \textbf{(D-1)}$$

where

E = mass transport rate toward the structure [g/s]

D_{eff} = "overall" effective diffusion coefficient [cm^2/s]

C_{vs} = vapor concentration at the source [$\mathrm{g/cm}^3$]

C_{vf} = vapor concentration in the soil just outside the building foundation [$\mathrm{g/cm}^3$]

L_T = distance from source to basement [cm]

A_B = cross-sectional area of foundation available for vapor flux [cm^2]

Note, the effective diffusion coefficient is calculated using the Millington-Quirk relationship (Millington and Quirk, 1961, and described in Appendix A) which accounts for the amount of air vs. water-filled porosity in the soil. Furthermore, a lens can be incorporated in the vapor model so the "overall" effective diffusion coefficient can consider a different soil unit between the source and the house. A clay lens with a high water content can dramatically reduce the overall diffusion coefficient and can result in much lower vapor concentrations inside the house.

Adjacent to the foundation, the transport of contaminants is assumed to occur by a combination of advective and diffusive transport mechanisms through cracks in the foundation slab. The steady-state, one-dimensional solution to the advection-dispersion equation for vapor transport through a crack (just another type of porous media) is given by:

$$E = Q_{soil} C_{vf} - \frac{Q_{soil}\left(C_{vf} - C_{indoor}\right)}{\left[1 - \exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right)\right]} \qquad \textbf{(D-2)}$$

where

E = entry rate of contaminant into the building [g/s]

Q_{soil} = volumetric flow rate of soil gas into the building [cm^3/s]

C_{indoor} = indoor air concentration in the building [g/cm^3]

C_{vf} = vapor concentration in the soil just outside the building foundation [g/cm^3]

D_{crack} = effective diffusion coefficient in foundation cracks [cm^2/s]

L_{crack} = thickness of the foundation [cm]

A_{crack} = area of cracks or openings through which vapors enter building [cm^2]

The above two equations are assumed to be equal at steady state allowing the contaminant concentration in the soil just outside the foundation to be calculated. Setting Equations D-1 and D-2 equal to each other and rearranging to solve for C_{vf}:

$$C_{vf} = \frac{\left[C_{vs} \left[\frac{D_{eff} A_B}{Q_{soil} L_T} \right] \left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}} \right) - 1 \right] + C_{indoor} \right]}{\left[\left[\frac{D_{eff} A_B}{Q_{soil} L_T} \right] \left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}} \right) - 1 \right] + \exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}} \right) \right]} \qquad \textbf{(D-3)}$$

Substituting D-3 into equation D-2 yields:

$$E = \frac{\left[\left[\frac{D_t^{eff} A_B C_{vs}}{L_T} \right] \left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}} \right) - \left[\frac{C_{indoor}}{C_{vs}} \right] \right] \right]}{\left[\left[\frac{D_T^{eff} A_B}{Q_{soil} L_T} \right] \left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}} \right) - 1 \right] + \exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}} \right) \right]} \qquad \textbf{(D-4)}$$

In equation D-3, the only unknown variable (not entered by the user) is the concentration in the building, C_{indoor}. This concentration can be estimated from a mass balance equation assuming no other contaminant sources or sinks in the building (sorption to walls or furniture). Assuming a well-mixed building this mass balance equation can be written as:

$$Q_B C_{indoor} = E \qquad \textbf{(D-5)}$$

where

Q_B = building ventilation rate (calculated from the number of air exchanges per day and the volume of the building) [m^3/s] where all the variables have been defined previously. Note, the emission rate, E, is calculated from equation D-4; the building ventilation rate, Q_B, is calculated from user input variables. Substituting Equation D-5 into Equation D-4 yields

$$C_{indoor} = \frac{C^*_{indoor}\left[\exp\left(\frac{Q_{soil}L_{crack}}{D_{crack}A_{crack}}\right)\right]}{\left[\exp\left(\frac{Q_{soil}L_{crack}}{D_{crack}A_{crack}}\right)+\left[\frac{D_{eff}A_B}{Q_BL_T}\right]+\left[\frac{D_{eff}A_B}{Q_{soil}L_T}\right]\left[\exp\left(\frac{Q_{soil}L_{crack}}{D_{crack}A_{crack}}\right)-1\right]\right]} \qquad \textbf{(D-6)}$$

where

$$C^*_{indoor} = \frac{D_{eff}A_BC_{vs}}{Q_BL_T} \qquad \textbf{(D-7)}$$

C^*_{indoor} represents the indoor vapor concentration corresponding to the case where vapors diffuse from the source through a bare soil foundation.

The volumetric soil gas flow rate into the basement, Q_{soil}, may be specified by the user or it is calculated from the area of cracks, A_{crack}, soil type and stratigraphy, pressure difference between atmospheric and building pressure, and basement geometry. If Q_{soil} is specified in RISC to be equal to zero, the vapor transport model will calculate it from (Johnson and Ettinger, 1991):

$$Q_{soil} = \frac{2\pi(\Delta P)k_vX_{crack}}{\mu\ln\left[2Z_{crack}/r_{crack}\right]} \qquad \frac{r_{crack}}{Z_{crack}} << 1 \qquad \textbf{(D-8)}$$

This equation is based on flow through a cylinder of length X_{crack} and radius r_{crack} located a depth Z_{crack} below ground surface. The rest of the variables used in D-8 are:

ΔP = pressure gradient between building and outside [g/cm-s^2]

Z_{crack} = depth below ground surface to foundation cracks [cm]

k_v = permeability of the soil to vapor flow [cm^2]

μ = viscosity of vapor [g/cm-s]

The crack length, X_{crack} , is an input parameter and can be conservatively assumed to be the total floor/wall seam perimeter distance. r_{crack} is defined as:

$$r_{crack} = \frac{\eta A_B}{X_{crack}} \qquad \textbf{(D-9)}$$

where

η = the ratio: A_{crack}/A_B so that 0 =< η =< 1

For intrinsic permeabilities of vapor flow, k_v, of less than 1E-8 cm^2 (fine sand soils), the soil gas flow rate through the cracks becomes so low that diffusion is the dominant transport mechanism and the solution is independent of k_v. For "larger" values of k_v, (greater than 1E-8 cm^2) the solution is dominated by the advective contribution. In the model output, the contribution from diffusion is estimated by setting k_v to a very low value.

D.4 SOURCE TERM

The source may be specified by entering total soil concentrations or by entering soil vapor concentrations. Using measured soil vapor concentrations has the following advantages:

- It eliminates the uncertainty in the model of estimating the source vapor concentrations from the equilibrium partitioning equation. This can be significant because of the complexities of partitioning when the chemicals are part of a mixture and because the soil properties like soil moisture and porosity are rarely known.
- The soil vapor concentration may be measured in the vadose zone between the source and the building. This approach can directly account for attenuation processes such as degradation and diffusion through different soil horizons (whose soil properties are not known) that the model may under-estimate. This can be very significant and many US State risk-based corrective action programs are developing protocols for starting with soil vapor concentrations rather than total soil concentrations.

Note that if the location of the soil vapor measurement is not close to the source, it is important to evaluate whether or not the soil vapor concentration has yet reached equilibrium. For example, if a recent subsurface chemical spill occurred in a silty clay and the soil vapor measurement point were 3 meters away, the vapor concentrations may not have yet reached their maximum values.

If there is no residual phase hydrocarbon present, the source vapor concentration is calculated from the total soil concentration using the following equation presented by Jury (1983, 1984, and 1990):

$$C_{vs} = \frac{C_T \rho_b K_H}{\theta_a K_H + \theta_w + \rho_b F_{oc} K_{oc}} \left(\frac{kg}{1E6mg} \right) \tag{D-10}$$

where

C_{vs} = vapor concentration at the source [g/cm^3]

C_T = total soil concentration of chemical *i* [mg/kg]

ρ_b = soil bulk density of the source area [g/cm^3]

F_{oc} = fraction organic carbon in soil [g oc/g soil]

K_{oc} = chemical-specific organic carbon partition coefficient [ml/g m^3/kg]

K_H = Henry's law constant [(mg/l)/(mg/l)]

θ_a = air-filled porosity of vadose zone [cm^3 of air/cm^3 total soil volume]

θ_w = water-filled porosity of vadose zone [cm^3 of water/cm^3 total soil volume]

If residual phase hydrocarbon (NAPL) is present, Raoult's Law is used with the component mole fraction

$$C_{vs} = \frac{x_i P_v^{\,i} MW_i}{RT} \tag{D-11}$$

where

x_i = mole fraction of component *i* in the hydrocarbon [mol/mol]

P_i^v = pure component vapor pressure of component *i* [atm]

MW_i = molecular weight of component *i* [g/mol]

R = the universal gas constant (82.1) [cm^3-atm/mol-K]

T = absolute temperature [K]

The model checks to see if residual-phase hydrocarbon is present and then calculates the source term accordingly. (The method for determining the residual limit is discussed in more detail in Appendix A, starting with Equation A-15.)

The mole fraction, x_i, is calculated from

$$x_i = \left(\frac{C_T}{C_{TPH}} \right) \left(\frac{MW_{TPH}}{MW} \right) \qquad \textbf{(D-12)}$$

where

C_T = total soil concentration of chemical *i* [mg/kg]

C_{TPH} = total soil concentration of TPH mixture [mg/kg]

MW_{TPH} = molecular weight of the mixture [g/mol]

MW_i = average molecular weight of component *i* [g/mol]

If the molecular weights of the component, *i*, and the mixture are similar, this roughly translates to the concentration of the component, *i*, over the concentration of total petroleum hydrocarbons (TPH) in the source.

D.5 DATA REQUIREMENTS OF THE SOIL VAPOR MODEL

The input data requirements for this model are presented in Table D-1.

Table D-1. Data Requirements for the Soil Vapor Model for Indoor Air
(Page 1 of 2)

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
UNSATURATED ZONE			
Porosity	cm^3/cm^3	0.01	0.5
Water content in diffusion zone	cm^3/cm^3	0	porosity
Hydraulic conductivity of the soil surrounding the foundation (used to estimate soil vapor flow)	m/day	1.0E-07	100
Soil Bulk Density	fraction	1.4	2.2
LENS (Optional)			
Porosity	cm^3/cm^3	0.01	0.5
Water content of lens	cm^3/cm^3	0	porosity
Lens thickness	m	site-specific	site-specific
TPH DATA (Optional)			
Molecular weight of TPH	g/mol	80	120
Concentration of TPH	mg/kg	site-specific	site-specific
FOUNDATION PARAMETERS			
Distance to foundation	m	site-specific	site-specific
Cross-sectional area of foundation perpendicular to vapor flow	m^2	site-specific	site-specific
Volume of house	m^3	site-specific	site-specific
Number of air exchanges per day	d^{-1}	residential: 12 industrial: 20	location/site-specific
Thickness of foundation	m	0	site-specific
Fraction of cracks in foundation	cm^3/cm^3	0	1

Table D-1. Data Requirements for the Soil Vapor Model for Indoor Air (Page 2 of 2)

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
PARAMETERS USED TO CALCULATE PRESSURE-DRIVEN FLOW			
Soil Gas Flow Rate Into Building *(Q_{soil})* (**or** next three parameters)	cm^3/s	*>0*	*location/site-specific*
Length of Foundation Perimeter (not needed if Q_{soil} specified)	m	0	site-specific
Depth Below Ground Surface of Foundation (not needed if Q_{soil} specified)	m	0	site-specific
Pressure Difference From Indoors to Outdoors (not needed if Q_{soil} specified)	g/cm^2-s	0	site-specific
CHEMICAL SPECIFIC DATA (individual chemical component)			
Molecular Weight	g/mol	chem-specific	chem-specific
Source Concentration: Soil Vapor Concentration, or Total Soil Concentration	mg/m^3 mg/kg	site-specific	site-specific
Solubility	mg/l	chem-specific	chem-specific
Diffusion Coefficient in Air	cm^2/s	chem-specific	chem-specific
Diffusion Coefficient in Water	cm^2/s	chem-specific	chem-specific
Henry's Law coefficient	(mg/l)/(mg/l)	chem-specific	chem-specific

D.6 LIMITATIONS OF THE SOIL VAPOR MODEL

1. This is a steady-state, constant and one-dimensional model. The source does not deplete due to vapor losses so mass is not conserved. This assumption has only a minor impact on the risk due to non-carcinogens (unless the source is

very small) since the highest seven-year running average intake is compared to the reference dose. It can have a more significant impact however on carcinogens (such as benzene) since the cumulative exposure over a long exposure duration (up to 30 years) forms the basis for the risk calculation.

2. There is no biodegradation of the vapors as they migrate through the soil.

D.7 REFERENCES

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Appendix

E

Vapor Transport From Groundwater Into Buildings

E.1 MODEL DESCRIPTON

The groundwater vapor transport model is based on the approach outlined in American Society of Testing and Materials' (ASTM's) Risk Based Corrective Action (RBCA) manual (ASTM, 1995). Vapor emissions from dissolved groundwater contaminants are estimated using a one-dimensional steady-state vapor diffusion model, where capillary fringe, vadose zone properties, and building foundation properties are considered in the estimation of diffusion properties.

> This is basically the same model as the one used in the Tier 1 spreadsheet and the ASTM RBCA guidance manual to calculate risk-based screening levels in groundwater that are protective of indoor inhalation. The enhancements made by the RISC software are twofold: (1) multiple soil horizons may be considered by using the lens and (2) the groundwater concentration under the house may be predicted using one of the groundwater models. This second option allows clean-up levels to be calculated for soil or groundwater that are protective of indoor inhalation for a plume extending downgradient.

This model considers the diffusion of vapors from groundwater through the vadose zone. The model ignores chemical degradation in the vadose zone and advection into the building (pressure-driven flow). Advection is ignored on the assumption that capillary fringe diffusion resistance dominates the problem. With the capillary fringe dominating transport, the equations for vapor transport into a building reduce to the ones presented in this appendix. Figure E-1 shows the problem geometry.

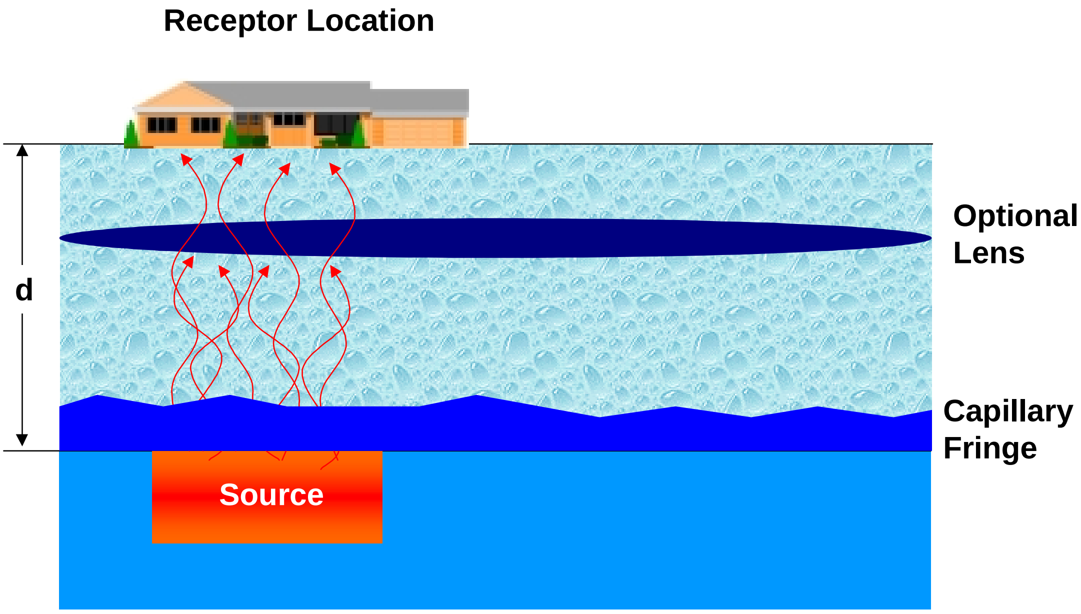

Figure E-1. Schematic of the Vapor Transport Model from Groundwater into Buildings.

E.2 APPLICATIONS OF THIS MODEL

This is a partial list of the main applications of the model:

- The source is assumed to be in the groundwater only. If the original source were in the vadose zone and the volatilization to indoor air pathway is being evaluated for a building close to the source, the soil to indoor air pathway will dominate the risk.
- The source size is assumed to be as large or larger than the footprint of the building.
- The chemicals must diffuse out of the groundwater, through the capillary fringe and through the vadose zone before reaching the building. If contaminants are located above the water table (e.g. the water table has dropped considerably and residual product is left in the vadose zone) then one of the soil vapor models should be used.
- If soil vapor concentrations have been measured above the water table and are to be used as the source term, one of the volatilization from soil models should be used.

- Vapor diffusion through the vadose zone is assumed to be steady-state. The source concentration in groundwater underneath the building can be specified by the user (a constant concentration) or it can be estimated using one of the groundwater models (transient source concentration).
- Biodegradation of the chemical vapors is not considered. This is appropriate for chemicals that do not degrade readily, that travel very short diffusion distances, and/or for screening level evaluations. BTEX constituents can have very high degradation rates (higher than in groundwater) under certain conditions.
- If measured soil gas concentrations have been taken between the groundwater and the source, it would be more appropriate to use one of the soil vapor models with a soil gas source term. The groundwater volatilization model estimates the soil gas concentration using Henry's Law and then estimates the diffusion rate through the capillary fringe. After that point, this model is identical to the Johnson and Ettinger model from a soil gas source (Appendix D) when building under-pressurization is not considered (set to zero).

E.3 TRANSPORT EQUATION AND PROCESSES

Steady-state one-dimensional diffusive vapor transport over a length, *d*, can be described by:

$$F = \frac{D_{eff}\left(C_{vs} - C_{vf}\right)}{L_d} \qquad \textbf{(E-1)}$$

where

F = volatile emission rate of the chemical constituent being modeled [g/cm^2/s]

D_{eff} = effective diffusion coefficient [cm^2/s]

C_{vs} = vapor phase concentration just above the water table in the capillary fringe [g/cm^3]

C_{vf} = vapor phase concentration in the soil at the building foundation [g/cm^3]

L_d = diffusion path length (distance from the water table to the foundation) [cm]

In this equation, the vapor phase concentration in the soil at the building foundation, C_{vf}, is assumed to be negligible ($C_{vf} << C_{vs}$) in comparison to the concentration in vapor at the water table.

E.4 SOURCE TERM

The vapor phase concentration at the water table is calculated using Henry's Law partitioning from the groundwater into the vapor phase concentration:

$$C_{vs} = C_{gw} K_H \left(\frac{L}{1000 cm^3} \right) \cdot \left(\frac{g}{1000 mg} \right) \qquad \textbf{(E-2)}$$

where

C_{vs} = vapor phase concentration just above the water table in the capillary fringe [g/cm^3]

C_{gw} = dissolved phase concentration at the top of the groundwater aquifer (water table - capillary fringe interface) [mg/l]

K_H = Henry's law constant [(mg/l)/(mg/l)]

If this model is linked with the Dissolved Phase Transport model (Appendix B) or the Saturated Soil Model (Appendix C) then the vapor flux in g/d is calculated for each time step. If this model is run in a stand-alone mode the user will be asked to specify a constant concentration in groundwater (C_{gw}) that is assumed to be directly under the house.

This model does not check to see if the dissolved phase concentration entered by the user (in a stand-alone mode) exceeds the effective solubility for the chemical. It is important that the user enter a concentration in groundwater that does not exceed the chemicals' effective solubility. This also applies to groundwater with non-aqueous phase liquids (NAPL) on the surface because the vapor concentrations are also limited by Raoult's Law (they cannot exceed the "effective vapor concentration"). Using Raoult's Law or calculating the effective solubility and multiplying by Henry's Law will result in the same equilibrium vapor concentration for a given TPH mixture.

E.4.1 Effective Diffusion Coefficient

The overall effective diffusion coefficient is calculated as a depth-weighted average of the effective diffusion coefficients in the capillary fringe, the vadose zone above the capillary fringe, the lens and the building foundation. The reason for considering the capillary fringe in the calculation is that the moisture content in the capillary fringe is usually much higher than the moisture content in the unsaturated zone. The smaller air-filled porosity in the capillary fringe will reduce the overall diffusion coefficient significantly. Following the approach in ASTM (1995) the overall diffusion coefficient is given by:

$$D_{eff} = (d_{cap} + d_v + d_{lens} + d_{bldg})\left[\frac{d_{cap}}{D_{eff\ cap}} + \frac{d_v}{D_{eff\ v}} + \frac{d_{lens}}{D_{eff\ lens}} + \frac{d_{bldg}}{\eta D_{eff\ bldg}}\right]^{-1} \qquad \textbf{(E-3)}$$

where

D_{eff} = overall effective gaseous diffusion coefficient from water table to the building foundation [cm^2/s]

$D_{eff\ cap}$ = effective gaseous diffusion coefficient in the capillary fringe [cm^2/s]

$D_{eff\ v}$ = effective gaseous diffusion coefficient in the vadose zone between the capillary fringe and the building foundation [cm^2/s]

$D_{eff\ lens}$ = effective gaseous diffusion coefficient in the lens [cm^2/s]

$D_{eff\ bldg}$ = effective gaseous diffusion coefficient in the building foundation [cm^2/s]

d_{cap} = thickness of the capillary fringe [cm]

d_v = thickness of the vadose zone above the capillary fringe and below the building foundation [cm]

d_{lens} = thickness of the lens [cm]

d_{bldg} = thickness of the building foundation [cm]

η = fraction of foundation that is cracks [cm^2/cm^2]

The effective diffusion coefficient in each zone is calculated using the Millington-Quirk relationship (Millington and Quirk, 1961):

$$D_{eff\ i} = D_{air} \frac{\theta_{ai}^{\ 3.33}}{\theta_{Ti}^{\ 2}} + \frac{D_{water}}{K_H} \frac{\theta_{wi}^{\ 3.33}}{\theta_{Ti}^{\ 2}} \qquad \textbf{(E-4)}$$

where

$D_{eff\ i}$ = effective gaseous diffusion coefficient in zone *i* [cm^2/s]

θ_{ai} = air-filled porosity in zone *i* [cm^3 of air/cm^3 total soil volume]

θ_{wi} = water-filled porosity in zone *i* [cm^3 of water/cm^3 total soil volume]

θ_T = total porosity in zone *i* [cm^3 pores/cm^3 total soil volume]

D_{air} = gaseous diffusion coefficient [cm^2/s]

D_{water} = liquid diffusion coefficient [cm^2/s]

K_H = Henry's Law constant [(mg/l)/(mg/l)]

E.4.2 Moisture Content

The moisture content in the four zones (capillary fringe, vadose zone, lens and building foundation) are explicitly specified for this model (unlike the Vadose Zone model, Appendix A). It is assumed that the region of the vadose zone under a building has no infiltration rate, therefore the moisture content cannot be calculated using the van Genuchten approach (discussed in Appendix A). The soil beneath the building is expected to have some moisture content that depends on the soil type and moisture content of adjacent soil.

E.4.3 Concentration in the Building

The total mass flux of contaminant entering the building is estimated from:

$$E = F \cdot A \qquad \textbf{(E-5)}$$

where

E = total mass flux of the chemical constituent entering the building[g/s]

A = cross-sectional area of the foundation (perpendicular to the vapor flux) [cm^2]

F = volatile emission rate of the chemical constituent being modeled (defined in Equation A-1) [g/cm^2/s]

The concentration of contaminant in the building, C_{bldg} (g/cm^3), is estimated by:

$$C_{indoor} = \frac{E}{Q_B}\left(\frac{m^3}{1E6cm^3}\right)\left(\frac{86400s}{d}\right) \qquad \textbf{(E-6)}$$

where

C_{indoor} = concentration of contaminant in building air [g/cm^3]

E = volatile emission rate of the chemical constituent being modeled [g/s]

$Q_{\boldsymbol{B}}$ = building ventilation rate (calculated from the number of air exchanges per day and the volume of the building) [m^3/d]

The building ventilation rate, Q_B, is calculated from the user input variables the define the volume of the building and the air exchange rate. Equation E-6 assumes that the entire flux of contaminant at the exterior of the building is pulled into the building and there is no reduction of the concentration (due to presence of concrete, etc.). It is also assumed that the air in the building is well mixed (including the basement air if a basement is present).

E.5 DATA REQUIREMENTS

The data requirements for the groundwater vapor transport model are shown in Table E-1. Note, the dissolved phase concentrations in the groundwater source are only used if the model is run in a stand-alone mode (not linked with the Vadose Zone or Saturated Soil models).

Table E-1. Data Requirements for the Groundwater Vapor Model.

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
UNSATURATED ZONE			
Porosity	cm^3/cm^3	0.01	0.5
Residual Water Content (irreducible)	cm^3/cm^3	0	porosity
Hydraulic Conductivity	m/day	1.00E-07	100
Distance from groundwater to foundation	m	site-specific	site-specific
FOUNDATION/BUILDING PARAMETERS			
Cross-Sectional Area for Volatile Flux	m^2	site-specific	site-specific
Volume of Building	m^3	site-specific	site-specific
No. of Air Exchanges per Day	d^{-1}	residential: 12 industrial: 20	location/site-specific
Fraction of Cracks (by area) in Building Foundation	cm^2/cm^2	site-specific	site-specific
CHEMICAL SPECIFIC DATA (individual chemical component)			
Concentration in Groundwater*	mg/l	site-specific	site-specific
Diffusion Coefficient in Air	cm^2/s	chem-specific	chem-specific
Diffusion Coefficient in Water	cm^2/s	chem-specific	chem-specific
Henry's Law Constant	(mg/l)/(mg/l)	chem-specific	chem-specific

* Only needed if the groundwater concentration is not calculated by another model.

E.6 ASSUMPTIONS AND LIMITATIONS OF GROUNDWATER VAPOR MODEL

1. It is assumed that diffusion through the capillary fringe is the dominant resistance to transport so that pressure-driven flow into the building can be neglected.
2. When the model is run in a stand-alone mode (not linked with a fate and transport model), the groundwater source concentrations are assumed to be constant (Figure E-1).
3. When the model is linked with a fate and transport model, the groundwater source concentrations calculated by this model at the receptor well are used as the source concentrations for the vapor transport model. The concentration in groundwater is assumed to remain constant over each time step. Figures E-2 and E-3 illustrate how the groundwater vapor transport model can be linked with two fate and transport models.

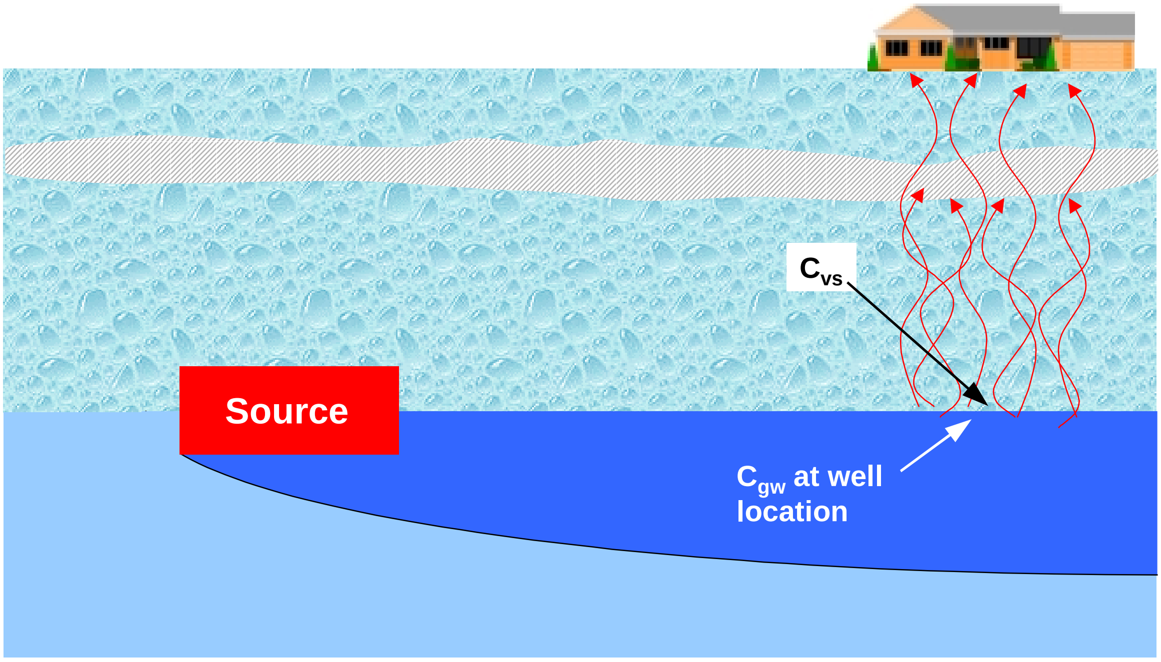

Figure E-2. Vapor Transport from Groundwater Using a Saturated Zone Fate and Transport Model to Estimate Source Concentrations

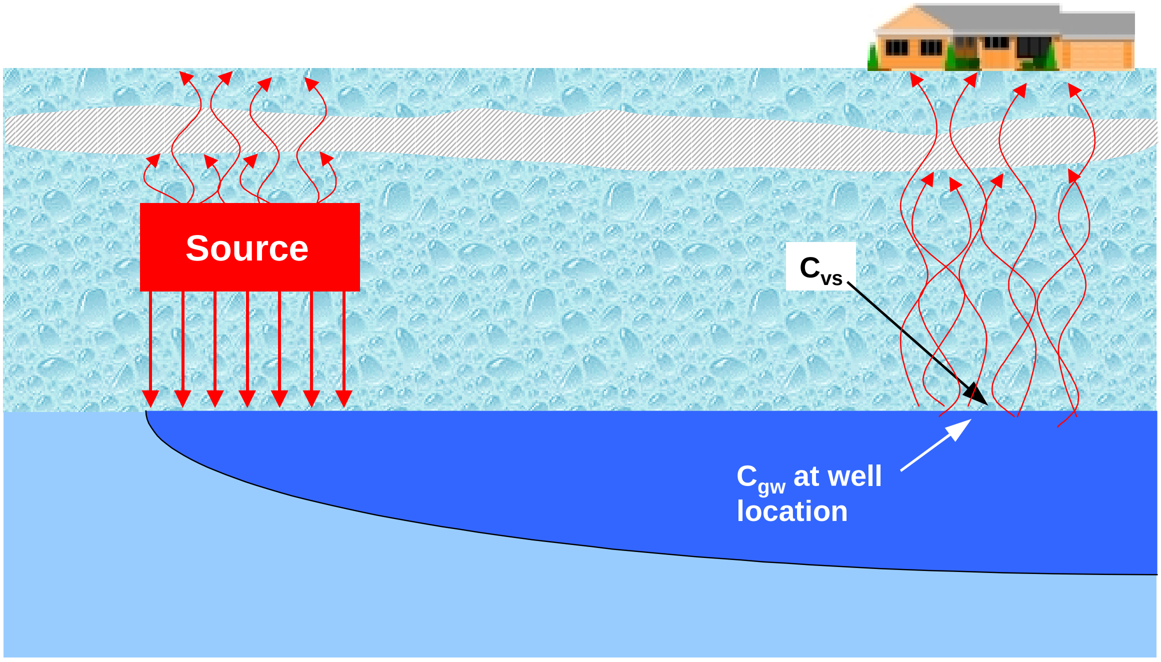

Figure E-3. Vapor Transport from Groundwater Using a Linked Vadose Zone and Dissolved Phase Transport Model

E.7 REFERENCES

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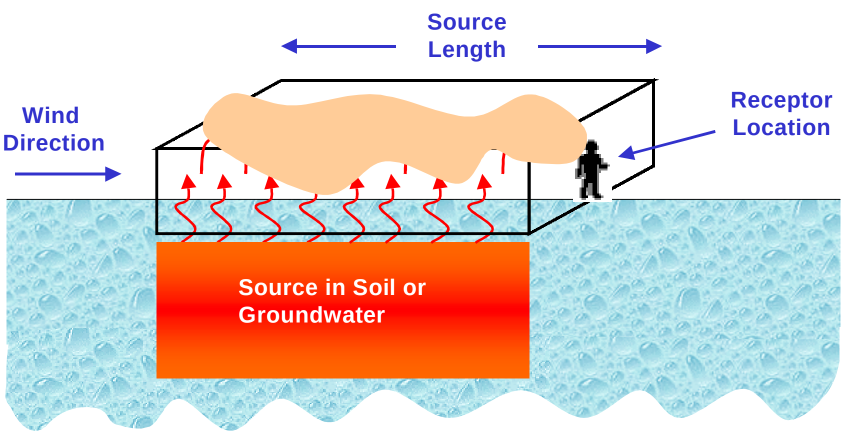
Appendix F

Outdoor Air Model

F.1 MODEL DESCRIPTION

The outdoor air model uses a "box" model to estimate a concentration in the breathing zone directly overlying contaminated soil. This model requires the volatile emission rate to be calculated by one of the soil vapor or groundwater emission models (Appendices D, E, J, or K) as an input. The approach is applicable for on-site exposures only (no distant downwind receptors). Figure F-1 shows the problem geometry.



Note: in the box model the receptor is always assumed to be located at the edge of the box downwind of the source. The most conservative approach is to make the length of the box equal to the longest source dimension.

Figure F-1. Schematic of the Outdoor Air Model.

F.2 APPLICATIONS OF THIS MODEL

This is a partial list of the main applications of the box model:

- This model is a screening model for estimating the worst case air concentrations for an on-site (directly over source) exposure.
- The box model uses the volatile emission flux estimates from one of the soil vapor or groundwater emission models (discussed in Appendices D, E, J or K).
- The volatile emissions are assumed to enter a "box" that is ventilated by the wind. Vertical dispersion of the chemicals out of the box is ignored.
- The receptor is always assumed to be at the downwind edge of the source.
- The wind is assumed to always blow in the direction of the receptor.
- The critical source dimension is the length of the source in the predominant direction of wind flow. If that direction is not known, the longest horizontal dimension of the source should be used for the most conservative assumption.
- Degradation and other loss mechanisms (such as deposition and photolysis) in the air are not considered.
- This model can be used to estimate concentrations in a trench or similar situations, however a reasonable "wind speed" (for the air exchange rate) must be chosen.

F.3 TRANSPORT EQUATION AND PROCESSES

The outdoor air model assumes that the volatile emissions leaving the contaminated soil enter a box-shaped area directly overlying the soil. The box is assumed to be ventilated by the wind and the contaminant is fully mixed. The air concentration is calculated by

$$C_{outdoor} = \frac{FL}{uH}\left(\frac{m}{100cm}\right) \tag{F-1}$$

where

$C_{outdoor}$= concentration in outdoor air [g/cm^3]

F = volatile emission rate from vadose zone impacted soil [g/cm^2/s]

L = length of the box in the direction of air flow (parallel to the wind) [m]

H = height of the box [m]

u = wind speed [m/s]

The vapor flux, *F*, is estimated in RISC using one of the volatile emission models. Note, this model does not have a variable for the width of the box, (i.e. the width of the source perpendicular to the wind direction). The width cancels out of the equation because it is used to calculate both the emission rate in the numerator and the air exchange rate in the denominator.

The user is encouraged to use site-specific wind speed data if available (from nearby weather station or from measurements). The USEPA Soil Screening Guidance Technical Background Document (1995) contains a table of reported average wind speeds for many major US cities. If this data is not available, a conservative value for average wind speed over an open site can be considered to be 2 m/s (4.5 mph).

F.3.1 Dimensions of Box

The height of the box is usually assumed to be the height of a person (~2 m). The length of the box should reflect the length of the vapor source in the predominant wind direction. It should **never** be set to a value less than the long dimension of the source because the model assumes that all of the soil emissions enter the box and are fully mixed. If the box dimensions are less than the source dimensions, the model assumes that the vapors are concentrating (which is not likely in open air). If the predominant direction of wind is not known, the length of the box could be set equal to the longest areal dimension of the source (this would be the most conservative approach).

Note, the size of the box should be chosen to equal the reasonable dimension of an area to which a receptor would be exposed over the entire exposure duration. For example, if a commercial scenario is being considered for an outdoor worker, the size of the box should reflect the area and time frame of exposure. The "box" could be the entire contaminated site over the entire day or only a portion of the site over a few hours.

F.4 DATA REQUIREMENTS

The data requirements for the outdoor air model are shown in Table F-1. Note, the emission rate is not input by the user, it is calculated by one of the volatilization models (either from a soil or groundwater source).

Table F-1. Data Requirements for the Outdoor Air Model.

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
BOX MODEL PARAMETER			
Length of box	m	Site-specific	site-specific
Height of box	m	1	2
Wind Speed	m/s	2	7

F.5 ASSUMPTIONS AND LIMITATIONS OF THE OUTDOOR AIR MODEL

1. The outdoor air model is for on-site exposures only and does not consider receptors located downwind or distant from the source area.
2. The size of the box should reflect a reasonable exposure area and the exposure duration used should be consistent with the time spent in the box by the potential receptor.
3. The length of the box should never be set to a value less than the respective length of the soil or groundwater source.
4. The air is considered to be fully mixed at all times.
5. The wind speed ventilates the box at a constant rate.
6. This model uses the volatile emissions calculated by one of the volatilization models as a source term.

Appendix
G

Volatilization In the Shower/ Volatilization From Sprinklers

G.1 MODEL OVERVIEW

The shower model in RISC is based on Foster and Chrostowski's paper entitled "Integrated Household Exposure Model for Use of Tap Water Contaminated With Volatile Organic Chemicals" (1986). Of the five shower models "on the market", this is the most conservative one, as evaluated by Carver et al (1991). However, the spread of concentrations predicted by the five models is relatively narrow; the Foster and Chrostowski (1986) model predicts a concentration only twice that of the least conservative model. The sprinkler model is a variation of the shower model and is described at the end of this appendix.

In the Foster and Chrostowski (1986) model, a two-film, gas-liquid mass transfer model is used to estimate the amount of chemical volatilized from the water. For the shower exposure, the total amount volatilized during the length of the shower is used to estimate the chemical concentration in shower air. The concentration in shower air is assumed to be fully mixed for the entire duration of the shower. The total mass volatilized is assumed to be in the shower stall at the beginning of the shower and to remain constant throughout the shower. The shower air is assumed to be stagnant (not exchanged with air outside of the shower). For the sprinkler scenario, the outdoor air concentration is calculated using a box model approach similar to the outdoor air model described in Appendix F. In this model, the mass volatilization *rate (rather than the total mass volatilized).* is calculated and the air is assumed to exchange via the wind. In both cases, the shower model is run during the risk calculation (Step 5).

This appendix is divided into two sections, one describing the shower model for a shower exposure and the other describing the sprinkler scenario.

G.2 SHOWER MODEL DESCRIPTION

The concentration in shower air is estimated from:

$$C_{sh} = \frac{M_{sh}}{V_{sh}} \qquad \textbf{(G-1)}$$

where

C_{sh} = air concentration in the shower stall [mg/m^3]

M_{sh} = mass of contaminant volatilized [mg]

V_{sh} = volume of air in the shower stall (or bathroom) [m^3]

The volume of the shower stall is a user input and should reflect the volume of air that the volatile chemicals can occupy. Foster and Chrostowski (1986) use a value of 3 m^3 in their paper for the volume of shower stall. Note that the smaller the volume of air, the higher the shower air concentration, therefore, the more conservative values for volume (e.g. RME value) will be smaller than the average value. The shower air concentration, C_{sh}, is used in the exposure equations (7-5a and 7-5b) to estimate chemical intake due to inhalation of volatile emissions in the shower. The air concentration is assumed to be constant over the entire exposure duration (length of shower).

The mass of contaminant volatilized is estimated from:

$$M_{sh} = f_v \bullet Q \bullet time_{sh} \bullet C_w \bullet \text{ 60 min/hr} \qquad \textbf{(G-2)}$$

where

M_{sh} = mass of contaminant volatilized [mg]

f_v = fraction of contaminant volatilized (calculated in Eqn. G-11) [mg/mg]

Q = volumetric flow rate of water [l/min]

$time_{sh}$ = duration for which the shower water is flowing [hr]

C_w = concentration of contaminant in shower water (tap water) [mg/l]

Estimation of volatile organic chemical (VOC) concentration in the shower air is based on two-film gas-liquid mass transfer theory. First, the volatilization rate of a VOC across the surface of a hypothetical shower droplet is estimated. The total mass volatilized is calculated by multiplying the volatilization rate by the droplet droptime (a user input). The Foster and Chrostowski (1986) approach assumes that the volatilization of the contaminant is limited by the rate of mass-transfer and not by Henry's Law equilibrium. The overall mass-transfer coefficient (K_L) is calculated from the following equation (from two-film boundary theory):

$$K_{\mathrm{L}} = \left[\frac{1}{k_l} + \frac{1}{K_H k_g} \right]^{-1} \qquad \textbf{(G-3)}$$

where

K_L = overall mass transfer coefficient [cm/hr]

K_H = Henry's Law constant for the contaminant [(mg/l)/(mg/l)]

k_g = gas-phase mass-transfer coefficient [cm/hour]

k_l = liquid-phase mass-transfer coefficient [cm/hour]

Equation G-3 describes the mass-transfer rate of a compound at an air-water interface where diffusion may be limited by both liquid- and gas-phase resistances. Empirical values of K_L, k_l, and k_g are situation-specific. Typical values of gas- and liquid-phase mass transfer coefficients (k_g and k_l) have been measured for CO_2 and H_2O and are used to estimate these parameters for other volatile compounds using the following relationships:

$$k_{g(VOC)} = k_{g(H_2O)}\left[\frac{18\ g/mol}{MW_{VOC}}\right]^{0.5} \tag{G-4}$$

$$k_{l(VOC)} = k_{l(CO_2)}\left[\frac{44\ g/mol}{MW_{VOC}}\right]^{0.5} \tag{G-5}$$

where

$k_{g(H2O)}$ = gas-phase mass transfer coefficient for water [cm/hr]

$k_{l(CO2)}$ = liquid-phase mass transfer coefficient for carbon dioxide [cm/hr]

18 = molecular weight of water [g/mol]

44 = molecular weight of carbon dioxide [g/mol]

MW_{VOC} = molecular weight of contaminant [g/mol]

The gas-phase mass transfer coefficient for water, $k_{g(H2O)}$ is assumed to be 3000 cm/hr. The liquid-phase mass transfer coefficient for carbon dioxide, $k_{l(CO2)}$, is assumed to be 20 cm/hr. The overall mass transfer coefficient, K_L (calculated in equation G-3), must be adjusted for the shower water temperature:

$$K'_{L(T_S)} = K_L\left[\frac{T_l\mu_s}{T_s\mu_l}\right]^{-0.5} \tag{G-6}$$

where

$K'_{L(Ts)}$ = temperature-adjusted overall mass transfer coefficient [cm/hr]

T_l = calibration water temperature of K_L [K]

T_s = shower water temperature [K]

μ_l = water viscosity at T_l [g/m-s]

μ_s = water viscosity at T_s [g/m-s]

The water viscosity is estimated from the following relationships (Weast, 1986) depending on the temperature of the water. Note, in the following equations, temperature is in degrees Centigrade.

If T < 20 ^{o}C: $\mu = 100 \cdot 10^{y}$

and

$$y = \frac{1301}{998.33 + 8.1855(T - 20) + 0.00585(T - 20)^{2}} - 3.30233 \qquad \textbf{(G-7)}$$

If T > 20 ^{o}C: $\mu = 1.002 \cdot 10^{y}$

and

$$y = \frac{-1.3272(T - 20) - 0.001053(T - 20)^{2}}{T + 105} \qquad \textbf{(G-8)}$$

Volatilization is assumed to be a first-order process, described by the differential equation:

$$\frac{dC_{sw}}{dt} = -K'_{L}\, aC_{sw} \qquad \textbf{(G-9)}$$

Integrating G-9 yields:

$$C_{sw} = C_{w} e^{-\frac{K'_{L}6t}{d(3600)}} \qquad \textbf{(G-10)}$$

where

C_{sw}	=	concentration of contaminant in shower droplet after time t [mg/l]
C_{w}	=	concentration of contaminant in shower water (tap water) [mg/liter]
a	=	specific interfacial area [cm^{2}-area/cm^{3}-volume]
d	=	shower droplet diameter [cm]
t	=	shower droplet drop time [sec]

In equation G-10, the interfacial area, *a*, has been replaced by the quotient "6/3600d". The ratio *6/d* represents the specific interfacial area per unit volume for a hypothetical shower droplet of diameter d$\left(\frac{area}{volume} = \frac{\pi d^{2}}{\frac{4}{3}\pi r^{3}}\right)$. The value 3,600 is the unit conversion factor used to convert K'_L from cm/hr to cm/sec. The larger the interfacial area for the hypothetical shower droplet, the more rapid the VOC volatilization into the shower stall air.

The aqueous concentration leaving the shower droplet (C_d) is obtained by the mass balance:

$$C_d = C_w(1 - e^{-K'_L t/600d}) \qquad \text{(G-11)}$$

where

C_d = concentration of contaminant leaving the shower droplet [mg/liter]

The term $(1 - e^{-K'_L t/600d})$ represents the fraction volatilized, f_v, used in Equation G-2 to calculate the total mass volatilized during the shower.

Table G-1. Data Requirements for the Shower Model.

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
SHOWER DATA			
Temperature of water	^oC	20	45
Volume of the shower stall	m^3	3	site-specific
Time in the shower (with water flowing)	min	>0	site-specific
Volumetric flow rate of the shower	l/min	>0	site-specific
Shower droplet drop time	s	>0	several seconds
CHEMICAL SPECIFIC DATA (individual chemical component)			
Molecular Weight	g/mol	chem-specific	chem-specific
Concentration in water	mg/l	site-specific	site-specific
Diffusion Coefficient in Air	cm^2/s	chem-specific	chem-specific
Diffusion Coefficient in Water	cm^2/s	chem-specific	chem-specific
Henry's Law coefficient	(mg/l)/(mg/l)	chem-specific	chem-specific

G.3 SPRINKLER VOLATILIZATION MODEL DESCRIPTION

The shower model can also be used to estimate concentration in outdoor air due to volatilization from water droplets emanating from a sprinkler. This exposure route may occur if impacted groundwater (or any impacted water) is used to irrigate residential gardens, where the potable water is obtained from another source (such as a municipal water supply). If the same water is also used for the potable water supply, the indoor groundwater routes will most likely dominate the risk assessment.

The outdoor air concentration in the vicinity of an operating sprinkler is calculated using the volatilization rate calculated by the shower model:

$$C_{air} = \frac{\dot{M}}{W \cdot H \cdot u} \qquad \textbf{(G-12)}$$

where

C_{air} = concentration of contaminant in outdoor air [mg/m^3]

$\dot{M}$ = mass of chemical volatilized per time [mg/s]

W = width of the box perpendicular to the direction of air flow [m]

H = height of the box [m]

u = wind speed [m/s]

The form of Equation G-12 is identical to the outdoor air model (or box model) described in Appendix F. The difference between the outdoor air model described here, and the shower model described above, is that the air in the shower stall is assumed to be stagnant, whereas the air around the sprinkler is assumed to be ventilated by the wind. Note the width of the box is assumed to be constant at 1 m since the actual width of the source does not affect the concentration calculation.

The mass volatilized from the sprinkler water is calculated from:

$$\dot{M} = Q_{sprinkler} \cdot f_v \cdot C_w \qquad \textbf{(G-13)}$$

where

$Q_{sprinkler}$ = flow rate of sprinkler [m^3/s]

The fraction volatilized, f_v, is calculated using equation G-11 ($f_v = 1 - e^{-K'_L t/600d}$). The input parameters should be chosen to reflect outdoor conditions:

- The drop time should represent the length of time that a particular droplet is available to contribute volatile emissions to the outdoor air 'box'. If the water infiltrates into the soil or moves out of the box, then it is assumed to no longer contribute to the volatile emissions. As such, this value may need to be increased to reflect puddled or standing water.
- The temperature of the water will most likely be less than that of shower water.
- The sprinkler droplet diameter is probably larger than that of shower water droplets (especially if the shower has a flow restrictor), however this is a difficult parameter to estimate or measure. The value could be left at the Foster and Chrostowski (1986) default to be conservative.

The data requirements for the irrigation volatilization model are listed in Table G-2.

Table G-2. Data Requirements for the Irrigation Volatilization Model.

	Units	Typical Range of Values	
		Minimum	Maximum
SPRINKLER DATA			
Temperature of water	°C		
Length of outdoor air box	m	site-specific	site-specific
Width of outdoor air box	m	1	1
Height of breathing zone	m	1	2
Wind speed	m/s	>0	5
Time in the sprinkler (with water flowing)	min	>0	site-specific
Volumetric flow rate of the sprinkler	l/min	>0	site-specific
Sprinkler droplet diameter	cm	>0	0.5
Sprinkler droplet drop time	s	>0	several seconds
CHEMICAL-SPECIFIC DATA (individual chemical component)			
Molecular Weight	g/mol	chem-specific	chem-specific
Concentration in water	mg/l	site-specific	site-specific
Diffusion Coefficient in Air	cm^2/s	chem-specific	chem-specific
Diffusion Coefficient in Water	cm^2/s	chem-specific	chem-specific
Henry's Law coefficient	(mg/l)/(mg/l)	chem-specific	chem-specific

G.4 REFERENCES

Carver, J.H., C.S. Seigneur, R.M. Block, T.M. Miller. 1991. Comparison of Exposure Models for Volatile Organics in Tap Water. Proceedings of Hazmacon. April 15, 1991. Santa Clara, California.

Foster, S.A. and P.C. Chrostowski. 1986. Integrated Household Exposure Model for Use of Tap Water Contaminated with Volatile Organic Chemicals. 79th Annual Meeting of the Air Pollution Control Association, Minneapolis, MN.

Weast, R.C., M.J. Astle and W.H. Beyer (eds.), 1986. CRC Handbook of Chemistry and Physics, 67th ed., CRC Press, Inc., Boca Raton, FL.

Appendix H

Tier 1 Look-Up Table

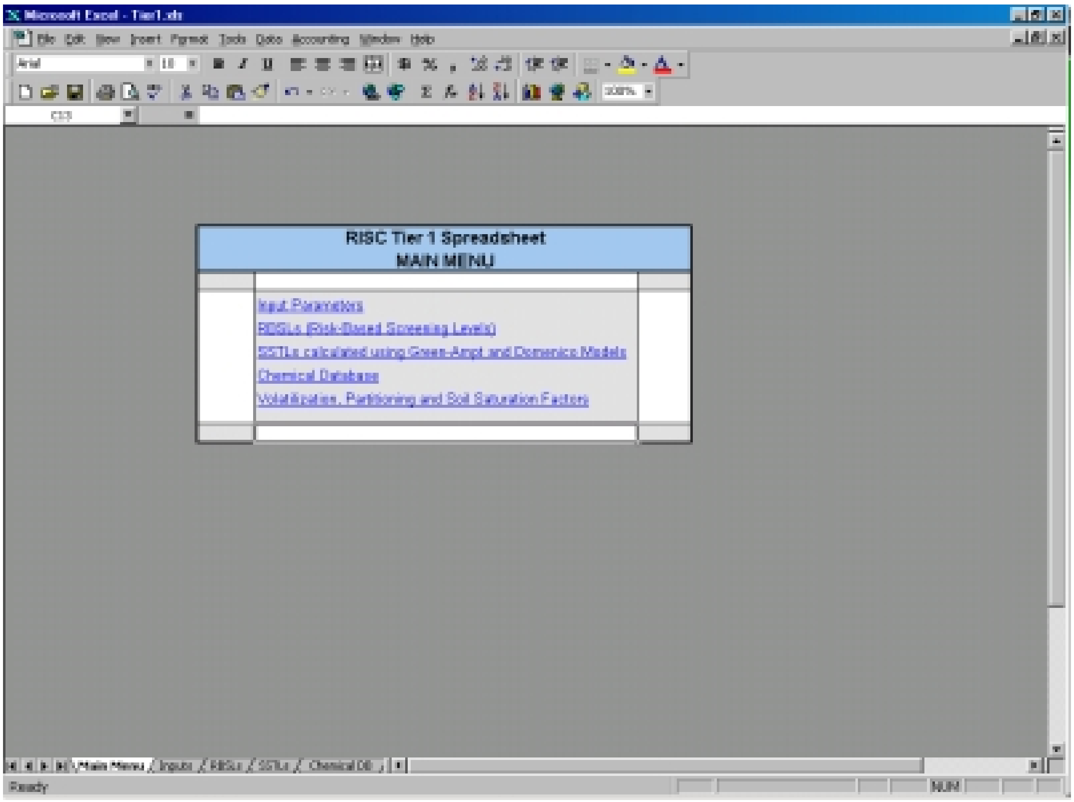
H.1 TIER 1 SPREADSHEET DESCRIPTION

The Tier 1 Look-Up Table is accessed by the “Tier 1 Levels” button on the main screen of the RISC interface. Selecting this button will bring up an Excel spreadsheet containing a Tier 1 spreadsheet based on the algorithms presented in the ASTM RBCA standard.

The spreadsheet is organized into a number of worksheets. There are two ways to navigate through the spreadsheet: (1) using the "Main Menu" the user can click on buttons to switch from one worksheet to another (each sheet has a button to return to the Main Menu), and (2) using the labeled worksheet tabs at the bottom of each Excel screen.

Table H-1 shows the Main Menu worksheet and Table H-2 shows the Inputs sheet with the labeled tabs at the bottom of the Excel screen.

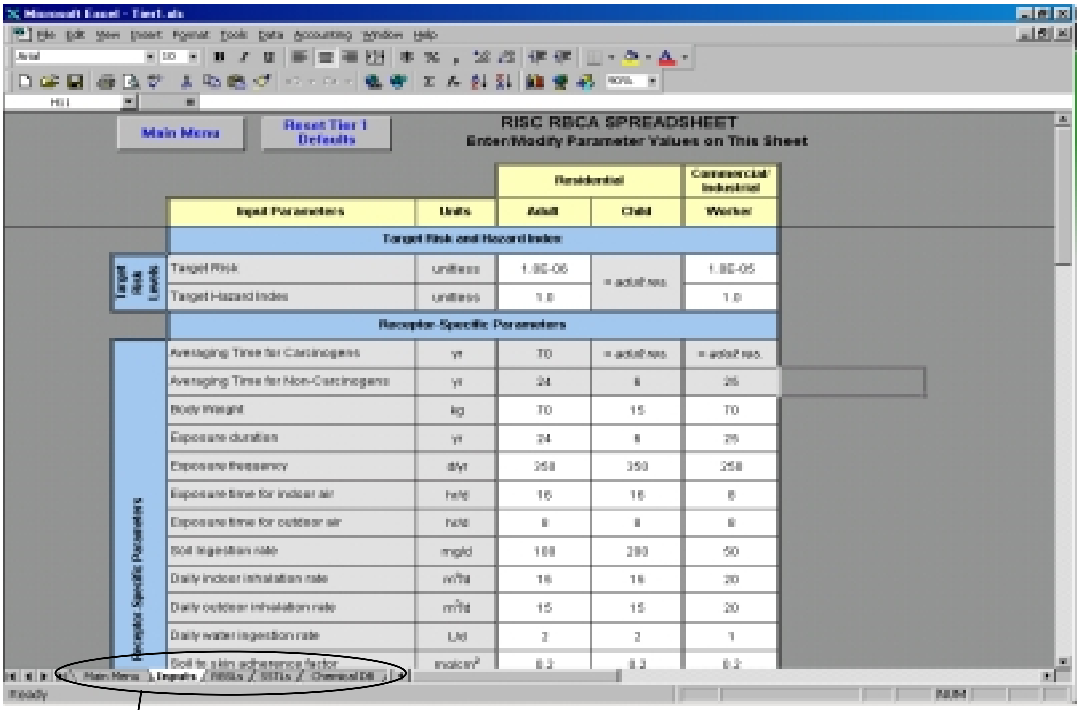
The worksheet, titled “Inputs”, contains the input variables that may be changed by the user. The worksheet, “RBSLs” (risk-based screening levels) contains the Tier 1 risk-based screening levels. The chemical database is in the worksheet entitled “Chemical DB”.



RISC Tier 1 Spreadsheet
MAIN MENU

Input Parameters
RBSLs (Risk-Based Screening Levels)
SSTLs calculated using Green-Ampt and Domenico Models
Chemical Database
Volatilization, Partitioning and Soil Saturation Factors

Figure H-1. Main Menu of the Tier 1 Spreadsheet



RISC RBCA SPREADSHEET
Enter/Modify Parameter Values on This Sheet

		Residential		Commercial/ Industrial
Input Parameters	Units	Adult	Child	Worker
Target Risk and Hazard Index				
Target Risk	unitless	1.0E-06	= adult res	1.0E-05
Target Hazard Index	unitless	1.0		1.0
Receptor-Specific Parameters				
Averaging Time for Carcinogens	yr	70	= adult res	= adult res
Averaging Time for Non-Carcinogens	yr	24	6	25
Body Weight	kg	70	15	70
Exposure duration	yr	24	6	25
Exposure frequency	d/yr	350	350	250
Exposure time for indoor air	hr/d	16	16	8
Exposure time for outdoor air	hr/d	8	8	8
Soil ingestion rate	mg/d	100	200	50
Daily indoor inhalation rate	m^3/d	15	15	20
Daily outdoor inhalation rate	m^3/d	15	15	20
Daily water ingestion rate	L/d	2	2	1
Soil to skin adherence factor	mg/cm^2	0.2	0.2	0.2

Worksheet Tabs

Figure H-2. "Inputs" Sheet Showing Worksheet Tabs

Tables H-1 through H-5 of this appendix present the equations contained in the Tier 1 spreadsheet for each of the five media considered: surficial soil, subsurface soil, groundwater, air, and water used for recreation (surface water).

The equations used to calculate the Tier 1 values are identical to the ones suggested in the ASTM's Risk-Based Corrective Action standard (ASTM, 1995) with the following exceptions:

- The equations used to calculate RBSLs for carcinogenic and non-carcinogenic health effects use two different receptor definitions:
  - For carcinogenic health effects under the residential land use scenario, the equations assume an additive child/adult receptor; that is, the receptor is assumed to be a young child for six years of the 30-year exposure duration and an adult for the remaining 24 years.
  - For non-carcinogenic health effects under the residential land use scenario, the equations assume that the receptor is always a child.
  - For both carcinogenic and non-carcinogenic health effects under the commercial/ industrial land use scenario, the equations assume the commercial/industrial receptor defined in the inputs sheet (which differs from the ASTM assumptions).
- Fate and transport effects in both the vadose and saturated zones can be incorporated in the Tier 1 spreadsheet (but not the ASTM guidance) by including the Green-Ampt algorithm and Domenico equation, respectively. However, if the user wants to match the numbers in the ASTM document, these modifications can be readily bypassed by placing the receptor at the source which, in turn, is placed at the water table.

Tables H-1 and H-2 present the equations used to calculate RBSLs for carcinogenic and non-carcinogenic effects, respectively. Table H-3 defines the exposure parameters used in the RBSL equations. The equations used to calculate the various volatilization factors, leaching factors, and effective diffusion coefficients are presented in Table H-4. The soil, building, surface and subsurface parameter variables used in the Table H-4 equations are defined in Table H-5.

To match the adult-only case of the ASTM standard or other software, assign adult parameters to the child case and make sure that the total exposure duration equals 30 years. For example, assign an exposure duration of 24 years for the adult and 6 years for the “child”.

H.2 GREEN-AMPT MODEL

In Tier 1, the vadose zone leaching algorithm assumes that the vadose zone source extends to the water table and assumes that there is no degradation or dispersion occurring in the vadose zone. The Green-Ampt model can be used as a model to predict the effects of degradation in the vadose zone. The Domenico model (described in the next section) is used to account for both dispersion and degradation in the saturated zone.

The Green-Ampt equation (1911) is used to calculate a minimal travel time for a wetting front to move through the vadose zone (from the source to the water table). The travel time is then used to estimate a vadose zone attenuation coefficient considering degradation processes. This algorithm is used by both the U.S. States of South Carolina and Ohio to estimate risk-based screening levels under their Underground Storage Tank divisions.

The Green-Ampt model assumes that water infiltrates through the vadose zone soil as a sharp wetting front. The volumetric water content above the wetting front is assumed to be completely saturated (equal to the total porosity). Since saturated conditions produce the highest permeability in the vadose zone (permeability decreases as soil moisture content decreases) this equation estimates the “fastest possible travel time”. Therefore it is conservative when used to calculate degradation losses.

Once the pore water velocity is calculated, the retarded velocity for each chemical is calculated. The chemical-specific travel time from the middle of the source to the groundwater is used to estimate degradation losses on the way to the groundwater. The SSTL (site-specific target level) sheet of the Tier 1 spreadsheet contains the new risk-based screening levels incorporating the Green-Ampt algorithm. Two different

SSTLs are generated: one using the "high-end" (or upper estimate) degradation rate and one using the "low-end" rate defined in the chemical database. The values of the degradation rates in the chemical database may be modified by the user as site-specific or new information becomes available.

For the default parameters in the Tier 1 spreadsheet, modifying the RBSLs using Green-Ampt produces no noticeable increase in clean-up levels for most chemicals. As the input parameters are changed to reflect site-specific conditions (e.g. lower infiltration rate, greater distance to groundwater) the SSTLs calculated with Green-Ampt may increase.

Table H-6 presents the Green-Ampt equations and Table H-7 presents the parameter definitions.

H.3 DOMENICO GROUNDWATER MODEL

In Tier 1, the exposure point in groundwater is assumed to be directly below the vadose zone source. The leaching and groundwater mixing algorithms do not account for dispersion or degradation in either the vadose or saturated zones. The Green-Ampt model described above is one way to account for degradation in the vadose zone.

The Domenico model is used to account for degradation and dispersion in groundwater. It is applicable for cases where the groundwater receptor point is downgradient of the source. The Domenico equation can be combined with either the ASTM soil leaching equation (LF_{sw}) or the leaching equation using the Green-Ampt equations. The SSTLs calculated for each of these options are shown on the "SSTLs" sheet in the Tier 1 spreadsheet.

H.4 REFERENCES

ASTM. 1995. Standard Guide to Risk-Based Corrective Action Applied at Petroleum Release Sites, ASTM E1739-95, Philadelphia, PA.

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Green, W.H. and G.A. Ampt. 1911. "Studies in Soil Physics. I. The Flow of Air and Water through Soils", *Journal of Agricultural Science*, 4:1-24.

Table H-1. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Carcinogenic Effects

(page 1 of 5)

RBSLs in SURFICIAL SOIL [mg/kg]

Ingestion Of Soil, Dermal Contact With Soil,

Inhalation Of Vapors and Particulates in Outdoor Air

Residential

$\mathrm{RBSL}_{\text{surf soil}} =$

$$\frac{TR}{\left[\begin{array}{l}\dfrac{\mathrm{EF_c}\times\mathrm{ED_c}}{\mathrm{BW_c}\times\mathrm{AT_{carc}}\times 365\,\dfrac{\mathrm{d}}{\mathrm{yr}}}\left[\left(\mathrm{SF_o}\times 10^{-6}\,\dfrac{\mathrm{kg}}{\mathrm{mg}}\times\left(\mathrm{ING(soil)_c}\times\mathrm{RAF_o}+\mathrm{SSA(soil)_c}\times\mathrm{M}\times\mathrm{RAF_d}\right)\right)+\left(\mathrm{SF_{inh}}\times\mathrm{INH(out\ air)_c}\times\left(\mathrm{VF_{ss}}+\mathrm{VF_p}\right)\right)\right]\\[2ex] +\dfrac{\mathrm{EF_a}\times\mathrm{ED_a}}{\mathrm{BW_a}\times\mathrm{AT_{carc}}\times 365\,\dfrac{\mathrm{d}}{\mathrm{yr}}}\left[\left(\mathrm{SF_o}\times 10^{-6}\,\dfrac{\mathrm{kg}}{\mathrm{mg}}\times\left(\mathrm{ING(soil)_a}\times\mathrm{RAF_o}+\mathrm{SSA(soil)_a}\times\mathrm{M}\times\mathrm{RAF_d}\right)\right)+\left(\mathrm{SF_{inh}}\times\mathrm{INH(out\ air)_a}\times\left(\mathrm{VF_{ss}}+\mathrm{VF_p}\right)\right)\right]\end{array}\right]}$$

Commercial/Industrial

$RBSL_{surf\ soil} =$

$$\frac{TR\times BW_i\times AT_{carc}\times 365\,\dfrac{d}{yr}}{EF_i\times ED_i\left[\left(SF_o\times 10^{-6}\,\dfrac{kg}{mg}\times\left(ING(soil)_i\times RAF_o+SSA(soil)_i\times M\times RAF_d\right)\right)+\left(SF_{inh}\times INH(out\ air)_i\times\left(VF_{ss}+VF_p\right)\right)\right]}$$

If the RBSL calculated for surficial soil exceeds the saturated soil concentration, C_{sat}, the target risk cannot be exceeded for any concentration and “SAT” is entered in the “RBSLs” worksheet. The equation used to calculate C_{sat} is defined in Table H-4.

Table H-1. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Carcinogenic Effects

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RBSLs in SUBSURFACE SOIL [mg/kg]

Inhalation of Outdoor Air

Residential and Commercial/Industrial

$$\mathrm{RBSL}_{\mathrm{sub\ soil}} = \frac{\mathrm{RBSL}_{\mathrm{out\ air}}}{\mathrm{VF}_{\mathrm{samb}}} \times 10^{-3} \frac{\mathrm{mg}}{\mu \mathrm{g}}$$

RBSLs in SUBSURFACE SOIL [mg/kg]

Inhalation of Indoor Air

Residential and Commercial/Industrial

$$RBSL_{sub\ soil} = \frac{RBSL_{ind\ air}}{VF_{sesp}} \times 10^{-3} \frac{mg}{\mu g}$$

RBSLs in SUBSURFACE SOIL [mg/kg]

Leaching to Groundwater and Ingestion of Groundwater

Residential and Commercial/Industrial

$$RBSL_{sub\ soil} = \frac{RBSL_{gw}}{LF_{sw}}$$

If the RBSL calculated for subsurface soil exceeds the saturated soil concentration, C_{sat}, the target risk cannot be exceeded for any concentration and “SAT” is entered in the “RBSLs” worksheet. The equation used to calculate C_{sat} is defined in Table H-4.

Table H-1. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Carcinogenic Effects

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RBSLs in GROUNDWATER [mg/l]

Ingestion of Groundwater

Residential

$$RBSL_{gw} = \frac{TR}{\left[\frac{ED_c \times EF_c \times ING(gw)_c \times SF_o}{BW_c \times AT_{carc}} + \frac{ED_a \times EF_a \times ING(gw)_a \times SF_o}{BW_a \times AT_{carc}}\right]} \times 365 \frac{d}{yr}$$

Commercial/Industrial

$$RBSL_{gw} = \frac{TR \times AT_{carc} \times BW_i}{SF_o \times EF_i \times ED_i \times ING(gw)_i} \times 365 \frac{d}{yr}$$

RBSLs in GROUNDWATER [mg/l]

Volatilization from Groundwater and Inhalation of Indoor Air

Residential and Commercial/Industrial

$$RBSL_{gw} = \frac{RBSL_{ind\ air}}{VF_{wesp}} \times 10^{-3} \frac{mg}{\mu g}$$

RBSLs in GROUNDWATER [mg/l]

Volatilization from Groundwater and Inhalation of Outdoor Air

Residential and Commercial/Industrial

$$RBSL_{gw} = \frac{RBSL_{out\ air}}{VF_{wamb}} \times 10^{-3} \frac{mg}{\mu g}$$

If the RBSL calculated for groundwater exceeds the solubility of the chemical in water, the target risk cannot be exceeded for any concentration and “>SOL” is entered in the “RBSLs” worksheet.

Table H-1. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Carcinogenic Effects

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RBSLs in Air [μg/m^3]

Inhalation of Indoor Air

Residential

$$RBSL_{ind\ air} =$$

$$\frac{TR}{\left[\frac{ED_c \times EF_c \times INH(ind\ air)_c \times SF_{inh}}{BW_c \times AT_{carc}} + \frac{ED_a \times EF_a \times INH(ind\ air)_a \times SF_{inh}}{BW_a \times AT_{carc}}\right]} \times 365\frac{d}{yr} \times 10^3\frac{\mu g}{mg}$$

Commercial/Industrial

$$RBSL_{ind\ air} = \frac{TR \times AT_{carc} \times BW_i}{SF_i \times EF_i \times ED_i \times INH(ind\ air)_i} \times 365\frac{d}{yr} \times 10^3\frac{\mu g}{mg}$$

RBSLs in Air [μg/m^3]

Inhalation of Outdoor Air

Residential

$$RBSL_{out\ air} =$$

$$\frac{TR}{\left[\frac{ED_c \times EF_c \times INH(out\ air)_c \times SF_{inh}}{BW_c \times AT_{carc}} + \frac{ED_a \times EF_a \times INH(out\ air)_a \times SF_{inh}}{BW_a \times AT_{carc}}\right]} \times 365\frac{d}{yr} \times 10^3\frac{\mu g}{mg}$$

Commercial/Industrial

$$RBSL_{out\ air} = \frac{TR \times AT_{carc} \times BW_i}{SF_i \times EF_i \times ED_i \times INH(out\ air)_i} \times 365\frac{d}{yr} \times 10^3\frac{\mu g}{mg}$$

Table H-1. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Carcinogenic Effects

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RBSLs in Surface Water for Recreational Use [mg/l]

Ingestion and Dermal Contact

Residential

$$\mathrm{RBSL_{sw}} = \frac{\mathrm{TR}}{\left[\dfrac{\mathrm{EF(sw)_c} \times \mathrm{ED_c} \times \mathrm{SF_o}}{\mathrm{BW_c} \times \mathrm{AT_{carc}} \times 365\dfrac{\mathrm{d}}{\mathrm{yr}}}\left(\mathrm{ING(sw)_c} + \mathrm{SSA(total)_c} \times \dfrac{\mathrm{PC}}{10^3\,\mathrm{cm^3/l}}\right) + \dfrac{\mathrm{EF(sw)_a} \times \mathrm{ED_a} \times \mathrm{SF_o}}{\mathrm{BW_a} \times \mathrm{AT_{carc}} \times 365\dfrac{\mathrm{d}}{\mathrm{yr}}}\left(\mathrm{ING(sw)_a} + \mathrm{SSA(total)_a} \times \dfrac{\mathrm{PC}}{10^3\,\mathrm{cm^3/l}}\right)\right]}$$

Commercial/Industrial

Scenario not considered

If the RBSL calculated for water used for recreation exceeds the solubility of the chemical in water, the target risk cannot be exceeded for any concentration and “>SOL” is entered in the “RBSLs” worksheet.

Table H-2. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Non-Carcinogenic Effects

(page 1 of 5)

RBSLs in SURFICIAL SOIL [mg/kg]

Ingestion Of Soil, Dermal Contact With Soil, Inhalation Of Vapors and Particulates in Outdoor Air

Residential

$$RBSL_{surf\ soil} = \frac{THQ \times BW_c \times AT_{haz} \times 365\,\frac{d}{yr}}{EF_c \times ED_c \left[\frac{\left(10^{-6}\,\frac{kg}{mg} \times \left(ING(soil)_c \times RAF_o + SSA(soil)_c \times M \times RAF_d\right)\right)}{RfD_o} + \frac{\left(INH(out\ air)_c \times \left(VF_{ss} + VF_p\right)\right)}{RfD_{inh}} \right]}$$

Commercial/Industrial

$$RBSL_{surf\ soil} = \frac{THQ \times BW_i \times AT_{haz} \times 365\,\frac{d}{yr}}{EF_i \times ED_i \left[\frac{\left(10^{-6}\,\frac{kg}{mg} \times \left(ING(soil)_i \times RAF_o + SSA(soil)_i \times M \times RAF_d\right)\right)}{RfD_o} + \frac{\left(INH(out\ air)_i \times \left(VF_{ss} + VF_p\right)\right)}{RfD_{inh}} \right]}$$

If the RBSL calculated for surficial soil exceeds the saturated soil concentration, C_{sat}, the target risk cannot be exceeded for any concentration and “SAT” is entered in the “RBSLs” worksheet. The equation used to calculate C_{sat} is defined in Table H-4.

Table H-2. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Non-Carcinogenic Effects

(Page 2 of 5)

RBSLs in SUBSURFACE SOIL [mg/kg]

Inhalation of Outdoor Air

Residential and Commercial/Industrial

$$\mathrm{RBSL}_{\mathrm{sub\ soil}} = \frac{\mathrm{RBSL}_{\mathrm{out\ air}}}{\mathrm{VF}_{\mathrm{samb}}} \times 10^{-3}\ \frac{\mathrm{mg}}{\mu\mathrm{g}}$$

RBSLs in SUBSURFACE SOIL [mg/kg]

Inhalation of Indoor Air

Residential and Commercial/Industrial

$$RBSL_{sub\ soil} = \frac{RBSL_{ind\ air}}{VF_{sesp}} \times 10^{-3}\ \frac{mg}{\mu g}$$

RBSLs in SUBSURFACE SOIL [mg/kg]

Leaching to Groundwater and Ingestion of Groundwater

Residential and Commercial/Industrial

$$RBSL_{sub\ soil} = \frac{RBSL_{gw}}{LF_{sw}}$$

If the RBSL calculated for subsurface soil exceeds the saturated soil concentration, C_{sat}, the target risk cannot be exceeded for any concentration and “SAT” is entered in the “RBSLs” worksheet. The equation used to calculate C_{sat} is defined in Table H-4.

Table H-2. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Non-Carcinogenic Effects

(page 3 of 5)

RBSLs in GROUNDWATER [mg/l]

Ingestion of Groundwater

Residential

$$RBSL_{gw} = \frac{THQ \times AT_{haz} \times BW_c \times RfD_o}{EF_c \times ED_c \times ING(gw)_c} \times 365 \frac{d}{yr}$$

Commercial/Industrial

$$RBSL_{gw} = \frac{THQ \times AT_{haz} \times BW_i \times RfD_o}{EF_i \times ED_i \times ING(gw)_i} \times 365 \frac{d}{yr}$$

RBSLs in GROUNDWATER [mg/l]

Volatilization from Groundwater and Inhalation of Indoor Air

Residential and Commercial/Industrial

$$RBSL_{gw} = \frac{RBSL_{ind\ air}}{VF_{wesp}} \times 10^{-3} \frac{mg}{\mu g}$$

RBSLs in GROUNDWATER [mg/l]

Volatilization from Groundwater and Inhalation of Outdoor Air

Residential and Commercial/Industrial

$$RBSL_{gw} = \frac{RBSL_{out\ air}}{VF_{wamb}} \times 10^{-3} \frac{mg}{\mu g}$$

If the RBSL calculated for groundwater exceeds the solubility of the chemical in water, the target risk cannot be exceeded for any concentration and ">SOL" is entered in the "RBSLs" worksheet.

Table H-2. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Non-Carcinogenic Effects

(page 4 of 5)

RBSLs in Air [μg/m^3]

Inhalation of Indoor Air

Residential

$$RBSL_{ind\ air} = \frac{THQ \times AT_{haz} \times BW_c \times RfD_{inh}}{EF_c \times ED_c \times INH(ind\ air)_c} \times 365 \frac{d}{yr} \times 10^3\ \frac{\mu g}{mg}$$

Commercial/Industrial

$$RBSL_{ind\ air} = \frac{THQ \times AT_{haz} \times BW_i \times RfD_{inh}}{EF_i \times ED_i \times INH(ind\ air)_i} \times 365 \frac{d}{yr} \times 10^3\ \frac{\mu g}{mg}$$

RBSLs in Air [μg/m^3]

Inhalation of Outdoor Air

Residential

$$RBSL_{out\ air} = \frac{THQ \times AT_{haz} \times BW_c \times RfD_{inh}}{EF_c \times ED_c \times INH(out\ air)_c} \times 365 \frac{d}{yr} \times 10^3\ \frac{\mu g}{mg}$$

Commercial/Industrial

$$RBSL_{out\ air} = \frac{THQ \times AT_{haz} \times BW_i \times RfD_{inh}}{EF_i \times ED_i \times INH(out\ air)_i} \times 365 \frac{d}{yr} \times 10^3\ \frac{\mu g}{mg}$$

Table H-2. Equations Used to Calculate Tier 1 Risk-Based Screening Levels (RBSLs) – Non-Carcinogenic Effects

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RBSLs in Water Used for Recreation [mg/l]

Ingestion and Dermal Contact

Residential

$$RBSL_{sw} = \frac{THQ \times RfD_o \times BW_c \times AT_{haz} \times 365\,\frac{d}{yr}}{EF(sw)_c \times ED_c \times ET(sw)_c \times \left(ING(sw)_c + SSA(total)_c \times PC \times 10^{-3}\,\frac{l}{cm^3} \right)}$$

Commercial/Industrial

Scenario not considered

If the RBSL calculated for water used for recreation exceeds the solubility of the chemical in water, the target risk cannot be exceeded for any concentration and “>SOL” is entered in the “RBSLs” worksheet.

Table H-3. Exposure Parameter Variables Used in Tables H-1 and H-2.

(page 1 of 2)

Parameters	Definitions	Units
AT_{carc}	averaging time for carcinogens	years
AT_{haz}	averaging time for non-carcinogens	years
$BW_{c,a,i}$	body weight (child, adult, commercial/industrial)	kg
C_{sat}	saturated soil concentration*	mg/kg
$ED_{c,a,i}$	exposure duration (child, adult, commercial/industrial)	years
$EF(sw)_{c,a}$	exposure frequency to water used for recreation (child, adult)	d/yr
$EF_{c,a,i}$	exposure frequency, for all pathways except water used for recreation (child, adult, commercial/industrial)	d/year
$ET(sw)_{c,a}$	exposure time to water used for recreation (child, adult)	hr/day
$ING(gw)_{c,a,i}$	groundwater ingestion rate (child, adult, commercial/industrial)	l/day
$ING(soil)_{c,a,i}$	soil ingestion rate (child, adult, commercial/industrial)	mg/d
$ING(sw)_{c,a}$	water ingestion rate during recreation (child, adult)	l/hr
$INH(ind\ air)_{c,a,i}$	indoor inhalation rate (child, adult, commercial/industrial)	
$INH(out\ air)_{c,a,i}$	outdoor inhalation rate (child, adult, commercial/industrial)	m^3/d
LF	leaching factor* (chemical-specific)	(mg/l)/(mg/kg)
M	soil to skin adherence factor	mg/cm^2
PC	skin permeability coefficient for chemicals in water (chemical-specific)	cm/hr
RAF_d	dermal relative absorption factor (chem.-specific)	mg/mg
RAF_o	oral relative absorption factor (chemical-specific)	mg/mg
RfD_{inh}	inhalation chronic reference dose	mg/kg-d
RfD_o	oral chronic reference dose	mg/kg-d
SF_{inh}	inhalation slope factor	1/(mg/kg-d)
SF_o	oral slope factor	1/(mg/kg-d)
$SSA(soil)_{c,a,i}$	skin surface area exposed to soil (child, adult, commercial/industrial)	cm^2
$SSA(total)_{c,a}$	total skin surface area exposed to water used for recreation (child, adult)	cm^2
THQ	target hazard quotient	unitless
TR	target individual excess lifetime cancer risk	unitless

*See Table H-4 for definition

Table H-3. Exposure Parameter Variables Used in Tables H-1 and H-2.

(page 2 of 2)

Parameters	Definitions	Units
VF_{ss}	volatilization factor from surficial soils to outdoor air (vapors) * (chemical-specific)	$(mg/m^3)/(mg/kg)$
VF_p	volatilization factor from surficial soils to outdoor air (particulates)* (chemical-specific)	$(mg/m^3)/(mg/kg)$
VF_{samb}	volatilization factor from subsurface soils to outdoor air* (chemical-specific)	$(mg/m^3)/(mg/kg)$
VF_{sesp}	volatilization factor from subsurface soils to indoor air* (chemical-specific)	$(mg/m^3)/(mg/kg)$
VF_{wesp}	volatilization factor from groundwater to indoor air* (chemical-specific)	$(mg/m^3)/(mg/l)$
VF_{wamb}	volatilization factor from groundwater to outdoor air* (chemical-specific)	$(mg/m^3)/(mg/l)$

*See Table H-4 for definition

Table H-4. Volatilization Factors, Leaching Factor, and Effective Diffusion Coefficients
(Page 1 of 3)

VF$_{ss}$: Volatilization factor from surficial soils to outdoor air (vapors) [(mg/m^{3}air)/(mg/kg soil)]

$$VF_{ss} = \frac{2W\rho_s}{U_{air}\delta_{air}}\sqrt{\frac{D_s^{eff}H}{\pi(\theta_{ws}+k_s\rho_s+H\theta_{as})\tau}}\times 10^3\ \frac{cm^3kg}{m^3g}$$

$$or:$$

$$VF_{ss} = \frac{W\rho_s d}{U_{air}\delta_{air}\tau}\times 10^3\ \frac{cm^3kg}{m^3g};\quad whichever\ is\ less$$

VF$_p$: Volatilization factor from surficial soils to outdoor air (particulates) [(mg/m^{3}air)/(mg/kg soil)]

$$VF_p = \frac{P_eW}{U_{air}\delta_{air}}\times 10^3\ \frac{cm^3kg}{m^3g}$$

VF$_{samb}$: Volatilization factor from subsurface soils to outdoor (ambient) air [(mg/m^{3}air)/(mg/kg soil)]

$$VF_{samb} = \frac{H\rho_s}{\left[\theta_{ws}+k_s\rho_s+H\theta_{as}\right]\left(1+\frac{U_{air}\delta_{air}L_s}{D_s^{eff}W}\right)}x10^3\ \frac{cm^3kg}{m^3g}$$

VF$_{sesp}$: Volatilization factor from subsurface soils to indoor (enclosed-space) air [(mg/m^{3}air)/(mg/kg soil)]

$$VF_{sesp} = \frac{\frac{H\rho_s}{\left[\theta_{ws}+k_s\rho_s+H\theta_{as}\right]}\left[\frac{D_s^{eff}/L_s}{ER\cdot L_B}\right]}{1+\left[\frac{D_s^{eff}/L_s}{ER\cdot L_B}\right]+\left[\frac{D_s^{eff}/L_s}{(D^{eff}{}_{crack}/L_{crack})\eta}\right]}x10^3\ \frac{cm^3kg}{m^3g}$$

Table H-4. Volatilization Factors, Leaching Factor, and Effective Diffusion Coefficients

(Page 2 of 3)

VF$_{wesp}$: Volatilization factor from groundwater to indoor (enclosed space) air
[(mg/m^{3}air)/(mg/l H_2O)]

$$VF_{wesp} = \frac{H\left[\dfrac{D_{ws}^{eff}/L_{gw}}{ER\ L_B}\right]}{1+\left[\dfrac{D_{ws}^{eff}/L_{gw}}{ER\ L_B}\right]+\left[\dfrac{D_{ws}^{eff}/L_{gw}}{(D_{crack}^{eff}/Lcrack)\,\eta}\right]} \times 10^3\ \frac{l}{m^3}$$

VF$_{wamb}$: Volatilization factor from groundwater to outdoor (ambient) air
[(mg/m^{3}air)/(mg/l H_2O)]

$$VF_{wamb} = \frac{H}{1+\left[\dfrac{U_{air}\delta_{air}L_{gw}}{WD_{ws}^{eff}}\right]} \times 10^3\ \frac{l}{m^3}$$

LF$_{sw}$: Leaching factor from subsurface soil to groundwater
[(mg/l H_2O)/(mg/kg soil)]

$$LF_{sw} = \frac{\rho_s}{\left[\theta_{ws}+k_s\rho_s+H\theta_{as}\right]\left(1+\dfrac{U_{gw}\delta_{gw}}{IW}\right)}\ x\ \frac{cm^3kg}{l\ g}$$

C$_{sat}$: Soil concentration at which dissolved pore-water and
vapor phases become saturated
[(mg/kg soil)]

$$C_{sat} = \frac{S}{\rho_s}\left[\theta_{ws}+k_s\rho_s+H\theta_{as}\right]\ x\ \frac{l\ g}{cm^3kg}$$

Table H-4. Volatilization Factors, Leaching Factor, and Effective Diffusion Coefficients

(Page 3 of 3)

$\mathbf{D_s^{eff}}$: Effective diffusion coefficient in soil based on vapor-phase concentration [cm^2/s]

$$D_s^{eff} = D^{air}\frac{\theta_{as}^{3.33}}{\theta_T^2} + D^{water}\left(\frac{1}{H}\right)\frac{\theta_{ws}^{3.33}}{\theta_T^2}$$

$\mathbf{D_{crack}^{eff}}$: Effective diffusion coefficient through foundation cracks [cm^2/s]

$$D_{crack}^{eff} = D^{air}\frac{\theta_{acrack}^{3.33}}{\theta_T^2} + D^{water}\left(\frac{1}{H}\right)\frac{\theta_{wcrack}^{3.33}}{\theta_T^2}$$

$\mathbf{D_{cap}^{eff}}$: Effective diffusion coefficient through capillary fringe [cm^2/s]

$$D_{cap}^{eff} = D^{air}\frac{\theta_{acap}^{3.33}}{\theta_T^2} + D^{water}\left(\frac{1}{H}\right)\frac{\theta_{wcap}^{3.33}}{\theta_T^2}$$

$\mathbf{D_{ws}^{eff}}$: Effective diffusion coefficient between groundwater and soil surface (depth-weighted average) [cm^2/s]

$$D_{ws}^{eff} = \frac{\left(h_{cap} + h_v\right)}{\left[\frac{h_{cap}}{D_{cap}^{eff}} + \frac{h_v}{D_s^{eff}}\right]}$$

Table H-5. Soil, Building, Surface, and Subsurface Parameters Used in Table H-4.

Parameters	Definitions	Units
d	lower depth of surficial soil zone	cm
D^{air}	diffusion coefficient in air (chemical-specific)	cm^2/s
D^{water}	diffusion coefficient in water (chemical-specific)	cm^2/s
ER	indoor air exchange rate	s^{-1}
f_{oc}	fraction organic carbon in soil	g OC/g soil
H	henry's law coefficient	$(cm^3\text{-}H_2O)/(cm^3\text{-air})$
h_{cap}	thickness of capillary fringe	cm
h_v	thickness of vadose zone	cm
I	infiltration rate of water through vadose zone	cm/yr
k_{oc}	carbon-water sorption coefficient	cm^3 H_2O/g OC
k_s	soil-water sorption coefficient (k_{oc} x f_{oc})	cm^3 H_2O/g soil
L_B	indoor air volume/infiltration area ratio	cm
L_{crack}	foundation thickness	cm
L_{gw}	depth to groundwater ($h_{cap}+h_v$)	cm
L_s	depth to subsurface soil sources	cm
P_e	particulate emission rate	$g/cm^2\text{-}s$
S	pure chemical solubility in water	mg/L
U_{air}	wind speed above ground surface in outdoor air mixing zone	cm/s
U_{gw}	groundwater Darcy velocity (gradient x hydraulic conductivity)	cm/yr
W	width of source area parallel to wind, or groundwater flow direction	cm
δ_{air}	outdoor air mixing zone height	cm
δ_{gw}	groundwater mixing zone thickness	cm
η	areal fraction of cracks in building foundation	$(cm^2$ cracks$)/(cm^2$ area$)$
θ_{acap}	volumetric air content in capillary fringe soils	$(cm^3$ air$)/(cm^3$ soil$)$
θ_{acrack}	volumetric air content in foundation cracks	$(cm^3$ air$)/(cm^3$ soil$)$
θ_{as}	volumetric air content in vadose zone soils	$(cm^3$ air$)/(cm^3$ soil$)$
θ_T	total soil porosity	$(cm^3$ voids$)/(cm^3$ soil$)$
θ_{wcap}	volumetric water content in capillary fringe soils	$(cm^3$ water$)/(cm^3$ soil$)$
θ_{wcrack}	volumetric water content in foundation cracks	$(cm^3$ water$)/(cm^3$ soil$)$
θ_{ws}	volumetric water content in vadose zone soils	$(cm^3$ $H_2O)/(cm^3$ soil$)$
ρ_s	soil bulk density	g/cm^3
τ	averaging time for vapor flux	s

Table H-6. Green-Ampt Equations Used to Calculate Attenuation Coefficients in the Vadose Zone (for SSTLs)

The Green-Ampt equation predicts pore water travel time from a vadose zone soil source to the water table. This travel time is then used to account for degradation in the vadose zone.

Time, t, for infiltrating water to move from the source to the water table (days):

$$t = \frac{\theta_a}{K_u}\left\{L - \left[\left(i - H_f\right)\ln\left(\frac{i + L - H_f}{i - H_f}\right)\right]\right\}\frac{1}{86400}\frac{day}{\text{sec}}$$

Vertical seepage velocity, V_s, of the water (cm/day):

$$V_s = \frac{L}{t}$$

Individual chemical velocity (considers retardation), V_c, (cm/day):

$$V_c = \frac{V_w}{1 + \left(\frac{\rho_b * K_d}{\theta_T}\right)}$$

The partition coefficient for organic chemicals, (ml/g) is calculated as:

$$K_d = K_{oc} \cdot F_{oc}$$

Travel time for the chemical to reach the water table, t_c, (days):

$$t_c = \frac{L}{V_c}$$

Green-Ampt attenuation coefficient, AF_{GrAm}, is then calculate using the first-order degradation equation:

$$AF_{GrAm} = \frac{C}{C_o} = e^{(-kt_c)}$$

RBSL in soil considering degradation in the vadose zone, RBSL (Green-Ampt) [mg/kg]:

$$RBSL_{(Green-Ampt)} = \frac{RBSL_s}{AF_{GrAm}}$$

Table H-7. Unique Input Parameters Required for the Green-Ampt Model (other parameters as defined previously)

Parameters	Definitions	Units
H_f	wetting front suction (matric potential) [see figure from Rawls (1989)]	cm
K_{sat}	saturated hydraulic conductivity of vadose zone	cm/sec
K_{su}	unsaturated hydraulic conductivity of vadose zone	cm/sec
L	distance from the bottom of the source to the water table, calculated as (depth to groundwater - depth to top of subsurface source/2.0)	cm
K_{su}	unsaturated hydraulic conductivity of vadose zone	cm/sec
t	time for water to travel from center of source to water table	d
V_s	vertical seepage velocity	cm/d
λ	chemical-specific degradation rate	1/d

The only "new" input parameters required for Green-Ampt the saturated hydraulic conductivity and the wetting front suction. The remainder of the above input parameters are calculated from the previously defined parameters.

Table H-8. Domenico Groundwater Model Equations Used to Calculate Attenuation Coefficients in Groundwater (for SSTLs)

$\mathbf{AF}_{\mathbf{dom}}$: Steady-state groundwater attenuation factor (along centerline of plume)
(Domenico)
[(mg/l)/(mg/l)]

$$AF_{dom} = \frac{C(x, y = 0, z = 0)}{C_o} = \exp\left\{\frac{x}{2\alpha_x}\left[1 - \sqrt{1 + \frac{4\lambda\alpha_x}{\upsilon}}\right]\right\}\left\{erf\left[\frac{W_y}{4\sqrt{\alpha_y x}}\right]\right\}\left\{erf\left[\frac{W_z}{2\sqrt{\alpha_z x}}\right]\right\}$$

x, y, and z are the distances downgradient, cross-gradient in the horizontal direction and vertically from the centerline of the plume.

Table H-9. Parameters Used in Table H-8, Groundwater Attenuation Factor.

Parameters	Definitions	Units
AF_{dom}	attenuation factor calculated using the Domenico model	(mg/l)/(mg/l)
C_o	dissolved concentration in groundwater at the source or directly underneath the soil source	mg/l
$C(x,y,z)$	dissolved concentration in groundwater at a downgradient location where x is in the direction of the groundwater flow on the centerline of the plume	mg/l
υ	groundwater seepage velocity (non-retarded) (Calculated as $\upsilon = k * i / \theta$, where θ = the porosity of the saturated zone)	cm/d
W_y	width of the groundwater source in the horizontal direction, perpendicular to groundwater flow (this is an input parameter, unique to the Domenico model)	cm
W_z	thickness of the groundwater source in the vertical direction, perpendicular to groundwater flow (assumed to be equal to the groundwater mixing zone height, δ_{gw})	cm
α_x	longitudinal dispersivity (in the direction of groundwater flow) (Calculated as $\alpha_x = 0.1 * x$)	cm
α_Y	transverse dispersivity (perpendicular to groundwater flow in the horizontal direction) (Calculated as $\alpha_y = \alpha_x / 3$)	cm
α_x	vertical dispersivity (Calculated as $\alpha_y = \alpha_x / 3$)	cm
λ	chemical-specific degradation rate	1/d

Appendix

I

Rationale For Selection Of Monte Carlo Distributions

Derivation of a Monte Carlo distribution for certain exposure parameters is discussed in this chapter. In developing these distributions, previously published distributions for parameters were used when available and appropriate. Many of the distributions were obtained from the American Industrial Health Council's Exposure Factors Sourcebook (1994). For several parameters published data were not available. In those cases distributions were developed by BP using best professional judgment and simple distributions (i.e. triangular or uniform). It is also important for users to recognize that these distributions are "defaults". They represent the potential behaviors expected across a range of facilities and areas of the USA. Before undertaking a Monte Carlo-based risk assessment, users should carefully consider whether the default distributions are representative of their specific situation and country.

I.1 BODY WEIGHT

These distributions are taken from the literature and are based upon measured data. The distributions have been truncated to preclude the possibility of including abnormally small or large individuals. The expected value (identical to the arithmetic average) of the distribution is identical to the typical and RME point estimates. Body weight is one of the few distributions where the RME point estimate is equal to the typical value and also the arithmetic average.

I.2 EXPOSURE DURATION

The distributions for adult residents and trespassers are based upon measured data for owners of homes. Distributions for other groups (renters, etc.) are also available, but owners were selected because they will result in conservative estimates of potential risk. The expected value (11.36 years) of this normal distribution is similar to the typical point estimate of 9 years. As expected, the RME point value (30 years) is substantially lower than the maximum of the distribution, because the 30 years is assumed to represent the upper 95th percentile, not the maximum, of the distribution of duration of residence.

The distribution for child residents (aged 1 to 6) is assumed to be uniform with a minimum of 1 year and maximum of 5 years - the maximum time a child is assumed to live adjacent to a site or facility.

The distribution of workers is based upon measured data and reflects a normal distribution pattern. The expected duration or residence (8.3 years) is about the same as the typical point estimate of 8 years. The maximum of the distribution is 50 years. Again, the RME point estimate is 25 years, and represents an upper percentile of the potential exposure of workers.

I.3 EXPOSURE FREQUENCY

I.3.1 Soil

All these distributions are based upon best professional judgement, are represented by a triangular distribution, and were developed to encompass the full range of potential exposure frequencies. The maximum of each distribution is equal to the RME point estimate and the expected value (which in a triangular distribution is the most likely value) is equal to the typical point estimate. The minimum of each distribution represents the lowest number of days each receptor is assumed to come into contact with soil. Note, that the assumptions for the worker represent someone whose job requires them to be outside a portion of the day. It is not intended to represent office workers.

I.3.2 Indoor Air, Outdoor Air and Drinking Water

This parameter is represented by a constant of 350 days for the adult and child receptor and 250 days for the worker. This assumes that a resident will breathe air and drink water during every day of the year, except for two weeks when they are on vacation, during all of the years they are exposed. Similarly, a worker is assumed to breathe air and drink water everyday that they are at work, which is assumed to be 250 days per year.

I.3.3 Swimming Frequency per Year

All these distributions are represented by a triangular distribution and are developed to encompass the full range of potential exposure frequencies. The maximum of each distribution (60 days) is about twice the RME point estimate (36 days) because the RME represents an upper percentile while the maximum is designed to represent the greatest number of days that a person would potentially swim (equal to every day during the summer). The minimum (0 days) represents the fewest days that a person could swim. The expected value (7 days), which in a triangular distribution is the most likely value, is the average number of days the USEPA reports that a person swims per year, and is equal to the typical point estimate.

I.3.4 Swimming Frequency per Day

The distribution of swimming exposure time per day is assumed to be triangular, with an expected point estimate value of 1 hour/day. Both the point estimate typical and RME values are assumed to be 2.6 hours/day, as recommended by USEPA (1988). USEPA describes this value as an estimate of the national average time per swimming event while on vacation. In this case, the RME value represents an average parameter value, rather than an upper-bound value, and is therefore equal to the typical value for this parameter.

I.4 TOTAL SKIN SURFACE AREA (SHOWERING/SWIMMING)

These normal distributions are taken from the literature and represent the natural variation in the skin surface area of receptors of the ages shown. The expected value of the distribution (the arithmetic average of a normal distribution) is identical to the typical point estimate value. The RME point values represent an upper percentile of the distribution of surface area for each receptor group and, thus, are less than the maximum.

I.4.1 Fraction Skin Exposed (Soil Contact/Wading)

All these distributions are based upon best professional judgment, are represented by a triangular distribution, and were developed to represent the range of skin surface area that may potentially be exposed to soil or water for each of the different receptors. The minimum of each distribution is equal to zero, because it is possible for a receptor to contact soil or water but not absorb any chemicals because they are wearing clothing. The expected value is the same as the typical point estimate value and represents the fraction of skin comprised by the hands and half of the forearms, which are the parts of the body assumed to be exposed most frequently. The maximum is identical to the RME point value and represents the fraction of skin comprised by the legs, feet, arms and hands. Exposure of these parts of the body are assumed to represent the highest fraction that could be exposed to soil or when wading in water.

I.4.2 Soil-on-Skin Adherence

A single distribution for soil adherence to skin is assumed for all receptors. The distribution is based upon measured data, however, insufficient data exist to determine the shape of the distribution. Consequently, a triangular distribution is assumed. The range of the distribution is based upon information in USEPA (1992). The expected value (0.2 mg/cm^2) is described by USEPA (1992) as “the best value to represent an average over all exposed skin”. The typical point estimate of 0.6 mg/cm^2 is the midpoint between the minimum and maximum values. The RME estimate of 1 mg/cm^2 is described by USEPA (1992) as representing a “reasonable upper value.”

I.5 INGESTION RATE

I.5.1 Soil

The distribution of soil ingestion rate for children was derived from the literature and is based upon measured data, following a normal distribution. The expected soil ingestion rate for children (86 mg/day) is close to the typical point estimate of 90 mg/day. The RME point estimate value (200 mg/day) is smaller than the distribution maximum, because 200 mg/day is assumed to represent the 95th percentile, not the maximum, of the distribution of child soil ingestion rate.

Soil ingestion rates for adult residents, trespassers, and workers are assumed to be approximately equal to one-half the soil ingestion rate of a child. For this reason, the expected (mean) and typical soil ingestion rates for these three receptors are approximately 40 mg/day. As for the child soil ingestion rate, the RME point estimate (100 mg/day) is less than the distribution maximum, because it represents the upper 95th percentile, not the maximum of the distribution.

I.5.2 Drinking water

The distributions for adults and children is taken from the literature and are based upon measured data using normal distributions. For adults, the distribution for the age group 20-65 is used. The expected water ingestion rate (1.27 L/day) is slightly higher than the typical point estimate value of 1.1 L/day. The RME point estimate value (2 L/day), recommended by EPA (1991), is lower than the distribution maximum, which is truncated to prevent unrealistically large estimates of water ingestion (greater than 3 L/day).

The distribution for the age group 1-11 is used for children. The typical point estimate value (0.5 L/day), assumed to be equal to one-half the adult’s typical drinking water ingestion rate, is slightly lower than the expected (mean) ingestion rate of 0.7 L/day. The RME point estimate value for the child (1 L/day) is assumed to equal one-half the adult RME point estimate value (2 L/day), and is truncated at 2 L/day to prevent unrealistically large water ingestion estimates.

The worker drinking water ingestion rate is assumed equal to one-half the adult drinking water ingestion rate, as recommended by EPA (1991). The expected water ingestion rate (0.63 L/day) is slightly higher than the typical point estimate value (0.5 L/day). As for the adult and child resident receptors, the distribution is truncated (at 2L/day) to prevent unrealistically large water ingestion rates.

I.5.3 Water While Swimming

The distribution of water ingestion rates while swimming is assumed to be uniform, ranging from 0 to 50 mL/hr. A uniform distribution is assumed because little data for this parameter are available.

The distribution maximum value is recommended in USEPA (1988), and is assumed to represent a worst-case estimate of water ingestion. A value of 10 mL/hr is assumed to represent the typical point estimate value. This distribution is used for all receptors exposed via swimming.

I.6 ACTIVITY TIME

I.6.1 Time Spent Outdoors

The distributions for time spent outdoors for both the adult resident and child resident are assumed to be triangular, with expected values derived from measured data from the literature. The ranges surrounding the expected values are determined using professional judgment. The typical point estimate value is assumed to equal the expected value, and the RME point estimate value is assumed to equal the distribution maximum, in the absence of additional data.

The distributions for the trespasser and the worker are assumed to be triangular, and are based upon professional judgment. As for the adult and child, the point estimate typical value is assumed to equal the expected value, and the RME point estimate is assumed to equal the distribution maximum. An expected value of 4 hours/day is assumed for workers, and an expected value of 1.5 hours/day is assumed for trespassers.

I.6.2 Time Spent Indoors

Similar to time spent outdoors, the distribution for time spent indoors is assumed to be triangular, with expected values of 18.3 and 19.6 hours derived from the literature for the adult and child resident receptors, respectively. For the worker, professional judgment is used to derive a triangular distribution with an expected value of 4 hours/day. For all receptors, the typical point estimate value is assumed to equal the expected value, and the RME point estimate value is assumed to equal the distribution maximum, because no additional data are available to determine median or upper-bound estimates.

I.7 INHALATION RATE

I.7.1 While Showering

For all receptors assumed to be exposed via this pathway, the inhalation rate while showering is assumed to be constant at 0.6 m^3/hour, as recommended by USEPA (1989). This parameter is best described by a constant distribution, because there is likely very little variability in the distribution.

I.7.2 While Indoors and Outdoors

For the adult and child resident receptors, the distribution is assumed as normal and taken from the literature based upon measured data. The point estimate typical value (0.83 m^3/hour) is derived assuming an inhalation rate of 20 m^3/day, as recommended by USEPA (1991), and is slightly higher than the expected inhalation rate of 0.79 m^3/hour for the adult and 0.72 m^3/hour for the child.

For the trespasser, a triangular distribution is derived from data in Anderson et al. (1985). The distribution minimum represents the average inhalation rate for the age group 10-18 (males) engaging in light activity. The average moderate activity inhalation rate for this group is used for the distribution maximum. The trespasser is assumed to spend one-half the exposure time engaging in light activity and one-half engaging in moderate activity. The expected value is the arithmetic mean of the minimum and maximum of the distribution. The typical point estimate value is assumed to equal the expected value, and the RME value is assumed to equal the distribution maximum.

A methodology similar to that used to derive the trespasser inhalation rate distribution is used to derive a distribution for worker inhalation rate. The distribution is based upon data in U.S. EPA (1985). The distribution is assumed to be triangular, with the expected value equal to the light activity inhalation rate for adult males. The distribution minimum is assumed to equal the resting inhalation rate for adult males, and the distribution maximum is assumed to equal the moderate activity inhalation rate for adult males. The typical point estimate value is assumed to equal the expected value, and the RME point estimate value is assumed to equal the distribution maximum. The RME point estimate also corresponds to EPA’s recommended inhalation rate for workers of 20 m^3/day (EPA, 1991).

I.8 SHOWER PARAMETERS

I.8.1 Flow Rate

This parameter is relevant only to residents (adult and child) and is taken directly from the analysis by Finley and Paustenbach (1994), who fit a lognormal distribution to shower flows determined from a water use study of 2,500 receptors conducted by James and Kuniman (1987).

I.8.2 Water Temperature

Again relevant to residents (adult and child), the values are taken directly from the judgment-based estimate of Smith (1994), with the Smith-reported degrees Kelvin converted to degrees Centigrade. Smith expects that the range of water temperatures should be fairly "narrow" as receptors have similar comfort levels. It is best represented as triangular.

I.8.3 Shower Volume

Relevant to residents (adult and child), this distribution is also taken directly from the judgment-based estimate of Smith (1994). If one assumes a shower stall must be something more than 2 m high to comfortably accommodate the average individual, the minimum value (2 m^3) would contemplate a stall something less than 1 meter in length and width, which are quite modest dimensions. The maximum of 6 m^3 would connote a quite generous "tub" structure of, say, 1 by 3 m. As a judgmental decision, the triangular distribution is considered reasonable.

I.8.4 Exposure Time While Showering

Relevant to residents (adult and child), this distribution is obtained directly from AIHC (1994), who fit a triangular distribution to survey data on 2,500 individuals keeping time-activity diaries (James and Kuniman, 1987).

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Appendix J

Vapor Transport Model Considering Degradation— Dominant Layer Model

J.1 MODEL DESCRIPTION

This vapor transport model is based on the “dominant layer model” described in “Assessing the Significance of Subsurface Contaminant Vapor Migration to Enclosed Spaces: Site-Specific Alternative to Generic Estimates” by Paul Johnson, Mariush Kemblowski, and Richard Johnson (1998). The model estimates the flux of contaminants through a three-layered vadose zone system and accounts for degradation. The layers correspond to a region near the source where no degradation is occurring, a middle layer where conditions are such that degradation can occur, and a near building or surface soil region where no degradation is assumed to occur. The user specifies the thickness of each layer based on observed conditions at the site.

This model may be used to estimate concentrations in both indoor air and outdoor air. It estimates the vapor flux at the top boundary. This flux term can then be combined with either the indoor air model or the outdoor air model to estimate air concentrations. When used to estimate air concentrations in buildings, the model can consider both diffusive and advective transport through the soil and into the building foundation. This part of the model is identical to the Johnson and Ettinger model (Johnson and Ettinger, 1991, Appendix D). Appendices D and F describe the indoor air model and outdoor air models, respectively.

The “dominant layer” model was developed because observations of field data of vapor concentration vs. depth curves indicate that there is often a region where degradation is occurring while a region exists above and below where diffusion dominates.

The subsurface region modeled corresponds to the region from the source to the ground surface (for estimating outdoor air) or the building foundation (for estimating indoor air). The following assumptions are made:

- the focus of the analysis is the transport of aerobically degradable chemical vapors under conditions where advection is negligible (although it can be included in the model),
- the subsurface properties (e.g., bulk density, porosity, moisture content, etc.) are assumed to be uniform and constant throughout each layer,
- the vapor source concentration is constant (or changes slowly compared to the simulation time),
- the dissolved and vapor concentrations of the chemical can be related by the chemical’s Henry’s Law Constant,
- the vapor source plan view dimensions are large in comparison with the depth to the vapor source, so that the problem can be reasonable approximated as being one-dimensional,
- the degradation rate is assumed to be first-order with respect to chemical concentration,
- the degradation rate is assumed to be equal to the product of the dissolved phase concentration of the chemical, the volumetric moisture content, and a first-order degradation constant.

Under these conditions, the subsurface can be depicted by the conceptual model shown in Figure J-1.

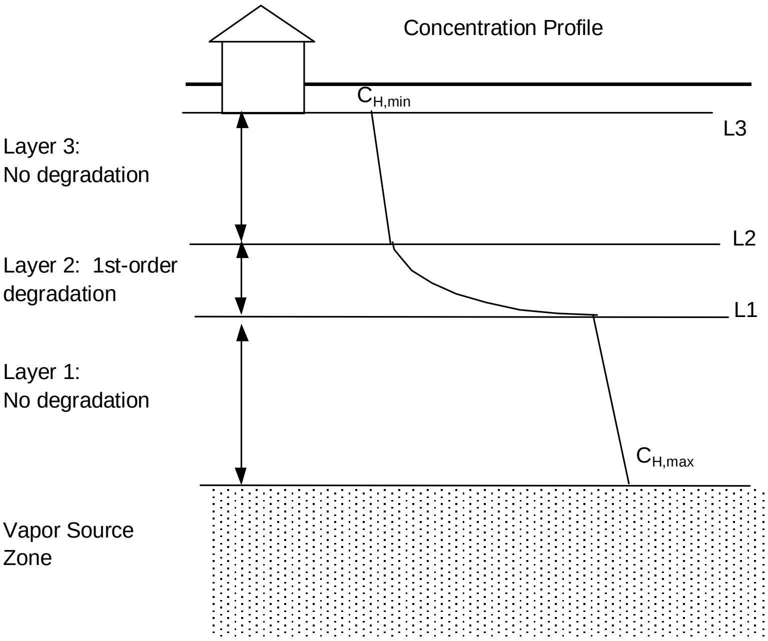

Figure J-1. Schematic of the Dominant Layer Vapor Transport Model.

Appendix K.1.2 discusses additional soil gas profile types and the applicability of the models in RISC to model the various soil gas profiles.

J.2 TRANSPORT EQUATIONS AND PROCESSES

The near steady state vapor-phase concentration profile for the scenario shown in Figure J-1 is given by:

Region 1 ($0<z<L_1$):

$$C_v(z) = C_{vs} - (C_{vs} - C_{v2})\left(\frac{z}{L_1}\right) \qquad \textbf{(J-1)}$$

Region 2 (L_1<z<L_2):

$$C_v(z) = \frac{C_{v3}\exp\left(\eta\,\frac{(L_1 - z)}{(L_2 - L_1)}\right) - C_{v2}\exp\left(\eta\,\frac{(L_2 - z)}{(L_2 - L_1)}\right)}{\exp(-\eta) - \exp(\eta)}$$

$$+ \frac{C_{v2}\exp\left(-\eta\,\frac{(L_2 - z)}{(L_2 - L_1)}\right) - C_{v3}\exp\left(-\eta\,\frac{(L_1 - z)}{(L_2 - L_1)}\right)}{\exp(-\eta) - \exp(\eta)} \tag{J-2}$$

Region 3 (L_2<z<L_3)

$$C_v(z) = C_{v3} - (C_{v3} - C_{v4})\left(\frac{z - L_2}{L_3 - L_2}\right) \tag{J-3}$$

and

$$\eta = \sqrt{\frac{\lambda_j \theta_m (L_2 - L_1)^2}{D_2^{eff} K_H}} \tag{J-4}$$

where

C_{vs} = vapor-phase concentration of chemical at source [g chemical/cm^3 vapor]

C_{v2}, C_{v3}, C_{v4} = vapor-phase concentration at top of layers 1, 2, and 3 [g chemical/cm^3 vapor]

z = distance measured up from the source [cm]

L_1, L_2, L_3 = distance to top of layers 1, 2, and 3, measured up from the source [cm]

θ_m = volumetric moisture content in the middle layer[cm^3/cm^3]

λ_j = first-order reaction rate constant (degradation rate) for chemical in middle layer [1/s]

K_H = Henry's Law Constant for chemical [(mg/l vapor)/(mg/l water)]

D_2^{eff} = overall effective porous medium diffusion coefficient for chemical in the middle layer[cm^2/s]

The parameter η represents a ratio of degradation rate to diffusion rate; therefore, it is expected that attenuation will increase with increasing η.

The effective diffusion coefficients for each layer are calculated using the Millington-Quirk relationship (Millington and Quirk, 1961, and described in Appendix A) which accounts for the amount of air vs. water-filled porosity in the soil.

$$D_i^{eff} = D_{air}\left(\frac{\theta_a^{3.33}}{\theta_T^2}\right) + \frac{D_{water}}{K_H}\left(\frac{\theta_m^{3.33}}{\theta_T^2}\right) \qquad \textbf{(J-5)}$$

where

D_i^{eff} = overall effective porous medium diffusion coefficient for chemical in the layer i [cm^2/s]

K_H = Henry's Law Constant for chemical [(mg/l vapor)/(mg/l water)]

D_{water} = molecular diffusion coefficient for chemical in water [cm^2/s]

D_{air} = molecular diffusion coefficient for chemical in air [cm^2/s]

θ_T = total porosity [cm^3/cm^3]

θ_a = volumetric air content [cm^3/cm^3]

J.2.1 Using the Dominant Layer Model for Indoor Air

Similar to Johnson and Ettinger (1991) for enclosed spaces the attenuation factor is calculated from:

$$\alpha = \frac{C_{indoor}}{C_{vs}} = \frac{1-\beta}{(1-\beta)\left(\frac{Q_B}{2\phi\gamma\psi}\right) + \left(\beta\left(\frac{Q_B}{Q_{soil}}\right) - 1\right)\left(\frac{1+\gamma\psi-4\psi^2}{2\gamma\psi^2}\right)} \qquad \textbf{(J-6)}$$

where:

$$\beta = 1 - \exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) \qquad \textbf{(J-7)}$$

$$\gamma = \left(\frac{D_1^{eff}}{D_2^{eff}} \right) \left(\frac{\exp(-\eta) - \exp(\eta)}{\eta} \right) \left(\frac{L_2 - L_1}{L_1} \right) \tag{J-8}$$

$$\psi = \frac{1}{\exp(-\eta) + \exp(\eta) - \gamma} \tag{J-9}$$

$$\phi = \left(\frac{A_B D_3^{eff}}{L_3 - L_2} \right) \frac{1}{\left[\sigma - (1/\psi) - \gamma + 4\psi \right]} \tag{J-10}$$

$$\sigma = \left(\frac{D_3^{eff}}{D_2^{eff}} \right) \left(\frac{\exp(-\eta) - \exp(\eta)}{\eta} \right) \left(\frac{L_2 - L_1}{L_3 - L_2} \right) \tag{J-11}$$

and the variables are defined as:

C_{vs} = vapor-phase concentration of chemical at source [g chemical/cm^3 vapor]

C_{indoor} = air concentration of chemical in building [g chemical/cm^3 air]

Q_{soil} = volumetric flow rate of soil gas into the building [cm^3/s]

D_{crack} = effective diffusion coefficient in foundation cracks [cm^2/s]

L_{crack} = thickness of the foundation [cm]

A_{crack} = area of cracks or openings through which vapors enter building: (flux area) x (fraction of floor that is cracks) [cm^2]

A_B = cross-sectional area of foundation available for vapor flux [cm^2]

Q_B = building air exchange rate [cm^3/s]

and η has been defined in Equation J-4. Refer to Appendix D for details on calculating Q_{soil} and D_{crack}. The other input parameters are user inputs.

The flux, E [g/s], from the vadose zone into the building can be calculated from a mass balance:

$$E = C_{indoor} * Q_B \tag{J-12}$$

J.2.2 Using the Dominant Layer Model for Outdoor Air

For outdoor air, the same equations are used as for the indoor air case (J-6 through J-11); only the soil gas flow rate, Q_{soil}, is set to near zero and the "building air exchange rate" is calculated from the user input wind speed and box height. The cross-sectional area for the outdoor air model is calculated as the product of the length of the source and 1 m since the width does not factor into the equation for estimating mixing in an outdoor box.

The following substitutions are made to equations J-6 through J-11:

Q_{soil} = 1E-20 (essentially zero) cm^3/s
Volume = *Height* * 1 m (width) * *Length*
Air Exchange Rate = *Wind speed* * *Height* * 1 m (width)

where

Volume = volume of the outdoor air “box” [m^3]
Height = height of the “box” [m] (a user input)
Length = length of the “box” in the predominant direction of wind [m] (a user input)
Air Exchange Rate = "Q_b" = ventilation rate of the “box” [m^3/s]
Wind speed = wind speed [m/s] (a user input)

From these variables the equivalent “Q_B” parameter [volumes/sec] may be calculated:

$$Q_B = \text{Volume/Vent Rate} \qquad \textbf{(J-13)}$$

The flux, E [g/s], out the soil surface is calculated similarly to the approach taken with the indoor air calculations:

$$E = C_{outdoor} * Q_B \qquad \textbf{(J-14)}$$

For additional discussion on the input parameters for this equation, refer to the “Box Model,” Appendix F.

J.3 SOURCE TERM

The dominant layer model (as all of the vapor models in RISC) may be run using a specified soil gas concentration or a total concentration in soil as the source term. Equations J-6 and J-1 require the soil vapor concentration, C_H^{max}, as a starting point. If soil gas concentration is used as the source term in RISC, then the user-specified value is used for C_H^{max}.

If the source term is entered as the total concentration in soil, then C_H^{max} is calculated from equilibrium partitioning equation or from the chemical's calculated effective solubility, whichever is less. This is the same approach used by the Vadose Zone model (Appendix A), the Saturated Soil model (Appendix C), and the other vapor models (Appendices D and J). See Appendix A for a detailed discussion on how the dissolved-phase concentration is determined from the user-input total concentration in soil. Note, this vapor model allows the user to specify values for soil bulk density, fraction organic carbon, moisture content, and porosity for the source zone which are separate from those used for the region where vapor transport is modeled. The reason for this is that the contamination may reside in a different unit than that where vapors migrate.

Once the dissolved-phase concentration (C_w) is calculated, the soil vapor source concentration is calculated from:

$$C_H^{\max} = C_w K_H \tag{J-15}$$

where

C_H^{max} = source vapor concentration at $z = L$ [g/cm^3]
C_w = dissolved-phase concentration [mg/l]
K_H = Henry's Law Coefficient [(mg/l)/(mg/l)]

J.4 EXAMPLE USING ACTUAL SITE DATA

This section presents an example problem using actual site data. The objectives are:

1. to evaluate field data,
2. to estimate model parameters to fit the data, and
3. to estimate a "minimum" vapor degradation rate for this soil system.

J.4.1 Evaluate Field Data

The example data used in this section is based on benzene data collected by BP (1997) and presented by Johnson et al (1998). Soil samples were collected from five regions below ground surface at an uncovered site. The results are plotted in Figure J- 2.

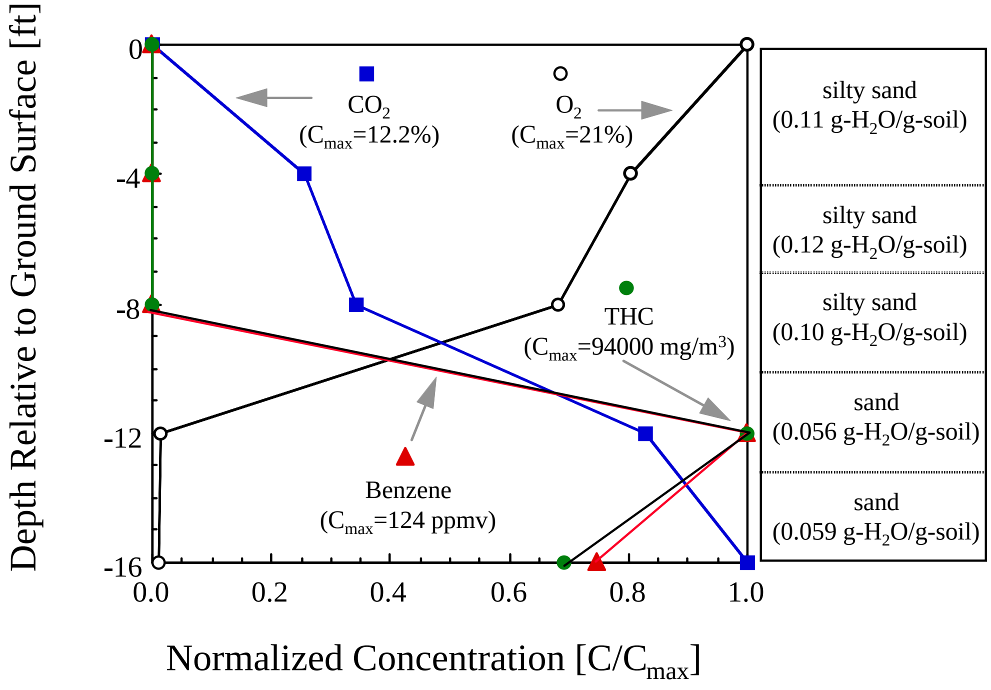

Figure J-2. Data Used for the Example Problem, from BP (1997).

The column on the right side indicates moisture content given on a weight basis. The plot indicates a sharp drop-off in the benzene concentration with a corresponding sharp increase in the oxygen concentration at 8 to 12 ft below ground surface (BGS). This type of behavior would not be predicted very well by a one-dimensional model, even if it considered degradation (Johnson et al, 1998). The sharp drop-off of benzene indicates the presence of a layer that seems to "dominate" the vapor transport process for benzene in this soil profile. There are several things to notice in this plot:

- The maximum concentration occurs at 12 feet BGS rather than at 16 feet BGS where the source was expected. There is no practical explanation as to why concentrations are higher at 12 feet BGS. However it is likely there is NAPL at 16 feet BGS so the model geometry will assume this scenario (maximum concentrations at 16 feet BGS). If the data in Figure J-2 were to be used explicitly, the source should probably be assumed to occur at 12 feet BGS.
- The benzene concentration drops from the maximum concentration at 12 feet BGS to zero at 8 feet BGS. There are no intermediate measurements of concentration vs. depth, making it difficult to determine the thickness of the middle layer where degradation is occurring.

These points must be considered when developing the geometry of the dominant layer model and selecting appropriate values for the parameters.

J.4.2 Estimate Model Parameters

Table J-1 presents the BP data that accompanied Figure J-2 as summarized by Johnson et al (1998).

Table J-1. Data Used For Example Problem (from BP, 1997)

Depth [ft BGS]	Soil Type	Water Content by Weight [g-H_2O/g-soil]	Volumetric Water Content, θ_m [cm^3/cm^3]*	Effective Diffusion Coefficient, D^{eff} [m^2/d]**
0-4	silty sand	0.11	0.19	0.016
4-7	silty sand	0.12	0.20	0.010
7-10	silty sand	0.10	0.16	0.023
10-13	sand	0.056	0.10	0.067
13-16	sand	0.059	0.10	0.062

* - assuming a bulk soil density of 1.7 g-soil/cm^3-soil

** - for $D^{air} = 0.09\ cm^2/s = 0.78\ m^2/d$

The data in Table J-1 does not show the air content or total porosity of the soil samples. It is not clear whether the effective diffusion coefficients were measured in the field or the porosities were estimated from the general soil types. In order for this data to be used in RISC, the air content must be estimated and the units must be converted. Assuming the effective diffusion coefficients in Table J-1 were measured, the volumetric air content value may be estimated from the D^{eff} and the volumetric water content using an iterative approach. Refer to the equation for calculating the effective diffusion coefficient in Appendix A (Equation A-13). Table J-2 presents the estimated air contents using the default value for the benzene diffusion coefficient in air from the RISC chemical database.

Table J-2. Estimated Total Porosity for the Example Problem

Measured Field Data					
Soil Sample Depth [ft BGS]	Effective Diffusion Coefficient [m^2/d]	Effective Diffusion Coefficient [cm^2/s]	Moisture Content [cm^3/cm^3]	Estimated Air Content [cm^3/cm^3]	Estimated Total Porosity [cm^3/cm^3]
0-4	0.016	1.9E-03	0.19	**0.17**	**0.36**
4-7	0.010	1.2E-03	0.20	**0.14**	**0.36**
7-10	0.023	2.7E-03	0.16	**0.19**	**0.35**
10-13	0.067	7.8E-03	0.10	**0.26**	**0.36**
13-16	0.062	7.2E-03	0.10	**0.25**	**0.35**

The information in Table J-2 must be grouped into three layers according to the major divisions observed on the concentration plot (Figure J-2). Assuming there is residual NAPL at 16 feet BGS, the vapor concentration at 12 feet BGS is assumed to be the same as at the source or slightly less. This zone will form the first layer. It is not clear where the first layer should end. However, because one of the objectives is to estimate a minimum reasonable degradation rate, a conservative approach is to make the dominant layer as large as possible. In this way the degradation process will have a longer vertical distance over which to operate and the degradation rate may be lower to obtain the same drop in concentration. To make the middle layer as large as possible it is assumed that the lower layer extends from 16 feet BGS to just above 12 feet BGS. Using that same reasoning and lacking additional information, the soil between 12 feet BGS and 8 feet BGS is chosen as the middle layer. This leaves the soil from 8 feet BGS to the ground surface as the top layer.

The model geometry for this example is shown in Figure J-3. Note that this geometry does not match the soil characterization provided by BP (1997). The reason, as stated above, is that the objective is to derive a degradation rate that is at the low end of the range that is expected to occur at the site. The air and water contents are chosen to equal the highest air content and lowest water content (i.e. the highest diffusion coefficient) of the soil regions in each of the layers. Not much effort is focused on the top layer because the measured data does not provide sufficient information to calibrate effective diffusion coefficients. The measured data points at 0 and 4 feet BGS are useful to indicate the absence of benzene vapors; however, they do not provide any useful information for the modeling effort. The data point at 8 feet BGS indicates that benzene concentration are reduced to non-detects somewhere below this point.

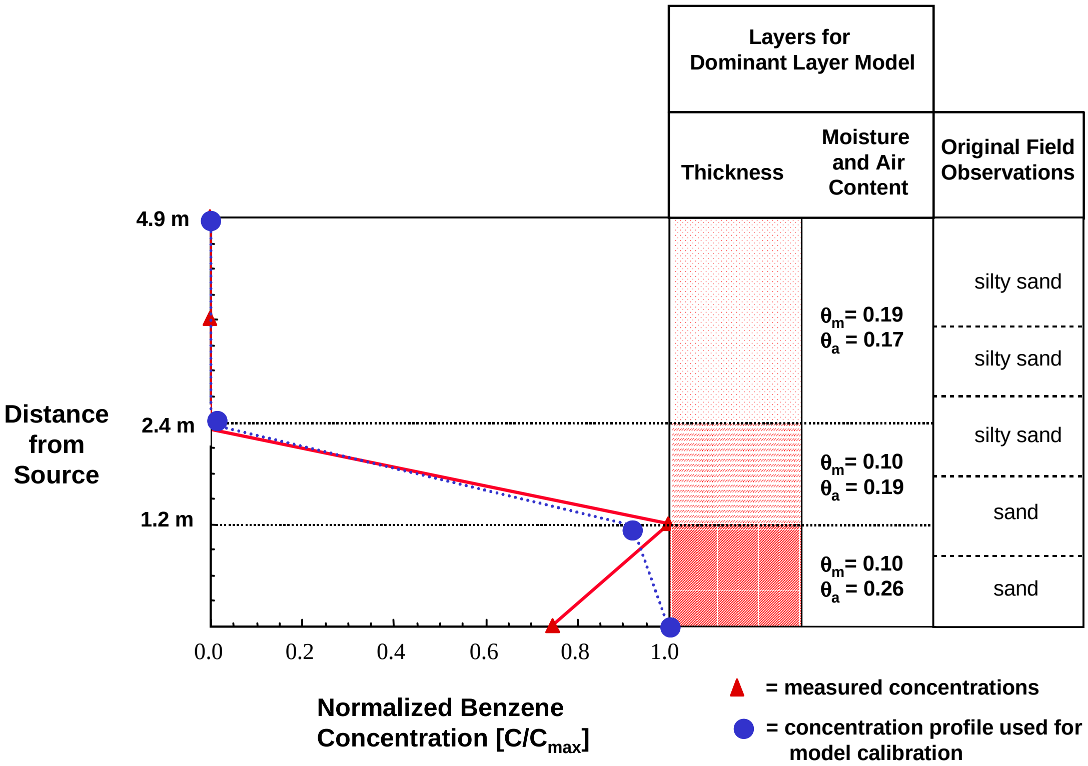

Figure J-3. Layers for the Dominant Layer Model.

The first model run used the measured effective diffusion coefficients presented in Table J-2 and a degradation rate for the middle layer equal to the high end value of 0.07/day reported by Howard et al (1991) (and tabulated in the RISC chemical database). The high degradation rate was chosen to start because it appears that the benzene concentrations drop off rapidly. Note, the degradation rates summarized in the RISC chemical database are representative of values reported in Howard (1991) for degradation in the saturated zone. Degradation rates in the vadose zone, where oxygen may be much more plentiful, may be much higher than saturated zone degradation rates. Figure J-4 shows the results of the "first run" using the reported diffusion coefficients.

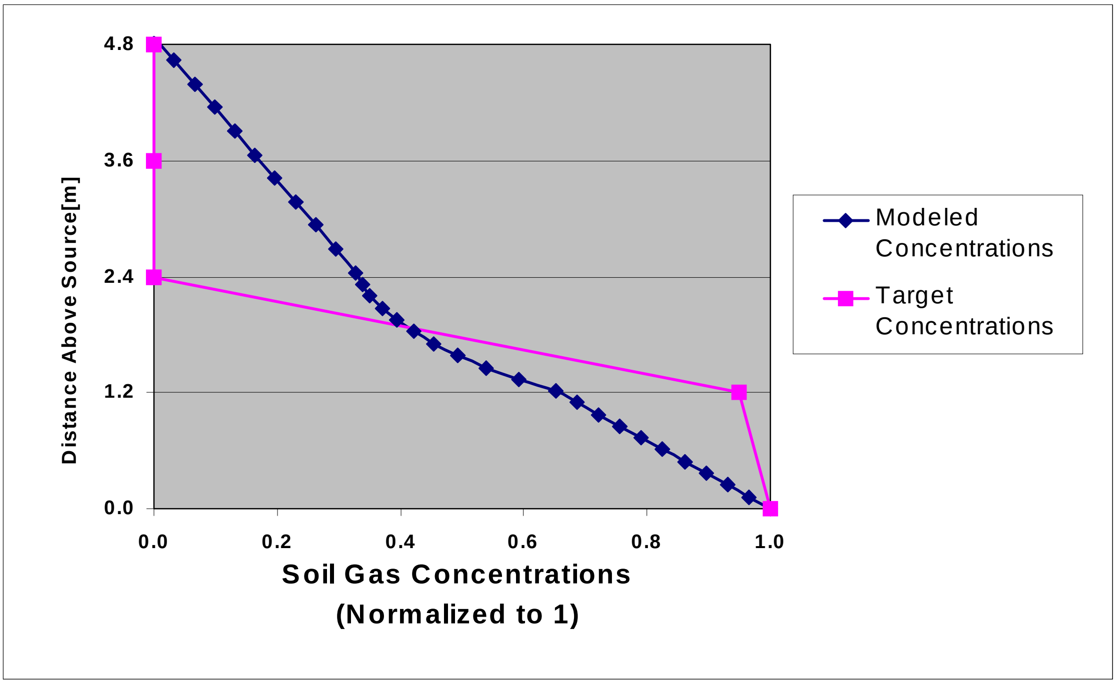

Figure J-4. Model Results Using the Reported Diffusion Coefficients, the "Base Case"

Figure J-4 shows that the model results do not predict the behavior measured in the field very well. The first thing to notice is that if the source is actually located at 16 feet BGS and there is very little concentration drop-off across the first layer, the diffusion coefficient in this lower layer may be much higher than the value reported. Alternatively, and more likely, there may be residual NAPL present at 12 feet BGS due to water table smearing of the source. However, the effects of changes in the diffusion coefficient will first be investigated.

J.4.3 Estimate Minimum Degradation Rate

The highest effective diffusion coefficient occurs in high porosity soil that is dry (water diffusion is very slow compared to air). Given the soil type of the lower layer, it is possible that the total porosity may actually be 0.40. For a "Dry Case" then, it is assumed that the air content is equal to 0.35 and the water content is equal 0.05 (about the residual moisture content of a sand which is being very conservative). Figure J-5 shows the model results using these assumptions for the lower layer.

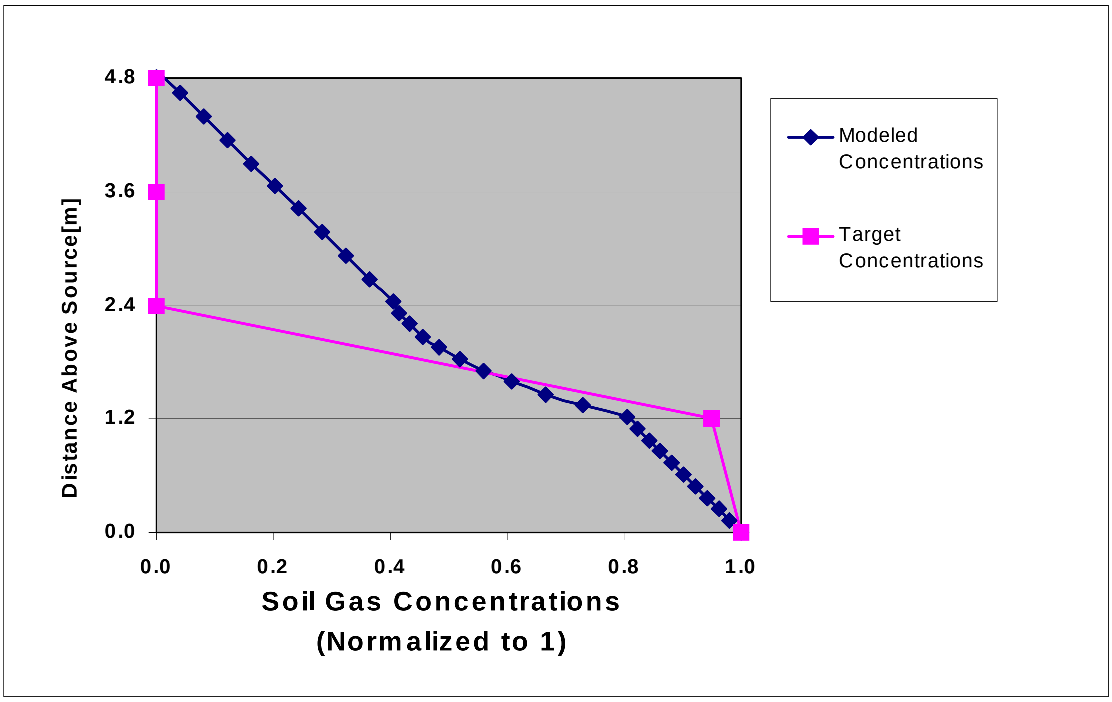

Figure J-5. Model Results for the "Dry Case" in Bottom Layer

Changing the diffusion coefficient (via the air content) changed the normalized concentration from 0.65 in the "Base Case" to 0.8 in the "Dry Case" shown in Figure J-5. This improved the model prediction at the interface between the bottom and middle layers somewhat. The concentration at this location may change more as the profile changes in the middle layer.

The next step is to focus on the middle layer. In this layer, there are essentially two major processes being modeled, degradation and diffusion. If the same degradation rate of 0.07/day is maintained in this iteration, the middle layer's predicted concentration profile in Figure J-5 suggests that the diffusion coefficient is too high relative to the data. Using the same approach as applied to the lower layer, but in reverse, it is assumed that the soil is wet in this layer. A low air content yields a small diffusion coefficient and therefore provides a longer duration for the degradation process. In this iteration, the water content is assumed equal to 0.3 and the total porosity equal to 0.35, with the degradation rate left at 0.07/day. The model results are shown in Figure J-6.

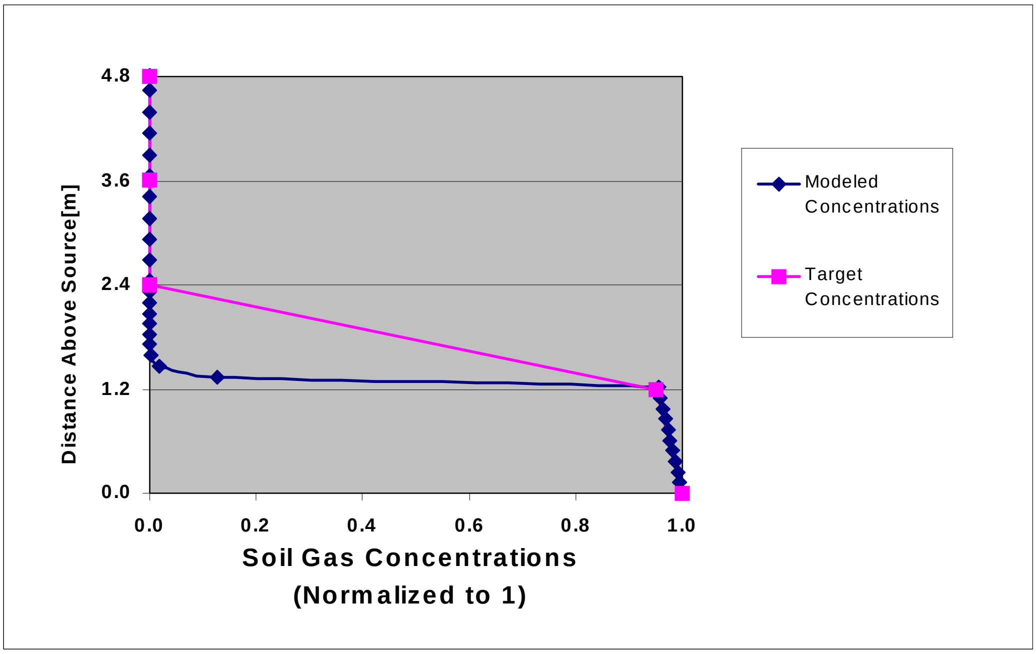

Figure J-6. Model Results Using a Dry Bottom Layer and a Wet Middle Layer

These results could actually match the measured site data because it is not known precisely at what depth the benzene exceeds non-detect levels. (Note how the concentration at the interface between the lower and middle layers increased to 0.95 in this iteration.) Since the degradation rate is relatively high however, this is not a "conservative" solution for the objectives of this example. It appears that the "minimum likely" degradation rate for this soil profile is less than 0.07/d. After several runs, a "best fit" was found using a degradation rate of 0.007/day (Figure J-7).

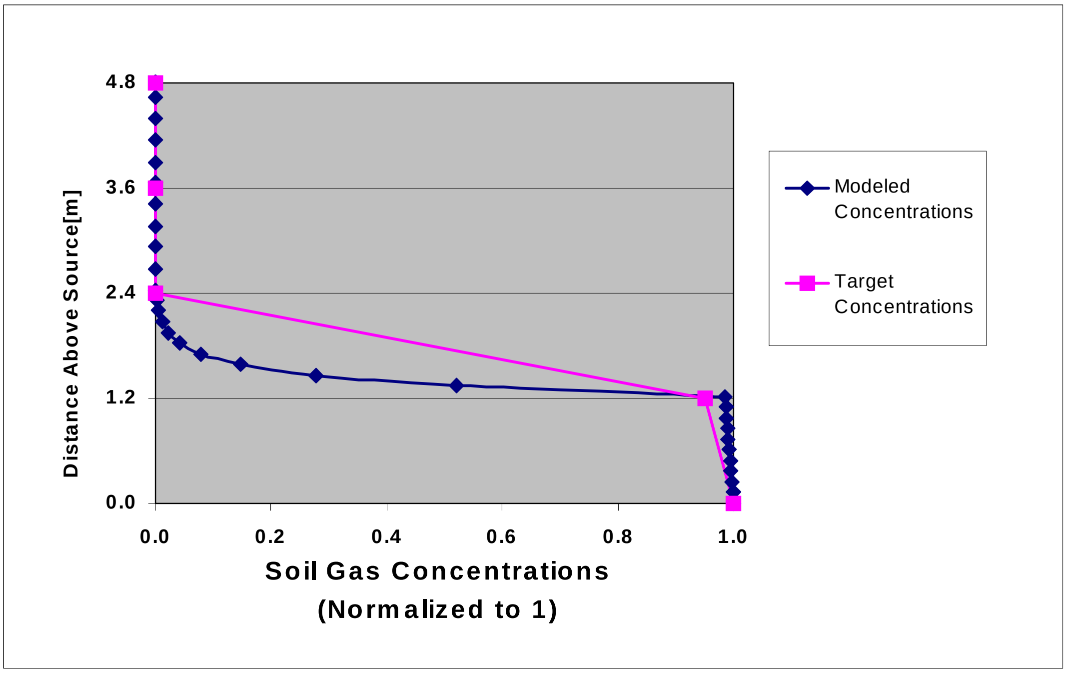

Figure J-7. Model Results With A Degradation Rate of 0.007/d

This example demonstrates how parameter estimating is used to develop the best curve fit using as much site data as possible and informed judgement when certain data are not available.

J.5 DATA REQUIREMENTS OF THE DOMINANT LAYER VAPOR MODEL

The input data requirements for this model are presented in Table J-1.

Table J-3. Data Requirements for the Dominant Layer Vapor Model

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
UNSATURATED ZONE			
Air content for each layer	cm^3/cm^3	0	porosity
Water content for each layer	cm^3/cm^3	0	porosity
Thickness of each layer	m	Site-specific	site-specific
CHEMICAL (individual chemical component)			
Diffusion coefficient in air	cm^2/s	Chem-specific	chem-specific
Diffusion coefficient in water	cm^2/s	Chem-specific	chem-specific
Henry's Law coefficient	(mg/l)/(mg/l)	Chem-specific	chem-specific
Degradation rate in the middle layer	1/day	Chem-specific	chem-specific
Source entered as a Soil Vapor Concentration:			
Soil vapor concentration	mg/l	Site-specific	site-specific
Source entered as a Total Soil Concentration:			
Source concentration	mg/kg	Site-specific	site-specific
Porosity in source region	cm^3/cm^3	0.01	0.5
Water content in source region	cm^3/cm^3	0	porosity
Fraction organic carbon in source region	m	1.00E-03	1
Soil bulk density in source region	fraction	1.4	2.2
Molecular weight of chemical	g/mol	Chem-specific	chem-specific
Solubility of chemical	mg/l	Chem-specific	chem-specific
Molecular weight of TPH	g/mol	80	120
Concentration of TPH	mg/kg	Site-specific	site-specific

J.6 LIMITATIONS OF THE DOMINANT LAYER VAPOR MODEL

1. This is a steady-state, constant and one-dimensional model. The source does not deplete due to vapor losses so mass is not conserved. This assumption has only a minor impact on the risk from non-carcinogens (unless the source is very small) since the worst seven-year running average intake is compared to the reference dose. It can have a more significant impact however on carcinogens (such as benzene) since the cumulative exposure over a long exposure duration (up to 30 years) forms the basis for the risk calculation.
2. The model assumes that degradation occurs only in the middle layer. The location and thickness of this layer must be specified by the user.

J.7 REFERENCES

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Johnson, P.C., and Ettinger, R.A., 1991. Heuristic Model for Predicting the Intrusion Rate of Contaminant Vapors into Buildings, *Environmental Science and Technology*, 25, 1445-1452.

Johnson, P.C., Kemblowski, M.W., and Johnson, R.L., December1998. Assessing the Significance of subsurface Contaminant Vapor Migration to Enclosed Spaces: Site-Specific Alternative to Generic Estimates, American Petroleum Institute Publication Number 4674.

Jury, .W.A., Russo, D., Streile, G. and Abid, H. El. 1990. "Evaluation of Volatilization by Organic Chemicals Residing Below the Soil Surface". *Water Resources Research*. 26(1). 13-20.

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Appendix
K

Vapor Transport Model Considering Degradation—Oxygen-Limited Model

This vapor transport model is based on the paper entitled, “An Oxygen-Limited Hydrocarbon Vapor-Migration Attenuation Screening Model” by Paul Johnson (1998, draft). The model estimates the flux of contaminants through the vadose zone and accounts for degradation. The unique feature of the model is that it calculates an oxygen profile while recognizing that there must be a minimum amount of oxygen present for degradation to occur. In the region where oxygen is below this user-specified minimum, degradation is assumed to be absent.

Section K.1 presents the model description and compares the features of this model with the other vapor models in RISC. Four generalized soil gas profile types are evaluated and the applicability of using the model for the profile type is discussed.

In Section K.2 the equations used to estimate the vertical profiles of chemical and oxygen concentration, the flux, and the indoor or outdoor air concentrations are presented. The source options, which are the same as for the other vapor models, are described. Sections K.4 and K.5 present the data requirements and summarize the model limitations, respectively.

K.1 MODEL DESCRIPTION

The Oxygen-Limited Vapor Model assumes that there is a region above the source that has depleted levels of oxygen where aerobic degradation cannot occur. The distance above the source at which the oxygen levels become high enough to support aerobic degradation, called "delta", is calculated by the model. The vadose zone properties are assumed to be homogeneous in the region modeled. The conceptual model is shown in Figure K-1.

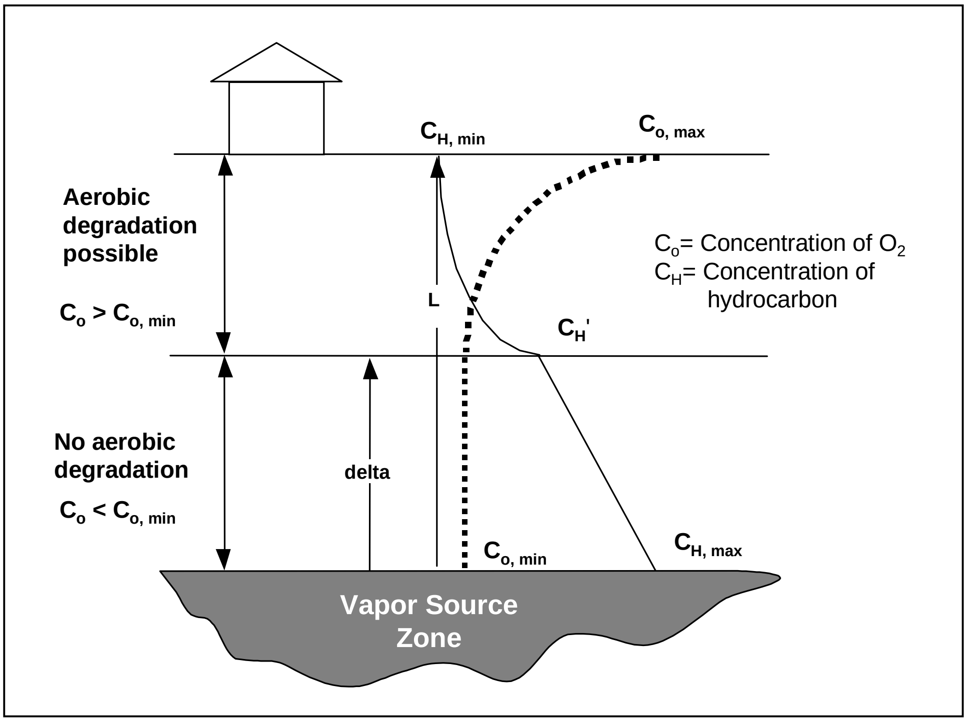

Figure K-1. Schematic of the Oxygen-Limited Vapor Transport Model.

In the region between the source and "delta," the transport is assumed to be diffusion-dominated, represented by the solid, straight line between $C_{H,max}$ and C_H' in Figure K-1. The term C_H' is the concentration of the hydrocarbon (or any chemical being modeled) at "delta". This concentration, C_H', is calculated by the model. The oxygen concentration in the region below "delta" remains constant at the minimum (or less) indicating that it is depleted and aerobic degradation cannot occur.

In the region between "delta" and the top boundary, the transport is a combination of degradation and diffusion processes, as represented by the curve between C_H' and $C_{H,min}$. The degradation is assumed to be first-order with respect to the contaminant concentration, i.e. it does not depend on the concentration of the oxygen other than the oxygen concentration must be greater than the minimum specified for aerobic degradation (a user input). In this region the oxygen concentration increases from the minimum concentration to the ambient oxygen concentration. This curve is calculated by the model and is dependent on the chemical's degradation rate and the chemical's stoichiometric coefficient (a measure of how much oxygen the chemical uses when it degrades). A constant flux of oxygen is assumed to occur across the top boundary refreshing the oxygen in the upper portion of the vadose zone.

The oxygen-limited model is based on the advection-dispersion equation written for the vapor phase transport of a single chemical in the vadose zone. The subsurface region modeled corresponds to the region from the source to the ground surface (for estimating outdoor air) or the building foundation (for estimating indoor air). In summary, the following assumptions are made:

- the focus of the analysis is the transport of an aerobically degradable chemical and oxygen vapors under conditions where advection is negligible (although it can be included in an indoor air scenario),
- the subsurface properties (e.g., bulk density, porosity, moisture content, etc.) are assumed to be uniform and constant over the region modeled,
- the vapor source concentration is constant (or changes slowly compared to the simulation time),
- the dissolved and vapor concentrations of the chemical can be related by the chemical's Henry's Law Constant,
- the vapor source plan view dimensions are large in comparison with the depth to the vapor source, so that the problem can be reasonably approximated as being one-dimensional,
- the degradation rate is assumed to be first-order with respect to chemical concentration as long as the oxygen concentration exceeds some lower threshold value,
- when the oxygen concentration is equal to or less than the lower threshold value, no degradation takes place, and
- the degradation rate is assumed to be equal to the product of the dissolved phase concentration of the chemical, the volumetric moisture content, and a first-order degradation constant.

K.1.1 Comparison With Other Vapor Models

The Oxygen-Limited Vapor Model differs from the Dominant Layer Model (Appendix J) in that it calculates the thickness of the layers where degradation occurs and does not occur in the vadose zone. In the Dominant Layer Model, the user specifies the thickness of each layer and it is assumed that degradation occurs in the middle layer (the dominant layer). In RISC, the Vapor Transport Model Without Degradation (Johnson-Ettinger Model) and the Vapor Transport Model from Groundwater into Buildings do not simulate degradation.

Table K-1 compares the transport processes modeled and the assumptions made by the four vapor models in RISC.

Table K-1. Transport Processes Modeled by the Vapor Models in RISC.

Assumption/ Fate and Transport Process	Vapor Model Without Degradation*	Dominant Layer Model	Oxygen-Limited Model	Vapor Model From Groundwater Into Buildings
Layering/ Heterogeneity	May have two layers (lens), each being homogeneous	May have three layers, each being homogeneous	Assumes homogeneous system	May have two layers (lens) along with the capillary fringe
Degradation	Not modeled	Assumed to occur in middle layer	Assumed to occur if O_2 levels are high enough	Not modeled
Model O_2 Concen-trations?	No	No	Yes	No
Considers Pressure-Driven Flow by Building?	Yes	Yes	Yes	No
Source Term	Soil gas or soil concentrations	Soil gas or soil concentrations	Soil gas or soil concentrations	Groundwater concentrations

*This is the Johnson-Ettinger model with the addition of an optional lens.

The Oxygen-Limited Model requires some unique input parameters such as an oxygen-transfer coefficient at the boundary. This input parameter may not be available at many sites and may be difficult to estimate. For this reason, until estimates of this flux parameter become more readily available, this model should be viewed as a screening level code for learning how vapor transport behaves.

This model may be used to estimate concentrations in both indoor air and outdoor air. When used to estimate air concentrations in buildings, the model can consider both diffusive and advective transport through the soil at the building foundation. This part of the model is identical to the Johnson and Ettinger model (Johnson and Ettinger, 1991, Appendix D). Appendices D and G describe the indoor and outdoor air models, respectively.

K.1.2 Applicability of the Model/Soil Gas Profile Types

This section briefly presents some generalized soil gas profile types and discusses the applicability of the Oxygen-Limited Model and the other vapor models in RISC to be used with various profile types.

Soil gas profiles can be largely grouped into four general types, depending on the behavior or trends of the hydrocarbon and oxygen concentration profiles with depth. These types are illustrated in Figure K-2.

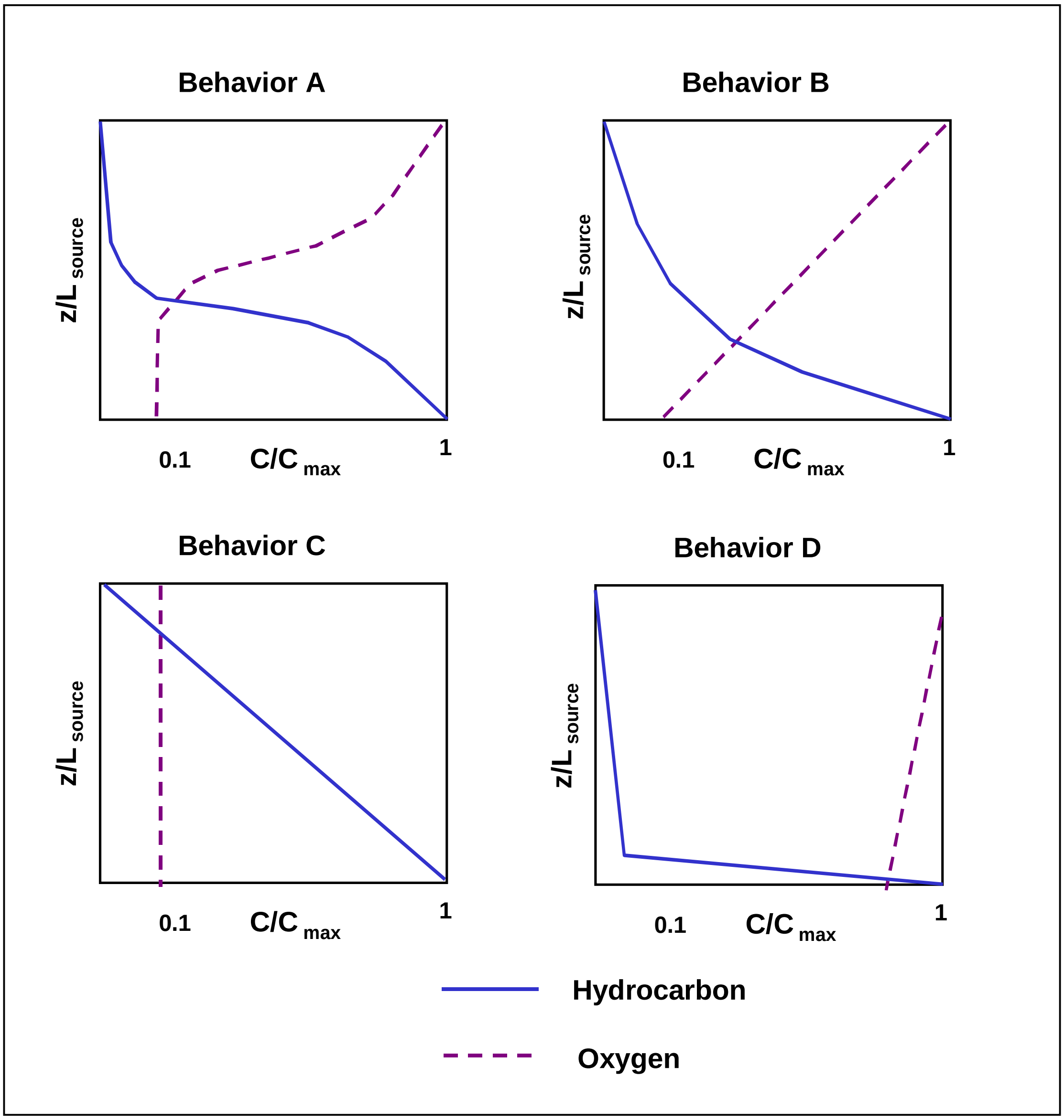

Figure K-4. Four Generalized Soil Gas Profiles

These four generalized behaviors are described in the following paragraphs.

Behavior A. This profile corresponds to the case where there is an oxygen-limited zone for some distance above the source where diffusion is the predominant fate and transport process (as illustrated by the straight line section). At some location above the source the oxygen levels become high enough to support aerobic degradation and the hydrocarbon rapidly decreases. This is the behavior depicted in detail in Figure K-1. The Oxygen-Limited Model was developed to model this type of behavior.

Behavior B. This behavior, illustrated by the parabolic curve, corresponds to the case where the oxygen profile never reaches asymptotic conditions. Aerobic degradation is assumed to be able to occur over the entire distance from the source to the top boundary. The Oxygen-Limited Model or the Dominant-Layer Model can be used to model this profile. In the Oxygen-Limited Model, this case would not be oxygen-constrained (in other words, there really is no reason to use the Oxygen-Limited Model and to determine parameter values for its more difficult input requirements).

Behavior C. Here the oxygen concentration is constant with depth and degradation of the hydrocarbon is not occurring. This profile often may correspond to soil gas concentrations found at capped sites or directly under foundations where oxygen transfer across the upper boundary is limited or eliminated. The predominant transport process controlling the movement of chemical in the vadose zone is diffusion, as indicated by the straight line for the hydrocarbon concentration. This case could actually be characterized by any of the vapor models in RISC, but would be easiest to model using the Vapor Model Without Degradation (Johnson and Ettinger) or the Dominant Layer Model with the degradation rate set equal to zero (if there were three different soil horizons).

Behavior D. In this case, the hydrocarbon is not oxygen-limited near the source region, therefore degradation can occur and the hydrocarbon profile drops off sharply. This can be an especially difficult situation to fit a model to because of the lack of precise field data with which to characterize the hydrocarbon concentration profile. Although the Oxygen-Limited Model could be applied in this case, the profile is not oxygen-constrained and it may be more readily represented by the Dominant Layer Model, adjusting the layer thicknesses as necessary.

K.2 TRANSPORT EQUATIONS AND PROCESSES

This section presents the equations used to calculate the distance to the aerobic degradation zone ("delta"), the vertical concentration profiles of both the chemical and oxygen, and the vapor flux out of the top boundary. Sections K.2.1 and K.2.2 present the equations used by RISC to estimate indoor and outdoor air concentrations, respectively, from the output of the Oxygen-Limited Model.

For the region $0<z<\delta$ where the oxygen concentration is below the minimum required for aerobic degradation:

chemical:

$$0 = D_{eff\_H} \frac{\partial^2 C_H}{\partial z^2} \qquad \textbf{(K-1)}$$

oxygen:

$$0 = D_{eff\_O2} \frac{\partial^2 C_{O2}}{\partial z^2} \qquad \textbf{(K-2)}$$

For the region $\delta<z<L$ where the oxygen concentration is not limited ($C_{02}>C_{02,min}$):

chemical:

$$0 = D_{eff\_H} \frac{\partial^2 C_H}{\partial z^2} - \frac{\lambda\theta_m}{K_H} C_H \qquad \textbf{K-3)}$$

oxygen:

$$0 = D_{eff\_O2} \frac{\partial^2 C_{O2}}{\partial z^2} - \beta \frac{\lambda\theta_m}{K_H} C_H \qquad \textbf{(K-4)}$$

where

C_H = vapor-phase concentration of chemical (or hydrocarbon) [g chemical/cm^3 vapor]

C_{02} = vapor-phase concentration of oxygen [g/cm^3]

z = distance measured up from the source [cm]

θ_m = volumetric moisture content [cm^3/cm^3]

λ_m = first-order reaction rate constant (degradation rate) for chemical [1/s]

K_H = Henry’s Law Constant for chemical [(mg/l vapor)/(mg/l water)]

D_{eff_H} = overall effective porous medium diffusion coefficient for chemical [cm^2/s]

D_{eff_O2} = overall effective porous medium diffusion coefficient for oxygen [cm^2/s]

β = stoichiometric coefficient [mg-O_2/mg-chemical degraded]

Note, the effective diffusion coefficient is calculated using the Millington-Quirk relationship (Millington and Quirk, 1961, and described in Appendix A) which accounts for the amount of air vs. water-filled porosity in the soil.

$$D_{eff\_H} = D_{air\_H}\left(\frac{\theta_a^{3.33}}{\theta_T^2}\right) + \frac{D_{water\_H}}{K_H}\left(\frac{\theta_m^{3.33}}{\theta_T^2}\right) \qquad \textbf{(K-5)}$$

$$D_{eff\_O2} = D_{air\_O2}\left(\frac{\theta_a^{3.33}}{\theta_T^2}\right) + \frac{D_{water\_O2}}{K_{H\,O2}}\left(\frac{\theta_m^{3.33}}{\theta_T^2}\right) \qquad \textbf{(K-6)}$$

where

$K_{H\text{-}O2}$ = Henry's Law Constant for oxygen [(mg/l vapor)/(mg/l water)]

K_H = Henry's Law Constant for chemical [(mg/l vapor)/(mg/l water)]

D_{water_H} = molecular diffusion coefficient for chemical in water [cm^2/s]

D_{water_O2} = molecular diffusion coefficient for oxygen in water [cm^2/s]

D_{air_H} = molecular diffusion coefficient for chemical in air [cm^2/s]

D_{water_O} = molecular diffusion coefficient for oxygen in air [cm^2/s]

θ_T = total porosity [cm^3/cm^3]

θ_a = volumetric air content [cm^3/cm^3]

The advection-dispersion equation is solved for the boundary conditions given below:

at $z = 0$: $$C_H = C_H^{\max} \ \textbf{ and } \ \frac{\partial C_O}{\partial z} = 0 \qquad \textbf{(K-7)}$$

at $z = \delta$: $$C_H = C'_H \ \textbf{ and } \ C_O = C_{O\,min} \qquad \textbf{(K-8)}$$

at z = L: $K_j\left(C_H - C_H^{amb}\right) = -D_{eff\_H}\left(\frac{\partial C_H}{\partial z}\right)$ **and** $K_O\left(C_O^{amb} - C_O\right) = D_{eff\_O}\left(\frac{\partial C_O}{\partial z}\right)$ **(K-9)**

where

$C_H^{\max}$ = source vapor concentration [g/cm^3]

C_H^{amb} = ambient chemical vapor concentration [g/cm^3]

C_O^{amb} = ambient oxygen vapor concentration [g/cm^3]

C'_H = chemical vapor concentration at $z = \delta$ [g/cm^3]

K_j = mass transfer coefficient for the chemical at the upper boundary [cm/s]

K_O = mass transfer coefficient for oxygen at the upper boundary [cm/s]

Note, the user has the option to enter a value for the oxygen rate transfer coefficient, K_O. If the number zero is entered, it will be calculated by the software according to the approaches presented under the sections entitled “Using the Oxygen-Limited Model for Indoor Air” and “Using the Oxygen-Limited Model for Outdoor Air” later in this appendix. The chemical mass transfer coefficient, K_j, is calculated by the software.

The last boundary condition given above (Equation K-9) is a generalized boundary condition that can simulate both open and semi-pervious upper boundaries. For example, as the ratio of the effective diffusion coefficient to the mass transfer coefficient approaches zero, the surface is open ($D_{eff\_H}/K_j \rightarrow 0$). For semi-pervious surfaces (pavement, foundations, etc.) the ratio of effective diffusion coefficient to mass transfer coefficient approaches infinity ($D_{eff\_H}/K_j \rightarrow$ infinity). From this point on, the ambient chemical vapor concentration above the soil (either in the building or outside) will be assumed to be much lower than the source concentration and the vapor phase concentrations in the soil column so that $C^{amb}{}_H$ may be neglected.

For the two regions in the soil column, using the above boundary conditions, the following solutions results:

For $0<z<\delta$ (no degradation region):

$$\frac{C_H}{C_H^{\max}} = 1 - \left(1 - \frac{C_H^{'}}{C_H^{\max}}\right)\left(\frac{z}{\delta}\right) \tag{K-10}$$

$$C_O = C_O^{\min} \tag{K-11}$$

For δ<z<L (region with first-order hydrocarbon degradation):

$$C_H = A_j e^{-\eta_j z} + B_j e^{\eta_j z} \tag{K-12}$$

$$C_O = \sum \beta j \left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(A_j e^{-\eta_j z} + B_j e^{\eta_j z}\right) + D_j z + E_j \tag{K-13}$$

where

$$\eta_j = \sqrt{\frac{\lambda_j \theta_m}{D_{eff\_H} K_H}} \tag{K-14}$$

$$A_j = \frac{C_H^{'} e^{-\eta_j \delta}}{e^{-2\eta_j L}\left[\dfrac{\eta_j \dfrac{D_{eff\_H}}{K_j} - 1}{\eta_j \dfrac{D_{eff\_H}}{K_j} + 1}\right] + e^{-2\eta_j \delta}} \tag{K-15}$$

$$B_j = C_H^{'}\left\{ e^{-\eta_j \delta} - \frac{e^{-\eta_j \delta}}{e^{-2\eta_j L}\left[\dfrac{\eta_j \dfrac{D_{eff\_H}}{K_j} - 1}{\eta_j \dfrac{D_{eff\_H}}{K_j} + 1}\right] + e^{-2\eta_j \delta}} \right\} \tag{K-16}$$

$$D_j = \frac{\left(C_O^{amb} - C_O^{\min}\right) - \left(1 + \frac{D_{eff\_O}}{K_O}\right)\left[\Sigma\beta_j\left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(B_j\eta_j e^{\eta_j\delta} - A_j\eta_j e^{-\eta_j\delta}\right)\right] + \left[\Sigma\beta_j\left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(A_j\eta_j e^{-\eta_j\delta} + B_j\eta_j e^{\eta_j\delta}\right)\right]}{\left[\frac{D_{eff\_O}}{K_O} + L - \delta\right]}$$

(K-17)

$$E_j = C_O^{\min} - D_j\delta - \Sigma\beta_j\left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(A_j\eta_j e^{-\eta_j\delta} + B_j\eta_j e^{\eta_j\delta}\right) \qquad \textbf{(K-18)}$$

Equations (K-10) through (K-18) describe the oxygen and chemical (or hydrocarbon) profiles in terms of the parameters C'_H and δ. In order to derive equations for C'_H and δ the flux of all chemicals (hydrocarbons) and oxygen are required to be continuous across the interface $z = \delta$ (the transition point between the non-degrading region and the region where degradation is taking place). These conditions provide two additional equations that can be used to solve for C'_H and δ:

$$C_H^{'} = \frac{C_H^{\max}}{1 + \left\{\frac{\eta_j\delta e^{-2\eta_j\delta}}{e^{-2\eta_j L}\left[\frac{\eta_j\frac{D_{eff\_H}}{K_j} - 1}{\eta_j\frac{D_{eff\_H}}{K_j} + 1}\right] + e^{-2\eta_j\delta}} + \eta_j\delta + \frac{\eta_j\delta}{e^{-2\eta_j L}\left[\frac{\eta_j\frac{D_{eff\_H}}{K_j} - 1}{\eta_j\frac{D_{eff\_H}}{K_j} + 1}\right] + e^{-2\eta_j\delta}}\right\}} \qquad \textbf{(K-19)}$$

$$0 = \Sigma\beta_j\left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(\frac{C_H^{\max} - C_H^{'}}{\delta}\right) - D_j \qquad \textbf{(K-20)}$$

To solve Equations K-19 and K-20, an iterative technique is used. First, an initial guess for the value of δ is chosen and Equation K-19 is used to calculate C'_H while Equations K-14 through K-16 are used to solve for *Aj*, *Bj*, and D_j. Then Equation K-20 is checked to see if the condition is satisfied. If not, a new value is chosen for δ

and the process is repeated. If the condition in Equation K-20 is satisfied, then the values for C'_H and δ, along with the other input parameters can be used with Equations K-12 and K-13 to solve for the chemical and oxygen profiles, respectively.

This approach (Equations K-10 through K-20) assumes that a region exists in the soil profile where the oxygen is too low for degradation to occur. This may not be the case. When there is no oxygen-limited region, Equations K-12 through K-18 still apply, however, δ now equals zero and $C'_H = C^{max}_H$ (the source concentration). For this situation Equations K-17 and K-20 for the D and E terms respectively must be replaced with:

$$D_j = \Sigma \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}} \right) \left(\eta_j A_j + \eta_j B_j \right) \tag{K-21}$$

$$E_j = C_O^{amb} - \left[\Sigma \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}} \right) \left(A_j \eta_j e^{-\eta_j \delta} + B_j \eta_j e^{\eta_j \delta} \right) \right] - D_j L - \frac{D_{eff\_O}}{K_O} \left[\Sigma \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}} \right) \left(- A_j \eta_j e^{-\eta_j \delta} + B_j \eta_j e^{\eta_j \delta} \right) + D_j \right] \tag{K-22}$$

To determine which case is applicable, the concentration of oxygen at $z = 0$ must be calculated and then compared with C^{min}_O:

$$C_O(z=0) = \Sigma \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}} \right) \left(A_j + B_j \right) + E_j \tag{K-23}$$

If the concentration of oxygen calculated with Equation K-23 is greater than C^{min}_O, then Equations K-12 through K-16 and K-21 through K-22 are used to calculate the soil gas profiles with $\delta = 0$ and $C'_H = C^{max}_H$. If the case is oxygen-limited, then Equations K-12 through K-20 are used.

The volatile emission flux per area leaving the source zone and upper boundary can be calculated from the following:

$$E(z=0)=D_{eff\_H}\frac{\left(C_H^{\max}-C_H'\right)}{\delta}\ ,\qquad if\ \delta>0 \tag{K-24}$$

$$E_{area}(z=0)=D_{eff\_H}\left(A_j\eta_j-B_j\eta_j\right),\quad if\ \delta=0\ \text{(i.e. CO>C}^{\text{min}}{}_{\text{O}}\text{)} \tag{K-25}$$

$$E_{area}(z=0)=D_{eff\_H}\left(A_j\eta_j e^{-\eta jL}-B_j\eta_j e^{\eta jL}\right) \tag{K-26}$$

where

E_{area} = flux per area through upper boundary [g/cm^2/s]

The flux estimate is then used with a dilution model to calculate indoor or outdoor air concentrations depending on which exposure pathway is chosen in the software.

K.2.1 Using the Oxygen-Limited Model for Indoor Air

For enclosed spaces the indoor air concentration is calculated from:

$$C_{building}=\frac{E_{area}A_B}{VQ_B} \tag{K-27}$$

where

$C_{building}$ = vapor concentration in the building [g/cm^3]

Q_B = building air exchange rate [building volumes/sec]

A_B = cross-sectional area for vapor flux [cm^2]

V = building air volume [cm^3]

E_{area} = contaminant flux per area at z = L [g/cm^2/s]

Modeling the flux from soil to enclosed spaces also affects the manner in which K_j and K_O are calculated. Note, the user has the option to specify a value for K_O.

The chemical mass transfer coefficient, K_j, for indoor air applications is calculated using the approach taken by Johnson and Ettinger (1991 and Appendix D):

$$K_j = \frac{Q_{soil}}{A_B} \frac{\exp\left(\dfrac{Q_{soil}\, L_{crack}}{D_{crack}\, A_B \eta}\right)}{\left[\exp\left(\dfrac{Q_{soil}\, L_{crack}}{D_{crack}\, A_B \eta}\right) - 1\right]} \tag{K-28}$$

where

Q_{soil} = volumetric flow rate of soil gas into the building [cm^3/s]

D_{crack} = effective diffusion coefficient in foundation cracks [cm^2/s]

L_{crack} = thickness of the foundation [cm]

A_{crack} = area of cracks or openings through which vapors enter building [cm^2]

η = fraction of cracks in A_B [cm^2-cracks/cm^2 total area]

Refer to Appendix D for details on calculating Q_{soil} and D_{crack}. The other input parameters are user inputs.

The approach that should be used for calculating K_O is not clear. It is hoped that with current research in the indoor air field, an approach will be developed for estimating K_O.

K.2.2 Using the Oxygen-Limited Model for Outdoor Air

For outdoor air, the air concentration is calculated from:

$$C_{air} = \frac{E_{area} L}{uH} \left(\frac{m}{100cm}\right) \tag{K-29}$$

where

C_{air} = concentration in air [g/cm^3]

E_{area} = emission rate per area from vadose zone impacted soil [$g/cm^2/s$]

L = length of the box parallel to the direction of air flow [m]

H = height of the box [m]

u = wind speed [m/s]

For additional discussion on the input parameters for this equation, refer to the "Box Model", Appendix F.

For open surfaces the following conditions apply:

$$\frac{\eta_j D_{eff\_H}}{K_j} << 1 \tag{K-30}$$

$$\frac{D_{eff\_O}}{K_O} << 1 \tag{K-31}$$

When outdoor air concentrations are being calculated in RISC using the oxygen-limited model, K_j is estimated from:

$$K_j = \frac{D_{eff\_H}}{d} \tag{K-32}$$

where

d = thickness of surface cover (a user-input) [cm]

For semi-pervious surfaces d should be set to the thickness of the semi-pervious cover. For an open surface d could be set to the thickness of the soil's stagnant air boundary layer thickness, following Jury et al. (1990). The simulations presented in Jury et al. (1990) used a value of 0.5 cm for both sandy soil and clayey soil. Jury et al. (1983) discuss ways of estimating values of the boundary thickness. The results of the model may not be very sensitive to changes in the thickness of the surface cover for an open surface (when using a reasonable range of values) so it may not be necessary to expend additional time refining the input value.

Similarly, the oxygen-transfer coefficient is calculated from:

$$K_O = \frac{D_{eff\_O}}{d} \tag{K-33}$$

Note, the user has the option to enter a value for the oxygen rate transfer coefficient, K_O. If a value of zero is entered for K_O, it will be code-calculated according to the approach presented above.

K.3 SOURCE TERM

The oxygen-limited model (as all of the vapor models in RISC) may be run using a specified soil gas concentration or a total concentration in soil as the source term. The equations presented in Equations K-19 and K-20 require the soil vapor concentration, C_H^{max}, of the chemical as a starting point. If soil gas is selected as the source term in RISC, then the user-specified value is used for C_H^{max}.

If the source term is to be entered as the total concentration in soil, then C_H^{max} is calculated from the equilibrium partitioning equation or from the chemical's calculated effective solubility, whichever is less. This is the same approach used by the Vadose Zone Model (Appendix A), the Saturated Soil Model (Appendix C), and the other vapor models (Appendices D and J). See Appendix A for a detailed discussion on how the dissolved-phase concentration is determined from the user-input total concentration in soil. Note, this vapor model allows the user to specify values for soil bulk density, fraction organic carbon, moisture content, and porosity in the source area as separate from those used for the modeled transport region. The reason for this is that the contamination may reside in a different unit than that where the vapor migrates.

Once the dissolved-phase concentration (C_w) is calculated, the soil vapor source concentration is calculated from:

$$C_H^{\max} = C_w K_H \qquad \textbf{(K-34)}$$

where

C_H^{max} = source vapor concentration at z = L [g/cm^3]

C_w = dissolved-phase concentration [mg/l]

K_H = Henry's Law Coefficient [(mg/l)/(mg/l)]

K.4 DATA REQUIREMENTS OF THE OXYGEN-LIMITED VAPOR MODEL

The input data requirements for this model are presented in Table K-1.

Table K-1. Data Requirements for the Oxygen-Limited Vapor Model.

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
Unsaturated Zone Parameters			
Porosity	cm^3/cm^3	0.01	0.5
Water content	cm^3/cm^3	0	porosity
Distance to building foundation or soil surface	m	site-specific	site-specific
Ambient O_2 concentration	%	0	21
Minimum O_2 concentration for degradation	%	2 (generally)	21
Oxygen mass transfer coefficient, KO	cm/s	0	
Chemical-Specific Parameters			
Diffusion coefficient in air	cm^2/s	chem-specific	chem-specific
Diffusion coefficient in water	cm^2/s	chem-specific	chem-specific
Henry's Law coefficient	(mg/l)/(mg/l)	chem-specific	chem-specific
Degradation rate in the middle layer	1/day	chem-specific	chem-specific
When Source is entered as a Soil Vapor Concentration:			
Soil vapor concentration	mg/m^3	site-specific	site-specific

Table K-1. Data Requirements for the Oxygen-Limited Vapor Model (concluded).

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
When Source is entered as a Total Soil Concentration:			
Source concentration	mg/kg	site-specific	site-specific
Porosity in source region	cm^3/cm^3	0.01	0.5
Water content in source region	cm^3/cm^3	0	porosity
Fraction organic carbon in source region	g OC/g soil	0.001	1
Soil bulk density in source region	g/cm^3	1.4	2.2
Molecular weight of chemical	g/mol	chem-specific	chem-specific
Solubility of chemical	mg/l	chem-specific	chem-specific
Molecular weight of TPH	g/mol	75	120
Concentration of TPH	mg/kg	site-specific	site-specific
When Model is Used to Predict Indoor Air Concentration:			
Cross-sectional area of foundation perpendicular to volatile emissions	m^2	site-specific	site-specific
Volume of house	m^3	site-specific	site-specific
Building air exchange rate	1/d	Residential: 12 Industrial: 20	location/ site-specific
Thickness of foundation	m	0	site-specific
Fraction of cracks in foundation	cm^3/cm^3	0	1
Qsoil: soil gas flow rate (OR next three parameters)	cm^3/s	0	site-specific
Length of foundation perimeter (not needed if Qsoil not equal to zero)	m	0	site-specific
Depth below foundation (not needed if Qsoil not equal to zero)	m	0	site-specific
Pressure difference from indoors to soil (not needed if Qsoil not equal to zero)	g/cm^2-s (pascals)	0	site-specific (probably at most 100)
When Model is Used to Predict Outdoor Air Concentration:			
Height of breathing zone	m	>0	site-specific
Length of "box" (length of source)	m	>0	site-specific
Wind speed	m	>0	site-specific

K.5 LIMITATIONS OF THE OXYGEN-LIMITED VAPOR MODEL

1. This is a steady-state, constant and one-dimensional model. The source does not deplete due to vapor losses so mass is not conserved. This assumption has only a minor impact on the risk from non-carcinogens (unless the source is very small) since the worst seven-year running average intake is compared to the reference dose. It can have a more significant impact however on carcinogens (such as benzene) since the cumulative exposure over a long exposure duration (up to 30 years) forms the basis for the risk calculation.
2. The model assumes that the oxygen-transfer coefficient can be estimated or is entered by the user. This term is difficult to estimate or measure in the field.
3. The model assumes that degradation occurs only when the oxygen in the vadose zone is above a minimum value. If the oxygen falls below that minimum, it is assumed that degradation ceases.

K.6 REFERENCES

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Appendix L

Surface Water Mixing And Sediment Partitioning Models

L.1 MODEL DESCRIPTION

The surface water mixing and sediment partitioning model is used to estimate the concentration in surface water and sediment assuming that a groundwater plume is discharging to surface water. In RISC, the groundwater concentration adjacent to the surface water body can either be directly entered by the user or it can be estimated by one of the groundwater fate and transport models.

The model has been formulated for two different types of water bodies:

- lakes, estuaries or large water bodies
- rivers, creeks or streams

The sediment model is a simple partitioning model (from the groundwater concentration) that predicts the concentration of the contaminant that is sorbed to the sediment (due to groundwater discharge) in the region where the contaminated plume passes through the sediments into the surface water. In the present model, no biodegradation is allowed as the plume enters the sediment interface.

Figure L-1 shows the model geometry from an areal perspective for the surface water model.

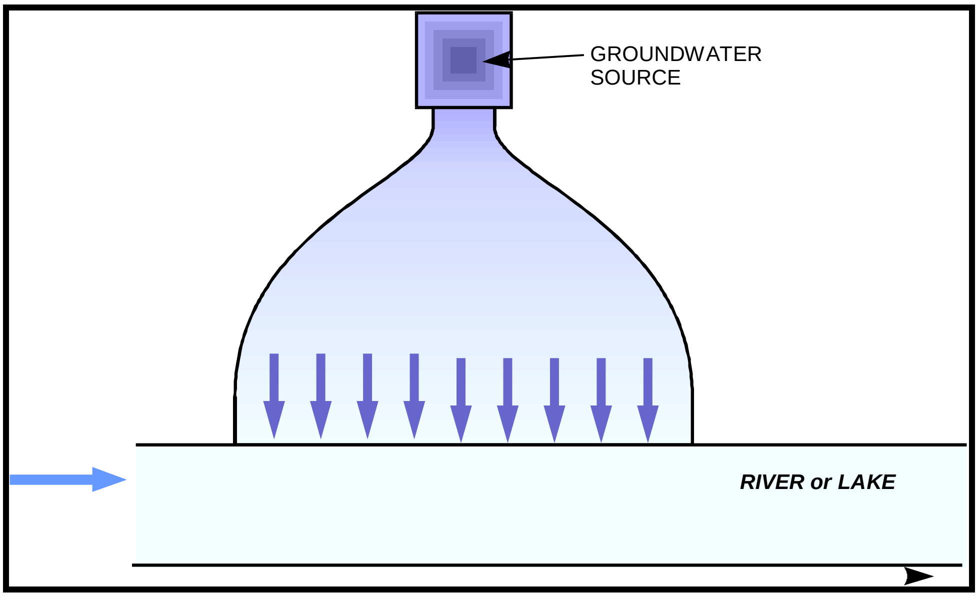

Figure L-1. Surface Water Mixing Model Geometry.

L.2 APPLICATIONS OF THIS MODEL

For human health risk assessments, surface water concentrations can either be entered by the user or they may be estimated with a mixing model (described in this appendix). These surface water concentrations will then serve as receptor point concentrations for the human health risk calculations associated with surface water pathways.

In an ecological assessment the surface water concentrations can be compared with surface water quality criteria and sediment concentrations compared with sediment criteria to evaluate potential ecological impact. In the ecological assessments the surface water and sediment concentrations can be input or estimated using one of the mixing models with a dissolved-phase groundwater plume as the source. This appendix describes the models used to estimate concentrations in surface water and sediment that emanate from a groundwater plume discharging to the surface water.

The main applications of the surface water mixing models are:

1. To estimate potential impacts to a surface water body from adjacent contaminated groundwater.
2. A source can be linked with a groundwater model to ascertain its impact on surface water.
3. If groundwater concentrations have been measured next to the surface water body (and they are at steady state) then the measured groundwater concentrations can be used as a source term. In this case the mixing model is not linked with a groundwater model.
4. To evaluate the potential length of groundwater impact along the surface water body shore.

L.3 TRANSPORT EQUATIONS AND PROCESSES

Water quality is normally simulated in surface water features through assumptions relating to the kinetics and mass transport. Two types of systems are normally considered:

- *Well mixed*, where the concentration through the surface water body (or specified control volume) is equal throughout. This is normally applied to lakes.

- *Incompletely mixed*, in which the contamination is not chemically homogenized. Incompletely mixed systems can also be described as “plug flow” or “mixed flow”. Plug flow models exist where advection dominates (applied to rivers), while mixed flow systems exist where both advection and diffusion/dispersion apply (applied to estuaries).

> Dispersion refers to the movement of contaminants as a result of variations of velocity in space while diffusion refers to the movement of mass due to the random motion.

The surface water mixing models in RISC are assumed to be well-mixed. The next two sections describe the surface water mixing and sediment partitioning models, respectively.

L.3.1 Surface Water Mixing Model

The surface water mixing model in RISC is based on a simple "well-mixed" model where the concentration through the water quality body is equal throughout. This approach is used by RISC to estimate the surface water concentration for both the river and lake options. The well mixed model does not account for advection or dispersion.

The well mixed model is based on the principle of mass balance:

$$V\frac{dC_{sw}}{dx} = W(t) - QC_{sw} - \mu_{sw}VC_{sw} \tag{L-1}$$

where:

$W(t)$	=	mass loading [mg/d]
V	=	volume of surface water for mixing [m^3]
C_{sw}	=	concentration of contaminant in surface water [mg/m^3]
t	=	time [d]
Q	=	inflow/outflow rate [m^3/d]
μ_{sw}	=	decay rate of chemical in surface water [d-1]
x	=	distance downgradient in the river (parallel to the surface water body edge) [m]

For rivers, the x-dimension is assumed to be parallel to the surface water body edge (downgradient in a river). The groundwater plume is assumed to intersect the surface water body at a right angle. For a lake scenario, it is assumed that the plume intersects the lake along a straight boundary perpendicular to the lake edge. The steady state solution to Equation L-1 is:

$$c = \frac{W}{Q + \mu_{sw}V} \tag{L-2}$$

Equation L-2 is used for both rivers and lakes; the only difference between the two is in the way in which the mixing volume is calculated. For rivers, the surface water mixing volume, V, is calculated as the product of the length of the plume and the cross-sectional area of the river, or that part of the river cross-section where mixing takes place. For lakes (or estuaries), the mixing volume is user-specified directly (it can equal either the total lake volume or a fraction thereof).

> Equation L-2 is very similar to Equation F-1 used for the outdoor air ("box") model (described in Appendix F). Equation L-2 assumes that there is a fixed volume of surface water (in this case the reach of the river or section of lake) that receives loading of contaminant (W) and that the contaminant is evenly mixed throughout the water volume. The water in the river reach or section of lake is flushed (or exchanged with fresh water) at the inflow rate. The inflow rate is similar to the wind speed in the box model.

The inflow/outflow rate, Q, is calculated from the user-specified input parameters values and is equal to the sum of the groundwater discharge and the inflow rate of surface water into the surface water volume:

$$Q = Q_{sw} + Q_{gw} \tag{L-3}$$

The mass loading rate, W, is calculated from:

$$W = Q_{sw}{*}C_o + Q_{gw}{*}C_{gw} \tag{L-4}$$

where

Q_{sw} = surface water inflow rate (upstream flow) [m^3/d]

C_o = upstream (background) concentration of contaminant in surface water [mg/m^3]

Q_{gw} = groundwater inflow rate [m^3/d]

C_{gw} = concentration of contaminant in groundwater inflow [mg/m^3]

L.3.2 Sediment Partitioning Model

The sediment concentrations are calculated using the equilibrium partitioning equation:

$$C_{sed} = C_{gw} K_d \tag{L-7}$$

where

C_{sed} = concentration in sediments [mg/kg]

C_{gw} = concentration in groundwater at centerline of plume estimated by RISC groundwater model or user-specified [mg/l]

K_d = soil-water partitioning coefficient [ml/g]

For inorganic chemicals, the soil-water partitioning coefficient, K_d, may be directly entered in the RISC chemical database (Step 1). For organic chemicals (chemicals that have an "ND" entered for the K_d in the chemical database), the partitioning coefficient is calculated as the product of the fraction organic carbon and the chemical's organic partitioning coefficient:

$$K_d = F_{oc} * K_{oc} \tag{L-8}$$

where

F_{oc} = fraction organic carbon in dry soil [g/g]

K_{oc} = chemical-specific organic carbon partition coefficient [ml/g]

Note, if the groundwater concentration, C_{gw}, is predicted by one of the RISC groundwater models, it will vary with time. In that situation, the estimated sediment concentrations will also vary with time.

L.4 EXAMPLES

The following two examples show how Equations L-2 through L-4 are used to estimate concentrations in surface water for rivers and lakes, respectively.

L.4.1 River Example

A river with inflow upstream of 900 m^3/d (approx. 10 l/s), groundwater inflow of 100 m^3/d and a generic contaminant concentration in groundwater of 316 mg/l (assumed to be steady state in this example). Other assumed or measured parameters include:

- Decay rate of contaminant in river 0.05/d.
- Length of polluted reach (where the groundwater plume intersects the surface water) = 100m
- River cross section of 5 m^2.
- Background contaminant concentration in river = 0

Calculations:

- Contaminant loading, W = 316 mg/l*100 m^3/d inflow*1000 l/m^3 = 31,600,000 mg/d or 3.16E7 mg/d
- Volume, V = 5 m^2 cross section*100 m reach = 500 m3
- Total outflow rate, Q = 900 m^3/d inflow upstream +100 m^3/d from groundwater = 1000 m^3/d

From Equation L-2, the concentration in the river is:

$$C_{sw} = \frac{W}{Q + kV} = \frac{3.16E7\,\frac{mg}{d}}{\left[1000\frac{m^3}{d} + \left(\frac{0.05}{d}\right)\left(500m^3\right)\right]} \frac{1m^3}{1000l} = 30.8mg/l$$

L.4.2 Lake Example

A lake with a total volume of 50,000 m^3, groundwater inflow rate of 100 m^3/d with a concentration 316 mg/l. The decay rate of the chemical in surface water has been estimated at 0.05/d and the inflow of surface water is 100 m^3/d. Mixing is assumed to occur throughout the entire lake volume.

Calculations:

- Mass loading, W = 316*100*1000 = 3.16E7 mg/d (as above)
- Outflow, Q = 100 m^3/d groundwater + 100 m^3/d surface water = 200 m^3/d

From Equation L-2, the concentration in the lake is:

$$C_{sw} = \frac{W}{Q+kV} = \frac{3.16E7\,\frac{mg}{d}}{\left[200\,\frac{m^3}{d} + \left(\frac{0.05}{d}\right)50{,}000m^3\right]} \frac{1m^3}{1000l} = 11.7mg/l$$

L.4.3 Adjusting the Mixing Volume for Large Surface Water Bodies

For large surface water bodies where it is unlikely that the groundwater mixes across the entire surface water body (e.g. large lakes or wide rivers), the mixing volume should be adjusted to represent the fraction of the total surface water volume available for mixing. Choosing an appropriate value for the mixing fraction will usually be a judgment call based on the site-specific information. In the lake example, if it were assumed that the groundwater only mixed with 1% of the total lake volume, the concentration would be estimated as:

$$C_{sw} = \frac{W}{Q_{gw} + Frac_{mix}\left(Q_{sw} + kV\right)} = \frac{3.16E6\,\frac{mg}{d}}{100\,\frac{m^3}{d} + 0.01\times\left[100\,\frac{m^3}{d} + \left(\frac{0.05}{d}\right)\left(50{,}000m^3\right)\right]} \frac{1m^3}{1000l} = 14mg/l$$

Note that the total surface water inflow rate, Q_{sw}, is adjusted along with the total surface water volume. Several points to consider when deciding whether or not to adjust the surface water mixing volume are:

- If the length of the reach is long relative to the cross-section of the river, the volume may not need to be reduced (the fraction for mixing would be equal to 1).
- If the river is flowing slowly and the cross-sectional area is not too large, it is probably a fairly good assumption that it is well mixed (the fraction should equal 1).
- Conversely, if the river (or lake) is flowing quickly and/or the thickness of the groundwater intersecting the river is small in comparison with the cross-section, then the mixing fraction should be adjusted to account for the reduced mixing potential.

L.4.4 Calculation of Groundwater Inflow Rate

In the above two examples, it is assumed that the groundwater inflow rate, Q_{gw}, and the contaminant loading rate, W, are known. Darcy's Law is used to estimate the groundwater inflow rate, Q_{gw}:

$$Q_{gw} = K_{sw} d_{sw} L_{reach} \left(\frac{h_{gw} - h_{sw}}{L_f} \right) \tag{L-5}$$

where:

Q_{gw} = groundwater inflow rate [m^3/d]

K_{sw} = hydraulic conductivity of the groundwater-surface water interface (**not necessarily** the hydraulic conductivity of the aquifer defined for the simulation of flow and transport within the aquifer) [m/d]

d_{sw} = thickness of groundwater that ends up discharging in the surface water body [m]. Note that this is user-specified and does not necessarily equal the total depth of the aquifer since, for partially penetrating conditions, some of the aquifer flow is beneath the surface water body.

L_{reach} = length of surface water reach receiving contamination [m]

L_f = distance along flow line between h_{sw} and h_{gw} [m]

h_{sw} = river/lake water level [m]

h_{gw} = groundwater hydraulic head [m]

The last term in Equation L-5 is the hydraulic gradient between the groundwater aquifer and the surface water. This hydraulic gradient may be different than the overall groundwater gradient away from the surface water body edge. Figure L-2 shows the cross-sectional schematic with the variables.

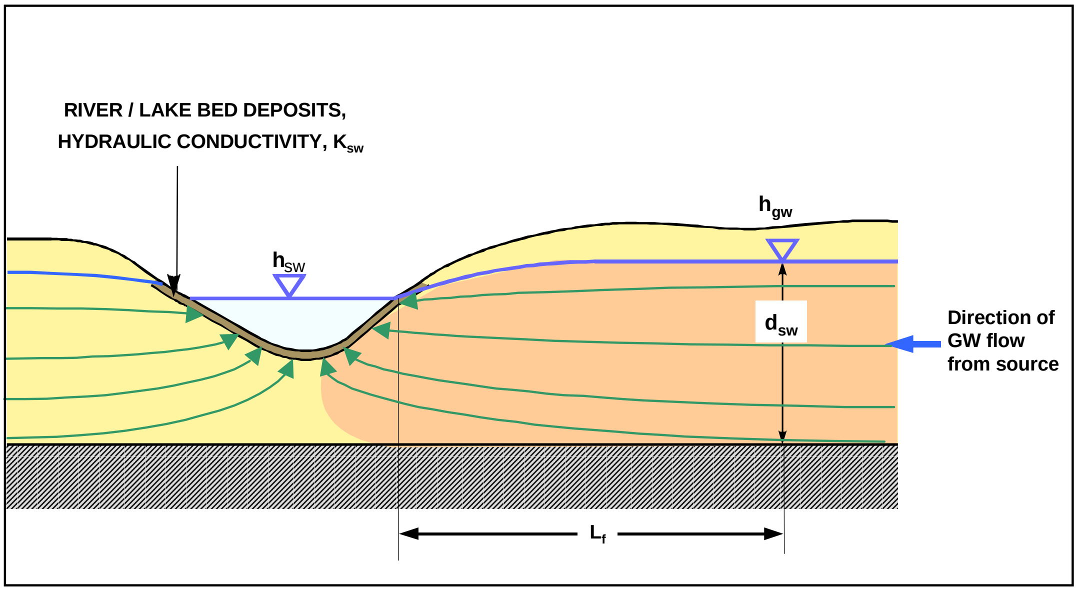

Figure L-2. Cross-Sectional Model Geometry.

L.4.5 Calculation of Length of Reach

The length of the reach, L_{reach}, where the groundwater plume impacts the surface water body is either directly entered by the user for the case where a groundwater model is not used, or it is calculated by the groundwater model in the linked situation. When the surface water mixing model is linked with a groundwater model, the length of the reach, L_{gw}, is a function of the plume width where it intersects the surface water body. Further, an assumption is made that the concentrations across the plume width is constant and the width of impact is calculated from the point at which the actual groundwater concentration drops to 5% of the centerline concentration when the plume is at steady state. Figures L-3 is an areal schematic showing how the length of the reach is calculated. Figure L-4 is a graph that compares the shape of the actual mass loading function with the conservative step loading rate assumed in the mixing model.

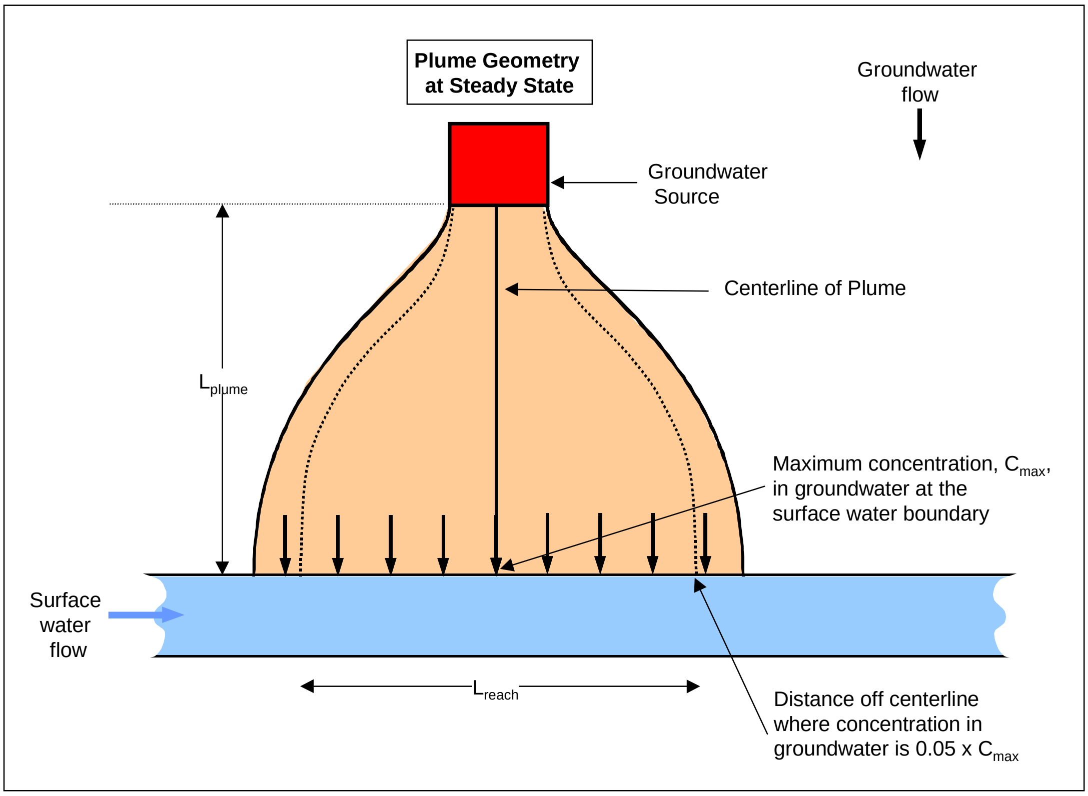

Figure L-3. Calculating the Length of the Reach

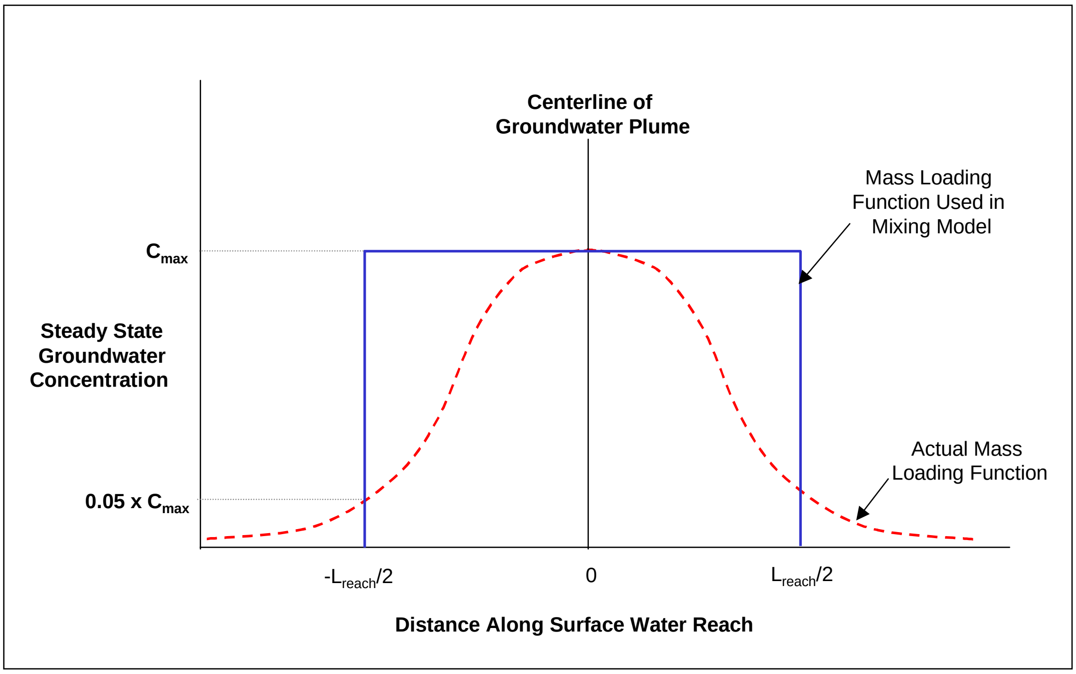

Figure L-4. Calculating the Mass Loading Function

The following equation (Domenico, 1987) is used to estimate the distance off the centerline at which the concentration becomes 5% of the centerline concentration:

$$C(x,y,z) = \frac{C_o}{4}\exp\left\{\frac{x}{2\alpha_x}\left[1-\sqrt{1+\frac{4\lambda\alpha_x}{\upsilon}}\right]\right\}$$
$$\left\{erf\left[\left(y+\frac{W_y}{2}\right)\frac{1}{2\sqrt{\alpha_y x}}\right]-erf\left[\left(y-\frac{W_y}{2}\right)\frac{1}{2\sqrt{\alpha_y x}}\right]\right\} \quad \textbf{(L-6)}$$
$$\left\{erf\left[\left(z+\frac{W_z}{2}\right)\frac{1}{2\sqrt{\alpha_z x}}\right]-erf\left[\left(z-\frac{W_z}{2}\right)\frac{1}{2\sqrt{\alpha_z x}}\right]\right\}$$

where:

$C(x,y,z)$ = steady-state concentration of chemical in groundwater at a location (x,y,z) [mg/l]

C_o = source concentration of chemical in groundwater [mg/l]

x = Cartesian coordinate in the direction of groundwater flow, measured downgradient of the groundwater source [m]

y = Cartesian coordinate in the transverse direction, measured from the centerline of the plume [m]

z = Cartesian coordinate in the vertical direction, measured positively downward from the water table [m]

W_y = width of the groundwater source in the cross-gradient direction [m]

W_z = vertical thickness of the groundwater source [m]

α_x = longitudinal dispersivity (in the direction of groundwater flow) [m] (assumed to be equal to 0.1 * L_{gw})

α_y = transverse dispersivity (perpendicular to the direction of groundwater flow) [m] (assumed to be equal to $\alpha_x/3$)

α_z = vertical dispersivity [m] (assumed to be equal to $\alpha_x/87$)

The length of the surface water reach is calculated by first using Equation L-6 to calculate the centerline concentration at the surface water body edge. Then L-6 is solved iteratively until it finds the distance cross-gradient where the groundwater concentration equals 5% of the centerline concentration. These concentrations will not likely match the concentrations calculated by the groundwater model in RISC. The important relationship calculated by Equation L-6 is the relative concentrations. The Domenico equation presented in L-6 assumes that the groundwater source is continuous and steady-state for the length of the simulation time. It therefore calculates a worst case width of the plume at the surface water body edge. This conservative value of the width is then used in Equation L-5 to estimate the groundwater loading to the surface water body. Note, the groundwater concentrations predicted by the RISC groundwater model are used to estimate the actual mass loading in Equation L-4; the groundwater concentration values in Equation L-6 are only used to estimate a worst case length of reach. The groundwater concentrations predicted by the RISC models are transient and therefore the loading rate to surface water will be a function of time as well.

L.5 DATA REQUIREMENTS

Table L-1 lists the data requirements for the surface water mixing and sediment partitioning models.

L.6 ASSUMPTIONS AND LIMITATIONS OF THE SURFACE WATER AND SEDIMENT MIXING MODELS

1. Impact on surface water and/or sediment caused by soil erosion, overland flow (runoff) or river upstream effects is not modeled.
2. Impact to surface water from a point discharge (e.g. a pipe) rather than a groundwater plume is ignored.
3. The mixing model assumes the aquifer discharges into the surface water body. If the river is a "loosing stream", then the groundwater will not impact the surface water body and the model should not be used.
4. The model should not be used if the groundwater plume flows underneath the river and does not discharge into it.
5. The sediment partitioning model assumes no biodegradation as the plume enters the sediment interface.

L.7 REFERENCES

Domenico, P.A., 1987, "An Analytical Model for Multidimensional Transport of a Decaying Contaminant Species," *Journal of Hydrology*, Vol. 91, p 49-58.

Table L-1. Data Requirements for the Surface Water Mixing and Sediment Partitioning Model

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
MEDIA-SPECIFIC PARAMETERS			
Distance to Surface Water Edge	m	Site-Specific	Site-Specific
Hydraulic Conductivity of Surface Water Bed	m/day	1.00E-07	100
Hydraulic Gradient Between Groundwater and Surface Water	m/m	Site-Specific	Site-Specific
Thickness of Groundwater Aquifer at Surface Water Edge	m	Site-Specific	Site-Specific
Surface Water Inflow/Outflow Rate	m^3/d	Site-Specific	Site-Specific
Cross-Sectional Area of River (only if River Mixing Option is chosen)	-	Site-Specific	Site-Specific
Total Volume of Surface Water (only if Lake Mixing Option is chosen)	m^3	Site-Specific	Site-Specific
Fraction of Surface Water Body Available for Mixing	-	Site-Specific	Site-Specific
Fraction Organic Carbon (in sediments)	g /g soil	0.001	0.2
SOURCE PARAMETERS (When not linked with a groundwater model)			
Length of Impacted Reach	m	site-specific	site-specific
Concentration of Chemical in Groundwater at Surface Water Body Edge	mg/l	site-specific	site-specific
CHEMICAL SPECIFIC DATA (individual chemical component)			
K_{oc}	ml/g	chem-specific	chem-specific
Degradation Rate in Surface Water	1/d	chemical- and site-specific	chemical- and site-specific

Appendix M

Summary Of National & International Status Guidelines For The Protection Of Aquatic Life

M.1 UNITED STATES - NATIONAL AMBIENT WATER QUALITY CRITERIA

The US Environmental Protection Agency (EPA) is required to derive, publish and update ambient water quality criteria for the protection of aquatic life and human health under Section 304(a) of the Clean Water Act. The most recent update to the criteria was published on December 10th, 1998 in the US Federal Register (Volume 63, No 237). The derivation process for National Ambient Water Quality Criteria (NAWQC) for protection of aquatic life is well documented (see *Guidelines for Deriving Numerical National Water Quality Criteria for the Protection of Aquatic Organisms and Their Uses*; EPA 1985).

The criterion derivation process for each chemical or quality parameter consists of a literature review phase followed by calculation of a criterion using a prescribed method for those parameters where sufficient data exist. For the derivation of a freshwater criterion, acute tests are required for species with breeding populations in North America from the following eight families:

- *Salmonidae* (salmonid fish) in the class *Osteichthyes*;
- a second family in the class *Osteichthyes*;
- a third family in the phylum *Chordata* (this phylum includes the class *Osteichthyes*);
- a planktonic crustacean;
- a benthic crustacean;

- an insect;
- a family in a phylum other than *Arthropoda* or *Chordata* (e.g. rotiferans, annelids, molluscs); and
- another insect or a family from a phylum not already represented.

Tests indicating the relationship between acute and chronic toxicity of a parameter are also required for aquatic species from at least three different families, which must include a fish, an invertebrate and at least one acutely sensitive freshwater species. In addition, one test on a freshwater plant or alga and one freshwater species bioconcentration factor are required.

Similar requirements exist for the derivation of marine criteria. The following calculation process is then performed for each chemical in the freshwater and marine environments:

- The calculation of a species mean acute value (SMAV) representing acute toxicity to each species represented;
- The calculation of a genus mean acute value (GMAV) representing acute toxicity to each genus represented;
- The calculation of a final acute value (FAV) protective of 95% of species against acute toxicity effects;
- The calculation of a final acute-chronic ratio (FACR) indicating the ratio between acute and chronic endpoints for aquatic life;
- The calculation of a final chronic value (FCV) protective of 95% of aquatic life against chronic toxicity effects. The FCV is calculated by applying the FACR to the FAV;
- Calculation of a final plant value (FPV) for protection of plant life; and
- Calculation of a final residue value (FRV) for protection against bioaccumulation effects.

The final criteria (i.e. the NAWQC) are published as a criterion maximum concentration (CMC) not to be exceeded in the short term (one-hour average), and a criterion continuous concentration (CCC) not to be exceeded in the long term (four-day average) more than once every three years on average.

The CMC is taken as half the value of the final acute value (FAV), and the CCC is selected as the lowest of the final chronic value, the final plant value and the final residue value from the calculation process above. An element of expert judgement is incorporated into the process and the derivation methodology may be revised for a given parameter following a round of public and scientific peer review. For the assessment of ecological impact of chemicals leaching from contaminated land, CCC values are considered to be appropriate indicators.

M.2 CANADA – WATER QUALITY GUIDELINES

Canadian Council of Ministers for the Environment (CCME) Water Quality Guidelines for protection of aquatic life are derived following guidelines published by the International Joint Commission Water Quality Board (IJC 1975) and the Ontario Ministry of the Environment (OMOE 1979, 1992). The goal is to protect all aquatic life stages during indefinite exposure to toxicants in water. All aquatic ecosystem components are considered if the data are available. Where limited data are available for a given chemical, CCME prefer to set an interim guideline to not specifying a guideline value.

For most water quality variables CCME have set a single maximum value not to be exceeded, with this value based on a long-term no-effect concentration.

Candidate chemicals for guideline derivation are selected from the following priority lists:

- CCME Task Force on Water Quality Guidelines Priority Pesticides List; and the
- Canadian Environmental Protection Act Priority Substances List.

In addition, chemicals of regional concern within Canada are selected with input from federal, provincial, and territorial agencies.

Published data on the following are reviewed:

- acute and chronic toxicity to aquatic biota;
- bioaccumulation potential;
- physico-chemical properties and information on fate and behaviour;
- patterns of production and use in Canada;
- background concentrations in Canada;
- genotoxicity; and
- guideline information from other jurisdictions.

Published toxicity studies are evaluated and classified as primary, secondary, or unacceptable, dependent upon the degree to which each study fulfils acceptable laboratory protocols. Specified minimum toxicological and environmental fate data set requirements must be met for a final guideline to be set. Where these requirements are not met, a less stringent set of requirements may be fulfilled to derive an interim guideline.

As with water quality criteria published by other jurisdictions, uncertainty factors are applied to selected ecotoxicity endpoints to derive a final guideline. When available, the lowest-observable-effects level (LOEL) from a chronic exposure study on the most sensitive *native Canadian* species is multiplied by a safety factor of 0.1 to arrive at the final guideline concentration. Alternatively, the lowest LC50 or EC50 from an acute exposure study is multiplied by an acute/chronic ratio or an appropriate uncertainty factor (this factor being set at 0.05 for non-persistent chemicals and 0.01 for persistent chemicals) to determine the final guideline concentration. The CCME guidelines represent concentrations protective of aquatic life from chronic exposure and no acute exposure guidelines are published.

M.3 EUROPE - ENVIRONMENTAL QUALITY STANDARDS

The European Community (EC) sets environmental quality standards (EQSs) for ‘priority list substances’, with these standards to be adopted by member states of the EC. Priority list substances include those named in List I of the Annex to Directive

76/464/EEC *on pollution caused by certain dangerous substances discharged into the aquatic environment of the community*. Water quality conditions for List I substances have been established in a series of "daughter Directives" (82/176/EEC, 83/513/EEC, 84/156/EEC, 84/491/EEC and 86/280/EEC amended by 90/415/EEC). There are two alternative methods for setting these conditions: member states may apply ‘end-of-pipe’ emission limit values based the best available techniques, or may base discharge permits on limits required to meet specified environmental quality objectives (i.e., EQSs) in the receiving body of water. The priority list is occasionally reviewed based on scientific evidence, the most recent review proposed by the European Commission in February 2000.

The methodology for derivation of EQSs for List I substances at the EC level is not published, although review of both eco-toxicity data and political/technical considerations is believed to be incorporated. EQSs published in EC daughter Directives to the Dangerous Substances Directive are quoted as continuous concentrations.

Numerical quality objectives for surface water are also specified for commercial salmonid and cyprinid fisheries waters in Directive 78/659/EC (ammonia, biological oxygen demand, chlorine, dissolved oxygen, nitrite, pH, phosphorous, chromium, copper, lead, nickel and zinc) and for shellfish waters in Directive 79/923/EC (dissolved oxygen and faecal coliform bacteria).

M.4 UNITED KINGDOM - ENVIRONMENTAL QUALITY STANDARDS

Environmental Quality Standards (EQS) for the protection of aquatic life are proposed and adopted in the UK from the following sources:

1. Adoption of the European Community EQS (chemicals named in List I of the Annex to Directive 76/464/EEC on pollution caused by certain dangerous substances discharged into the aquatic environment of the community).

2. Set by the DETR (Department of the Environment, Transport and the Regions) in the Surface Waters (Dangerous Substances)(Classification) Regulations (1989-1998) and/or the Surface Waters (Fishlife)(Classification) Regulations (1997). Regulations are published separately for England & Wales and for Scotland, under the Water Resources Act 1991.
3. Proposed by the WRc plc under contract to the DETR and awaiting passage into the Regulations.
4. Set by the Environment Agency (the UK regulatory body) in R&D reports, for the purposes of monitoring industrial discharge consents or dealing with specific contamination problems associated with chemicals without quality standards from the above sources.

For those standards not adopted directly from EC legislation, the EQS concentration is derived based upon review of the published literature on chemical eco-toxicity, using expert judgement and the application of uncertainty factors where necessary. Strict guidance has not been set on data quality and the application of uncertainty factors to toxicity endpoints. Review of selected R&D documents published by WRc plc reveals that order-of-magnitude uncertainty factors (i.e. 10, 100, etc) may be applied to acute toxicity data for sensitive aquatic species in order to derive an EQS. Background concentrations in the UK, physico-chemical properties, bioaccumulation potential and guidelines set by other jurisdictions are also considered in the derivation process.

Some or all of the following criteria may be published for a given chemical; Maximum Allowable Concentration (MAC) and Annual Average (AA) for each of inland (freshwater), estuarine and marine waters.

Specific monitoring regimes are not stipulated in the regulations for determining AA concentrations – this is left to the Environment Agency’s judgement. For the purposes of contaminated land assessment, AA concentrations are generally used in preference to MACs.

M.5 AUSTRALIA AND NEW ZEALAND - WATER QUALITY GUIDELINES

The Australian Water Quality Guidelines for Fresh and Marine Waters were first published by the Australia and New Zealand Environment and Conservation Council (ANZECC) under the National Water Quality Management Strategy in 1992. They were set largely by review of guidelines used by other jurisdictions, primarily the 1991 CCME Water Quality Guidelines for the protection of aquatic life, and the 1986 US Environmental Protection Agency's National Ambient Water Quality Criteria.

The ANZECC water quality guidelines have been revised and a draft version has been available for review since 1999. It is expected that they will be cleared for release in April 2001. Information on the new guidelines and the release date are available from the web site:

http://www.environment.gov.au/water/quality/guidelines/index.html.

Review of these revised guidelines was coordinated by Environmental Research Institute of the Supervising Scientist (ERISS), part of the Science Group of Environment Australia. The values shown in Table M-1 for ANZECC were obtained from the 1999 draft version.

M.6 ACKNOWLEDGEMENTS

This chapter was written by URS Dames and Moore UK (James Walker) under contract to BP.

Table M-1. Surface Water Quality Criteria Database in RISC

		U.S.				UK				New Zealand/ Australia		European Community		Canada	
		AWQC[1]				UKEQS[2]				ANZECC[3]		EC WQO[4]		CCREM[5]	
		Freshwater		Marine		Freshwater		Marine		Freshwater	Marine	Freshwater	Marine	Freshwater	Marine
Chemical	Comments	Continuous[6] ug/l	Maximum[7] ug/l	Continuous[6] ug/l	Maximum[7] ug/l	AA[8] ug/l	MAC[9] ug/l	AA[8] ug/l	MAC[9] ug/l	ug/l	ug/l	AA[8] ug/l	AA[8] ug/l	ug/l	ug/l
Acenaphthene	see PAHs (total)													5.8 I	
Acenaphthylene	see PAHs (total)														
Acetone	no guideline														
Anthracene	see PAHs (total)									0.06	0.06			0.012 I	
Arsenic		150	340	36	69	50		50		1.6	1.6			50	12.5
Barium	no guideline														
Benzo(a)anthracene	see PAHs (total)													0.018 I	
Benzene						30	300	30	300	230	170			370	110
Benzo(a)pyrene	see PAHs (total)									0.3	0.3			0.015 I	
Benzo(b)fluoranthene	see PAHs (total)														
Benzo(g,h,i)perylene	see PAHs (total)														
Benzo(k)fluoranthene	see PAHs (total)														
Beryllium															
Bis(2ethylhexyl)phthalate										2	2				
Butyl benzyl phthalate	no guideline														
Cadmium		2.2 H	4.3 H	9.3	43	5		2.5		0.013 H	1.7	5	2.5	0.03 I H	0.12
Carbon Disulfide	no guideline														
Carbon Tetrachloride						12		12		240	240	12	12	13.3 I	
Chlorobenzene										32	32			1.3 I	25 I
Chloroform (trichloromethane)						12		12		170	170			1.8 I	
Chromium (III)		74 H	570 H							9 H	9			8.9 I	56 I
Chromium (IV)		11	16	50	1100					1.1	3.1			1	1.5
Chromium (total)						10 H		5						2	
Chrysene	see PAHs (total)														
Copper		9 H	13 H	3.1	4.8	3 H		5		0.33 H	0.029			2 H	
Cresol(m)	no guideline														
Cresol(o)	no guideline														
Cresol(p)	no guideline														
Cyanide		5.2	22	1	1					1	1			5	
Dibenz(a,h)anthracene	see PAHs (total)														
Dichloroethane (1,1)	no guideline														
Dichloroethane (1,2) (EDC)						10		10		1100	1100	10	10	100 I	
Dichloroethene (trans 1,2)	no guideline														
Dichloroethene(trans 1,1-)										610	610				
Dichloroethylene (cis 1,2)										610	610				
Dimethylbenza(a)anthracene (7,12)	see PAHs (total)														
Dimethylphenol (2,4)	no guideline														
di-n-Butylphthalate															
Dinitrotoluene (2,4)										13	13				
di-n-Octylphthalate	no guideline														
Dioxane (1,4)	no guideline														
Ethylbenzene										86	86			90 I	
Ethylene Dibromide	no guideline														
Fluoranthene	see PAHs (total)									0.7	0.7			0.04 I	
Fluorene	see PAHs (total)													3.0 I	
Indeno(1,2,3CD)pyrene	see PAHs (total)														
Lead		2.5 H	65 H	8.1	210	10 H		10						2 H	
Mercury		0.77	1.4	0.94	1.8	1		0.3		0.013	0.029	1	0.3	0.1	
Methanol	no guideline														

Table M-1. Surface Water Quality Criteria Database in RISC

		U.S.				UK				New Zealand/ Australia		European Community		Canada	
		AWQC[1]				UKEQS[2]				ANZECC[3]		EC WQO[4]		CCREM[5]	
		Freshwater		Marine		Freshwater		Marine		Freshwater	Marine	Freshwater	Marine	Freshwater	Marine
Chemical	**Comments**	Continuous[6] ug/l	Maximum[7] ug/l	Continuous[6] ug/l	Maximum[7] ug/l	AA[8] ug/l	MAC[9] ug/l	AA[8] ug/l	MAC[9] ug/l	ug/l	ug/l	AA[8] ug/l	AA[8] ug/l	ug/l	ug/l
Methyl ethyl ketone	no guideline														
Methylene Chloride										3100	3100				
Methyl napthalene (2)	see PAHs (total)														
MTBE	EPA 1999	51	151	17	50										
Naphthalene						10	100	5	80	0.3	8.4			1.1 I	1.4 I
Nickel		52 H	470 H	8.2	74	20 H		15		0.7 H	32.6			65 H	
Nitrobenzene										60	60				
PAHs (total)															
PCBs			0.014		0.03									0.001	0.01
Phenanthrene	see PAHs (total)									2	2			0.4 I	
Phenol										6	21			4 P	
Pyrene	see PAHs (total)													0.025 I	
Pyridine	no guideline														
Selenium		5		71	290					1.4	1.4			1	1
Silver			3.4 H		1.9					0.005	0.18			0.1	
Styrene														72 I	
Tetrachloroethane (1,1,2,2)										200	200				
Tetrachloroethene (PCE)						10		10		82	82	10	10	111 I	
Tetraethyl Lead	no guideline														
Toluene						50	500	40	400	170	170			2 I	215 I
TPH Aliphatic C5-6	no guideline														
TPH Aliphatic C6-8	no guideline														
TPH Aliphatic C8-10	no guideline														
TPH Aliphatic C10-12	no guideline														
TPH Aliphatic C12-16	no guideline														
TPH Aliphatic C16-35	no guideline														
TPH Aromatic C5-7	no guideline														
TPH Aromatic C7-8	no guideline														
TPH Aromatic C8-10	no guideline														
TPH Aromatic C10-12	no guideline														
TPH Aromatic C12-16	no guideline														
TPH Aromatic C16-21	no guideline														
TPH Aromatic C21-35	no guideline														
Trichloroethane (1,1,1)						100	1000	100	1000	130	130				
Trichloroethane (1,1,2)						400	4000	300	3000	270	470			21 I	
Trichloroethylene (TCE)						10		10				10	10		
Vanadium						20 H		100		6	10				
Vinyl Chloride										100	100				
Xylenes						30	300	30	300	61	61				
Zinc		120 H	120 H	81	90	300 H DF		10 DF		2.4 H	2.7	300 H DF	10 DF	30	

Notes:

1 - United States Environment Protection Agency Ambient Water Quality Criteria
2 - United Kingdom Environmental Quality Standards (statutory and proposed)
3 - Australia and New Zealand Environment and Conservation Council, Guidelines for Fresh and Marine Water Quality (Draft, July 1999)
4 - European Commission Water Quality Objective
5 - Canadian Council of Ministers for the Environment Freshwater Aquatic Life Guideline
6 - Criteria Continuous Concentration (CCC) - 4-day average not to be exceeded more than once every three years on average
7 - Criteria Maximum Concentration (CMC) - one-hour average not to be exceeded more than once every three years on average
8 - Annual Average concentration
9 - Maximum Allowable Concentration

DF - Applies to designated fishery waters
H - Hardness-dependent. Where a single value is given this applies to a water hardness of 100 mg/l CaCO3, otherwise a range is quoted
I - Interim Guideline
P - Criterion applies to total phenols
pH - pH-dependent. Criterion applies to pH7
* - The UK Surface Waters (Dangerous Substances)(Classification) Regulations (1989) state that the total concentration of aldrin + dieldrin + endrin+ isodrin should not exceed 0.03 ug/l, with endrin not to exceed 0.005 ug/l

Appendix N

Sediment Quality Criteria

N.1 REVIEW OF SEDIMENT CRITERIA FOR THE PROTECTION OF AQUATIC ECOLOGY

This appendix presents sediment screening values that were reviewed for inclusion in RISC. The screening values are presented in Table N-1. A wide range of sediment quality criteria has been published by various sources, the majority of which are North American. The lack of criteria with national status in North America and elsewhere is largely due to ongoing debate regarding the most appropriate means of criteria derivation, and indeed whether the use of criteria for screening purposes is in itself an appropriate means of assessment of contaminated land and water.

The terms ‘criterion’, ‘screening value’, ‘benchmark’, ‘guideline’ and ‘standard’ have particular definitions under certain jurisdictions. However, they are viewed as interchangeable in this report, denoting concentrations appropriate for use in a first tier screening of the potential for ecological receptors to suffer adverse effects as a result of exposure to chemical contamination.

Part of the *problem* with sediments is that criteria for specific compounds are developed from bioassay sampling of real sediments extracted from a water body. Invariably these sediments are impacted by more than just the target compound for which a screening criteria is desired. Since it is difficult to isolate the effect due to the compound of concern, any observed effect is generally attributed to the specific compound. Criteria that result are therefore normally quite conservative since all the toxicity is assigned to the target compound.

It is usual for organizations to present a range of sediment criteria corresponding to various degrees of certainty that adverse effects will be observed in sediment/aquatic ecosystems. Many of the criteria published for organic contaminants are dependent upon the fraction of organic carbon present in the sediment. The criteria presented in Table N-1 have been normalized to 1% organic carbon where this is the case.

The following sections detail the eleven sources of sediment criteria that have been reviewed.

N.2 NOAA (1995)

The National Oceanic and Atmospheric Administration (NOAA) has published marine sediment criteria in the form of Effects Range–Low (ER-L) and Effects Range–Median (ER-M) values (Long *et al*, 1995). NOAA annually collects and analyses sediment samples from coastal marine and estuarine sites throughout the United States, and data from this ongoing survey were used to evaluate three alternative approaches to the derivation of sediment criteria:

- equilibrium partitioning (EqP) from water quality criteria;
- spiked-sediment toxicity testing; and
- evaluation methods for simultaneously collected biological and chemical field survey data.

Chemical concentrations observed or predicted by these three methods to be associated with biological effects were ranked, and the lower 10th percentile (the ER-L) and median (ER-M) concentrations were identified. For screening purposes, sediment concentrations below the ER-L are considered to be highly unlikely to be associated with adverse effects to marine organisms, and concentrations above the ER-M are more likely than not to be associated with toxic effects. These marine ER-L and ER-M values were recalculated by Long *et al* (1995) after omitting a small amount of freshwater data included in original calculations by Long & Morgan (1991) and adding more recent data.

N.3 NOAA (1998)

NOAA have also produced screening quick reference tables (‘SQuiRTs’) for freshwater and marine sediments (NOAA, 1998). These tables were developed for internal use by the NOAA Coastal Resource Co-ordination Branch (CRCB) and hence do not represent official NOAA policy. A range of screening values are quoted in the tables, including the ER-L and ER-M values published in 1995 (see Section 2 above) and the following values:

- Lowest *Hyallela azteca* Threshold Effects Level (TEL) measured by US EPA Assessment and Remediation of Contaminated Sediment (ARCS) project for the Great Lakes. Hence some of these values correspond to ARCS Threshold Effect Concentrations - see Section 5).
- Threshold Effects Level (TEL) – calculated as the geometric mean of the 15th percentile of the toxic effect concentrations data set and the median of the no-effect concentrations data set. Observed concentrations below the TEL are rarely expected to produce adverse effects.
- Probable Effects Level (PEL) – calculated as the geometric mean of the median of the effects data set and the 85th percentile of the no-effects data set. Concentrations above the PEL may be expected to frequently result in adverse effects.
- Apparent Effects Threshold (AET) developed for use in Puget Sound, Washington State (hence some values are identical to the Washington State marine sediment criteria – see Section N.8). An AET is the highest non-toxic concentration observed in a biological toxicity test. The AET quoted is the lowest AET from a range of five different marine tests – the amphipod bioassay, a benthic community impacts test, the Microtox bioassay, the oyster larvae bioassay and the echinoderm larvae bioassay. At concentrations above an AET, effects may always be expected in the chosen organism.
- Upper Effects Threshold (UET) derived for freshwater sediment in an analogous manner to the marine AET.

N.4 FDEP (1994)

The Florida Department of Environmental Protection (FDEP) approach (MacDonald 1994) is similar to the NOAA approach. The updated and revised data set used by Long *et al* (1995) was also used by MacDonald (1994) to calculate Threshold Effects Levels (TELs) and Probable Effects Levels (PELs). However, unlike the ER-Ls and ER-Ms, the TELs and PELs also incorporate chemical concentrations observed or predicted to be associated with no adverse biological effects (no-effects data). Specifically, the TEL is the geometric mean of the 15th percentile in the effects data set and the 50th percentile in the no-effects data set. The PEL is the geometric mean of the 50th percentile in the effects data set and the 85th percentile in the no-effects data set. Therefore, the TEL represents the upper limit of the range of sediment contaminant concentrations dominated by no-effects data. The PEL represents the lower limit of the range of contaminant concentrations that are usually or always associated with adverse biological effects.

N.5 US EPA ARCS (1996)

These criteria were produced by the US National Biological Service for the EPA Great Lakes National Program Office as part of the Assessment and Remediation of Contaminated Sediment (ARCS) Project. The criteria were based upon the following sediment toxicity tests:

- 14-day and 28-day reduction in survival, growth, or sexual maturation of the amphipod *Hyalella azteca*; and
- 14-day reduction in survival or growth of the midge *Chironomus riparius*.

Three methods were used to calculate Sediment Effect Concentrations from the results of each of these three tests:

- the NOAA method for calculation of ER-Ls (Effects Range – Low) and ER-Ms (Effects Range – Median) (see Section N.2);
- the FDEP method for calculation of Threshold Effect Levels (TELs) and Probable Effect Levels (PELs) (see Section N.4),
- the Apparent Effects Threshold (AET) method to calculate high No-Effect Concentrations (NECs).

One of the three ER-L and three TEL values for each chemical was selected as the representative threshold effect concentration (TEC). Similarly, a representative probable effect concentration (PEC) was selected for each chemical from the three ER-Ms and three PELs. A representative high no effect concentration (NEC) also was selected for each chemical from the three NECs.

The TECs are conservative screening values, below which effects are not expected to occur. NECs and PECs, respectively, are intended to discriminate chemicals that may contribute to toxicity (effects are less likely than not) from those that probably contribute to toxicity (effects more likely than not).

N.6 US EPA OSWER (1996)

The US EPA's Office of Solid Waste and Emergency Response (OSWER) Ecotox Thresholds (ETs) are intended for screening contaminants at CERCLA 'Superfund' sites in the US, and are defined as 'media-specific contaminant concentrations above which there is sufficient concern regarding adverse ecological effects to warrant further site investigation' (USEPA, 1996, 1999).

The preferred method for determining sediment ETs is to use the sediment quality criteria (SQC) values proposed by the USEPA (USEPA 1993a–c), which are derived by equilibrium partitioning (EqP) from aquatic chronic values calculated as part of the process of deriving national ambient water quality criteria (NAWQCs).

For chemicals without USEPA-proposed SQCs, a sediment quality benchmark (SQB) is used. The SQB is calculated in the same manner as the SQC except that a

Secondary Chronic Value (SCV) for the protection of aquatic life is used in place of NAWQC data. SCVs from either the US EPA Great Lakes Water Quality Initiative, Oak Ridge National Laboratory (see Section N.9), or USEPA OSWER were used, providing that acute toxicity values for the water flea *Daphnia* were used in their calculation. Because of the derivation process, both SQCs and SQBs are dependent on the organic carbon content of sediment (the values presented are normalized to 1% organic carbon).

An ER-L value from NOAA (1995, see Section 2) is used if neither an SQC nor an SQB is available. OSWER noted that there is relatively low correlation between observed incidence of toxic effects and exceedence of the sediment ER-Ls for mercury, nickel, and total PCBs, and that the ETs for these four chemicals should therefore be used cautiously. In addition, for those chemicals with the potential to bioaccumulate to toxic levels in upper trophic wildlife (e.g., PCBs and lead), the USEPA state that benchmarks may be under-conservative at some sites (US EPA, 1999).

The USEPA have produced software to calculate site-specific ETs by adjusting for pH and hardness in surface water and total organic carbon in sediment. The software is freely available from the USEPA internet site (US EPA, 1999), and produces ETs for freshwater and marine sites.

N.7 US EPA REGION IV (1995)

US EPA Region IV (1995) has recommended the NOAA and FDEP sediment values as potential lower screening criteria for use at ‘Superfund’ sites. Although these sediment screening values have been developed from studies conducted predominantly in marine environments, communication with the authors of the studies indicate that corresponding values being developed from a freshwater database were within a factor of three of the marine based numbers. The screening values have therefore been recommended for use at freshwater sites until specific freshwater criteria are developed.

When the Contract Laboratory Program's (CLP) practical quantification limit (PQL) is above the effect level, the screening value defaults to the PQL. For those contaminants whose screening values are based on the PQL, data reported below the required quantification limit should be compared to the Effects Level number. The CLP PQL, Effects Level and final criteria are presented in Table N-1.

N.8 WASHINGTON STATE (1995)

The state of Washington has developed sediment management standards for a range of inorganic and organic compounds (WSDE, 1995). The management standards are specific to Puget Sound in Washington State and should therefore be used with caution elsewhere. Information was not available on the derivation of the standards, although some values correspond with the AETs quoted by NOAA (1998, see Section N.3), suggesting that these values may not be protective of all species.

N.9 ORNL (1997)

The Oak Ridge National Laboratory (ORNL) has published sediment quality benchmarks (SQBs) derived by equilibrium partitioning (EqP) from EPA National Ambient Water Quality Criteria and ORNL’s own secondary chronic values for the protection of aquatic life (Jones *et al*, 1997). These secondary chronic values were derived by an approach similar to that adopted in the Great Lakes Water Quality Initiative. The EqP approach has been advocated by the US EPA (1993d) for developing criteria for non-ionic organic chemicals, and requires a water quality criterion, K_{oc} value, and a measured or assumed site-specific total organic carbon (TOC) value. SQBs are normalized in Table N-2 assuming 1% TOC.

For polar organic chemicals, it is noted by ORNL that adsorption mechanisms other than hydrophobicity may significantly increase the fraction of the chemical sorbed to the sediment particles and EqP is likely to overestimate the free (bioavailable) chemical concentration. SQBs for polar non-ionic organic chemicals are therefore conservative benchmarks.

N.10 OMEE (1993)

The Ontario Ministry of the Environment (OMEE) has published sediment quality guidelines based on Ontario sediments and benthic species from a wide range of geographical areas within the province (Persaud *et al.* 1993). The lowest effect level (Low) is the level at which actual eco-toxic effects become apparent. The severe effect level (Severe) represents contaminant levels that could potentially eliminate most benthic organisms.

The species-absence endpoint used to derive these guidelines is described as under-conservative, suggesting the values may not be adequately protective. OMEE values for organic chemicals are normalized to 1% organic carbon in Table N-1.

N.11 RIZA (1989)

The Netherlands Institute for Inland Water Management and Waste Water Treatment (RIZA) has calculated eco-tox values for freshwater and sediment (Stortelder *et al,* 1989). Eco-tox values are derived in one of two ways:

- For non-bioaccumulating chemicals, the lowest No Observed Effect Concentration (NOEC) from a review of chronic toxicity tests was used.
- For bioaccumulating substances, toxicity to fish-eating mammals was considered using bioconcentration factors to extrapolate from water and sediment to aquatic organism tissue concentration.

N.12 ENVIRONMENT CANADA (1995)

Environment Canada have published interim sediment quality guidelines (ISQGs) for the protection of aquatic life for both freshwater and marine (including estuarine) sediments. Environment Canada's Guidelines and Standards Division is the technical secretariat for the Water Quality Task Group of the Canadian Council of Ministers of the Environment (CCME).

The ISQG derivation protocol relies on both the NOAA approach and the spiked-sediment toxicity test approach. Spiked-sediment toxicity data are currently available for only a few substances, such as cadmium, copper, fluoranthene, and pyrene. Therefore, the threshold effect levels (TELs) calculated using the NOAA approach are most likely to be adopted as ISQGs. The probable effect levels (PELs), also calculated using this approach, provide additional information regarding the potential for observing adverse biological effects at higher concentrations.

Sediment chemical concentrations below the ISQGs are not expected to be associated with any adverse biological effects, while concentrations above the PELs are expected to be frequently associated with adverse biological effects. Chemical concentrations between the ISQGs and PELs represent the range in which effects are occasionally observed.

N.13 CONCLUSIONS

A range of sediment quality criteria was reviewed for use in screening potential harm to ecological receptors. By virtue of their derivation process, some criteria are more appropriate for a first tier screen than others. The following criteria were considered for inclusion in RISC:

- NOAA (1995 & 1998) marine ER-Ls and freshwater TELs;
- FDEP (1994) marine TELs;

- US EPA ARCS (1996) freshwater TECs;
- US EPA OSWER (1996) freshwater and marine ecotox thresholds;
- US EPA Region IV (1995) freshwater/marine effects values;
- ORNL (1997) freshwater sediment benchmarks;
- OMEE (1991) freshwater ‘Low’ screening values;
- RIZA (1989) freshwater ecotox values; and
- Environment Canada (1995) freshwater and marine ISQGs.

N.14 REFERENCES

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Table N-1. Sediment Quality Criteria Database in RISC

Chemical	**Note**	**NOAA** (1998)		**NOAA** (1998)	**NOAA** (1995)
		Freshwater		Marine/Estuarine	
		PEL *mg/kg*	UET *mg/kg*	AET *mg/kg*	ER-M *mg/kg*
Acenaphthene			0.29	0.13	0.5
Acenaphthylene			0.16	0.071	0.64
Acetone	no criterion				
Anthracene			0.26	0.28	1.1
Arsenic		17	17	57	70
Barium	no criterion				
Benzo(a)anthracene		0.385	0.5	0.96	1.6
Benzene	no criterion				
Benzo(a)pyrene		0.782	0.7	1.1	1.6
Benzo(b)fluoranthene				1.8	
Benzo(g,h,i)perylene			0.3	0.67	
Benzo(k)fluoranthene			13.4	1.8	
Beryllium	no criterion				
Bis(2-ethylhexyl)phthalate	no criterion				
Butyl benzyl phthalate	no criterion				
Cadmium		3.53	3	2.7	9.6
Carbon disulfide	no criterion				
Carbon tetrachloride	no criterion				
Chlorobenzene	no criterion				
Chloroform (trichloromethane)	no criterion				
Chromium (III)	no criterion				
Chromium (IV)	no criterion				
Chromium (total)		90	95	96	370
Chrysene		0.862	0.8	0.95	2.8
Copper		197	86	390	270
Cresol (-m)	no criterion				
Cresol (-o)	no criterion				
Cresol (-p)	no criterion				
Cyanide	no criterion				
Dibenz(a,h)anthracene			0.1	0.23	0.26
Dichloroethane(1,1-)	no criterion				
Dichloroethane(1,2-)	no criterion				
Dichloroethene(trans 1,2-)	no criterion				
Dichloroethene(trans 1,1-)	no criterion				
Dichloroethene(cis 1,2-)	no criterion				
Dimethylbenz(a)anthracene(7,12-)	no criterion				
Dimethylphenol(2,4-)	no criterion				
Di-n-butyl-phthalate	no criterion				
Dinitrotoluene(2,4-)	no criterion				
Di-n-octylphthalate	no criterion				
Dioxane(1,4-)	no criterion				
Ethylbenzene				0.004	
Ethylene dibromide	no criterion				
Fluoranthene		2.355	1.5	1.3	5.1
Fluorene			0.3	0.12	0.54
Indeno(1,2,3-CD)pyrene			0.33	0.6	
Lead		91.3	127	430	218
Mercury		0.486	0.56	0.41	0.71
Methanol	no criterion				
Methylethyl ketone	no criterion				
Methylene chloride	no criterion				
Methylnaphthalene(2-)				0.064	0.67
MTBE	no criterion				
Naphthalene			0.6	0.23	2.1
Nickel		35.9	43	110	51.6
Nitrobenzene	no criterion				
PAHs (total)			12		44.792
PCBs (total)		0.277	0.0026	0.13	0.18
Phenanthrene		0.515	0.8	0.66	1.5

Table N-1. Sediment Quality Criteria Database in RISC

Chemical	**Note**	**NOAA** (1998)		**NOAA** (1998)	**NOAA** (1995)
		Freshwater		Marine/Estuarine	
		PEL *mg/kg*	UET *mg/kg*	AET *mg/kg*	ER-M *mg/kg*
Phenol	no criterion		0.048		
Pyrene		0.875	1	2.4	2.6
Pyridine	no criterion				
Selenium				1	
Silver			4.5	>0.56	3.7
Styrene	no criterion				
Tetrachloroethane (1,1,2,2-)	no criterion				
Tetrachloroethene (PCE)				0.057	
Tetraethyl lead	no criterion				
Toluene	no criterion				
TPH aliphatic C10-C12	no criterion				
TPH aliphatic C12-C16	no criterion				
TPH aliphatic C16-C35	no criterion				
TPH aliphatic C5-C6	no criterion				
TPH aliphatic C6-C8	no criterion				
TPH aliphatic C8-C10	no criterion				
TPH aromatic C10-C12	no criterion				
TPH aromatic C12-C16	no criterion				
TPH aromatic C16-C21	no criterion				
TPH aromatic C21-C35	no criterion				
TPH aromatic C5-C7	no criterion				
TPH aromatic C7-C8	no criterion				
TPH aromatic C8-C10	no criterion				
Trichloroethane(1,1,1-)	no criterion				
Trichloroethane(1,1,2-)	no criterion				
Trichloroethene (TCE)	no criterion				
Vanadium	no criterion				
Vinyl chloride	no criterion				
Xylenes				0.021	
Zinc		315	520	410	410

Notes:

PEL Probable Effects Level
UET Upper Effects Threshold
AET Apparent Effect Threshold
ER-M Effects Range - Median

Appendix
O

Vegetable Uptake

This appendix presents the approach used by RISC to estimate the vegetable uptake and vegetable ingestion factors used in the human health risk calculations. It also presents the models reviewed during this study. It is assumed that contaminant uptake in vegetables may occur from them either being grown in contaminated soil or from being irrigated with contaminated groundwater. There are other mechanisms that can also contaminate vegetables, such as particulate deposition, however these mechanisms are not modeled in RISC.

O.1 CONCENTRATION IN VEGETABLES

The concentration in vegetables (or produce) is assumed to be either a function of soil concentration or of irrigation water concentration. For soil, the calculation takes the form of:

$$C_v = C_{soil} B_v \tag{O-1}$$

where:

C_v = concentration of chemical in vegetables [mg chemical/mg vegetable]

C_{soil} = concentration of chemical in soil [mg/kg]

B_v = uptake factor from soil [mg chemical/kg vegetable per mg chemical/kg soil]

When the vegetables are being irrigated with contaminated groundwater the calculation takes the form of:

$$C_v = C_{water} CF \qquad \textbf{(O-2)}$$

where:

C_v = concentration of chemical in vegetables [mg chemical/mg vegetable]

C_{water} = concentration of chemical in irrigation water [mg/l]

CF = water-vegetable concentration factor [g chemical/kg vegetable per mg chemical/l water]

Both the soil uptake factor, B_v, and the water concentration factor, CF, have been divided into two component factors for purposes of modeling exposure in RISC. One is for root vegetables (using the notation B_v) and the other for above-ground leafy portion of plants, B_{va}.

The next section reviews the most commonly used models for estimating the produce uptake factors.

O.2 VEGETABLES UPTAKE MODELS

The approaches used by most regulatory agencies in the U.S. derive from one of two empirical studies, both of which essentially fit observed ratios of soil-to-plant chemical concentrations as a function of the lipid solubility of the compound. There is one additional modeling approach with authors from regulatory agencies which is based on conceptual understanding of chemical transport in soil and plants (Trapp et al, 1994). However, this model is complex, has a numerical solution, and has only been validated against data with a single pesticide. It is, therefore, not presented here.

The empirical models are discussed below, but due to their dependence on K_{ow}, these approaches do not apply to inorganic compounds. An empirical model for inorganics is discussed in a separate section.

O.2.1 Travis and Arms Empirical Model

The first of the empirical models is that of Travis and Arms (1988). These investigators equated the ratio (as B_{pr}) of chemical concentration in plants (above-ground parts of the plant) to soil concentrations as reported in the literature for 29 chemicals. (Note: as described below, Travis and Arms and all the information found in this literature review is limited to vegetable uptake. As such, produce uptake factors for these equations have been denoted as B_v rather than B_{pr}).

Travis and Arms fit a linear regression to log transformed B_v on log K_{ow}, so that, to the extent the data used by Travis and Arms are representative, B_v for any organic compound may be calculated as:

$$\log B_v = 1.588 - 0.578 \ \log K_{ow} \qquad \textbf{(O-3)}$$

where:

B_v = uptake factor from soil [mg chemical/kg **dry weight** vegetable per mg chemical/kg soil]

log K_{ow} = chemical-specific log octanol/water partitioning coefficient [(l/kg) (see Chapter 11 of the main text for definition)]

The use of this B_v provides an estimate of mass of chemical per dry weight of produce, which can be converted to wet weight by multiplying the result by (1-plant moisture content). Each plant will be somewhat different, but a general value for plant moisture content is 0.85 (based on inspection of moisture listed in the re-draft of the *Exposure Factors Handbook; USEPA, 1998).*

The Travis and Arms equation was used for virtually all produce risk assessments prior to about 1994 and continues to be applied in many cases to the present. As such, there is good precedent for its application in risk assessment. It also has the advantage of being extremely simple. Among the difficulties with the Travis and Arms approach are:

- Because the equation relies on bulk soil concentration, it cannot be adjusted for soils of different organic carbon content. Presumably, the soils that form the data are representative, but accounting for various soil parameters might lead to a more refined estimate.

- Nothing was done by Travis and Arms to account for potential uptake by mechanisms other than translocation into the root. Thus, the observations of Travis and Arms may also be due to particulate deposition and/or foliar uptake of gaseous chemicals.

> It is assumed that deposition and foliar uptake of chemicals are of limited relevance for the compounds and the mechanisms of soil contamination being modeled by RISC.

- The data used by Travis and Arms were all derived from above-ground vegetables. Therefore, the method has been criticized as being of questionable use for other plant types (fruits and root vegetables).
- Inspecting the data in the Travis and Arms paper, there appears to be 2 or 3 "outlier" compounds that may be over-influencing the regression equation.

For the reasons listed in the above bullets, the USEPA has suggested that other approaches may be more appropriate. Therefore, the model no longer enjoys unqualified acceptance by U.S. regulatory agencies.

O.2.2 Briggs Empirical Model

As mentioned above, a majority of the criticisms of Travis and Arms were expressed by the USEPA, who suggested an alternative model for estimating chemical uptake into root vegetables. This is the model of Briggs, et al (1982). The Briggs equations were obtained from several documents (USEPA, 1993; Ryan, et al, 1988). The equations are again empirical, and in this case are derived from Briggs' experiments of growing barley shoots in water containing various compounds.

Briggs actually provides a series of equations to derive concentrations in different parts of the plant. The root equation is:

$$RCF = 10^{0.778 \log K_{ow} - 1.52} + 0.82 \qquad \textbf{(O-4)}$$

where:

RCF = the root concentration factor [mg chemical/kg produce per mg chemical/l water]

Briggs performed a portion of his experiments in macerated barley roots, the results of which - because the cellular structure of the plant would presumably be broken - should provide a partitioning factor from the growth fluid into the cell wall or other membranes in plant organelles. In fact, the exponential portion of equation (O-4) provides that partition constant. Briggs further assumed that the aqueous content of the plant would be of equivalent concentration to the external (growth) fluid. Briggs estimated the water content of the root to be 82%. Thus, the overall equation (O-4) represents the sum of partitioning to plant cell membranes plus equi-concentration cell water, which is 0.82 of the total weight of the root. The assumption of equal concentration between growth fluid and cell water seems unlikely because this would only occur once equilibrium were established (because a chemical has to pass through the cell wall in order to be present in cell water). However, the assumption would be reasonable for those plants whose growing period is sufficient to establish equilibrium and it should be an “upper bound” estimate for others.

Note that, because Briggs worked with aqueous systems, the *RCF* is not useful for determining the ratio of vegetable concentration to total soil. However, if one assumes that the same ratio of plant-to-pore water chemical concentration would hold, Briggs’ equation may be re-written as:

$$B_{vr} = \frac{RCF * \rho_b}{\theta_w + (1 - \theta_t) * K_d \rho_s} \approx \frac{RCF}{K_d} \qquad \textbf{(O-5)}$$

where:

B_{vr} = soil-to-root uptake factor [mg chemical/kg wet weight root per mg chemical/kg soil]

ρ_b = soil bulk density [g/cm^3]

θ_w = volumetric water content of soil [cm^3/cm^3]

ρ_s = soil bulk density [g/cm^3]

θ_t = total porosity of soil [cm^3/cm^3]

K_d = equilibrium partitioning coefficient [l/kg or ml/g]

This equation provides a wet weight (or "bulk weight") concentration in the plant root. Although this equation circumvents the "root vegetable difficulty" in the eyes of the USEPA, it does have some difficulties:

- Risk assessment of the produce pathway becomes more complex when multiple produce types have to be evaluated separately.
- Briggs' experiments utilized compounds with fairly low log K_{ow} (in the 2-3 range). The curve fit is an uncertain extrapolation if used for compounds with higher K_{ow}. Indeed, Poulder, et al (1995) have noted that this model substantially overestimates polynuclear aromatic hydrocarbon (PAH) concentrations in plant roots.
- Briggs' barley shoots have very different architecture than typical root vegetables (e.g. potatoes, carrots, turnip), so that the spatial distribution of chemical may be important. That is, if compounds move slowly into the root, their highest concentration would be at the surface. The surface represents a large proportion of a barley root, but a small portion of the mass of a potato, carrot, etc.

To respond to the last difficulty, USEPA (1993) suggested using a reduction factor to estimate the overall concentration of chemical in edible roots. The suggested value was 0.01 for "lipophilic" compounds (this is slightly less than the ratio of surface area to volume of a carrot, but USEPA also notes that washing root vegetables reduces the B_{vr} to a value even lower than this - thus it is a conservative adjustment). It is unclear what USEPA regards as lipophilic (they were considering chlorinated dioxins specifically), but it seems appropriate to consider at least PAHs lipophilic, so that the Briggs approach would utilize the following equation:

$$B_{vr} = \frac{0.01RCF}{K_d} \tag{O-6}$$

where the variables have been defined above.

Despite the disadvantages noted above, equation (O-6) does have the advantage of regulatory acceptance in the United States, as well as providing the opportunity to account for site-specific factors, such as fraction organic carbon (F_{oc}), unavailable to Travis and Arms. (Note: the selection of F_{oc} in a risk model may be very important and F_{oc} in a garden is expected to be substantially higher than F_{oc} in site soils that have not been optimized to grow edible vegetables).

In recommending the Briggs root equation, USEPA (1993) suggested the Travis and Arms equation could be used for all other produce estimates. However, because Briggs derived other equations, it is interesting to consider how they compare to estimates derived by Travis and Arms.

Briggs developed an empirical equation from the barley shoot experiments to estimate chemical concentrations in the "transpiration stream" of the plant (i.e. the concentration of chemical traveling in the water being carried through plant xylem):

$$TSCF = 0.748 e^{-\frac{(\log K_{ow} - 1.78)^2}{2.44}} \qquad \textbf{(O-7)}$$

where:

TSCF = the transpiration stream concentration factor, relating chemical concentration in xylem water to water in which the plant was grown [(mg/l)/(mg/l)]

Additionally, Briggs performed experiments with macerated barley stems to derive an empirical partitioning factor into the cell walls or other organelles of this part of the plant. Applying the same assumption used for roots - that cell water in the stem would be of equivalent concentration as the donor fluid and comprises 82% of the wet weight of the plant, a so-called stem concentration factor, *SCF*, equation was developed:

$$SCF = 10^{0.951 \log K_{ow} - 2.05} + 0.82 \qquad \textbf{(O-8)}$$

where:

SCF = stem concentration factor [mg chemical/kg stem per mg chemical/l transpiration steam fluid]

As with equation (O-4), the exponential portion of equation (O-8) represents partitioning into cell walls/organelles of the plant and 0.82 accounts for cell water content of chemical. Note that in an intact plant the "donor fluid" for stem uptake would be that in the transpiration stream. Thus, it was suggested by Ryan, et al (1988) that a stem concentration factor, B_{vst}, which related stem concentrations to chemical in soil could be derived by multiplying *SCF* by the *TSCF* and assuming that concentrations in soil moisture would behave as the growth fluid in Briggs' experiments (approximated by dividing the uptake equation by K_d). Thus, B_{vst} is:

$$B_{vst} = \frac{SCF \times TSCF}{K_d} \qquad \textbf{(O-9)}$$

where:

B_{vst} = soil-to-stem uptake factor [mg chemical/kg stem per mg chemical/kg soil]

TSCF = transpiration stream concentration factor [mg chemical/l transpiration stream fluid per mg chemical/l growth fluid]

K_d = equilibrium dissociation constant [ml/g or l/kg]

This ratio may be used to determine <u>wet weight</u> concentrations of chemicals in the stem.

Ryan, et al (1988) suggested that the stem equation may be used to calculate chemical concentrations in above-ground plants (in this case, it might be appropriate to use B_{va} to describe the parameter). Because Briggs worked with barley shoots, there is little distinction between stem and leaves. However, stem and leaf parts may be significantly different in edible plants so it may be appropriate to distinguish between the two. To evaluate the differences, the Briggs' stem equations were compared with those of Travis and Arms. This comparison is reported in the next section.

It should be noted that all Briggs equations are derived entirely from data on vegetables and therefore, like the Travis and Arms equation, may be of questionable use for estimating chemical concentrations in fruit. Indeed, there are no known studies suggesting how to estimate organic chemical concentration in fruit. All U.S. regulatory agencies apply vegetable uptake factors to fruit crops.

O.2.3 Uptake Factors for Inorganic Compounds

As mentioned previously, an uptake model based on K_{ow} is clearly inapplicable to inorganic compounds. As an alternative, the USEPA has in several guidance documents recommended the use of a set of “default” uptake factors published by Baes, et al (1984). Baes, et al have used several methods to develop uptake factors. For the most part, Baes, et al report the geometric mean of observed soil-to-plant concentration ratios, although there are some additional evaluations extrapolating findings from one element to another within periodic groups. These default values may be questionable however, because Baes, et al show clearly that the uptake ratios vary with the concentration of the elements in the soil. Thus, the geometric mean uptake factor will over- or underestimate uptake, depending on the concentration of the element at the study site. Nonetheless, the Baes, et al data is generally accepted, therefore it is recommended in RISC for metals.

The pertinent soil-to-plant factors are provided in Figures 2.1 and 2.2 (not included in this appendix) of the Baes, et al report, which relate to yet another subset of plant parts:

- the vegetative portions of the plant (stem and leaves), denoted in Baes, et al as B_v ,
- the reproductive portions of the plant (tubers, flowers, seeds, fruits), denoted as B_r .

All uptake factors reported in Baes, et al relate dry weight plant concentrations to dry weight soil concentrations. Therefore, to determine wet weight, one should multiply the estimated dry weight concentration by (1-water content).

It is important not to confuse Baes’ notation with the notation that was used in the previous sections discussing uptake factors for organic compounds, because they indicate transfer to different plant parts.

O.3 COMPARISON OF ESTIMATES VERSUS OBSERVATIONS

The relationship of the various soil-to-plant uptake factors to K_{ow} are plotted in Figures O-1 and O-2.

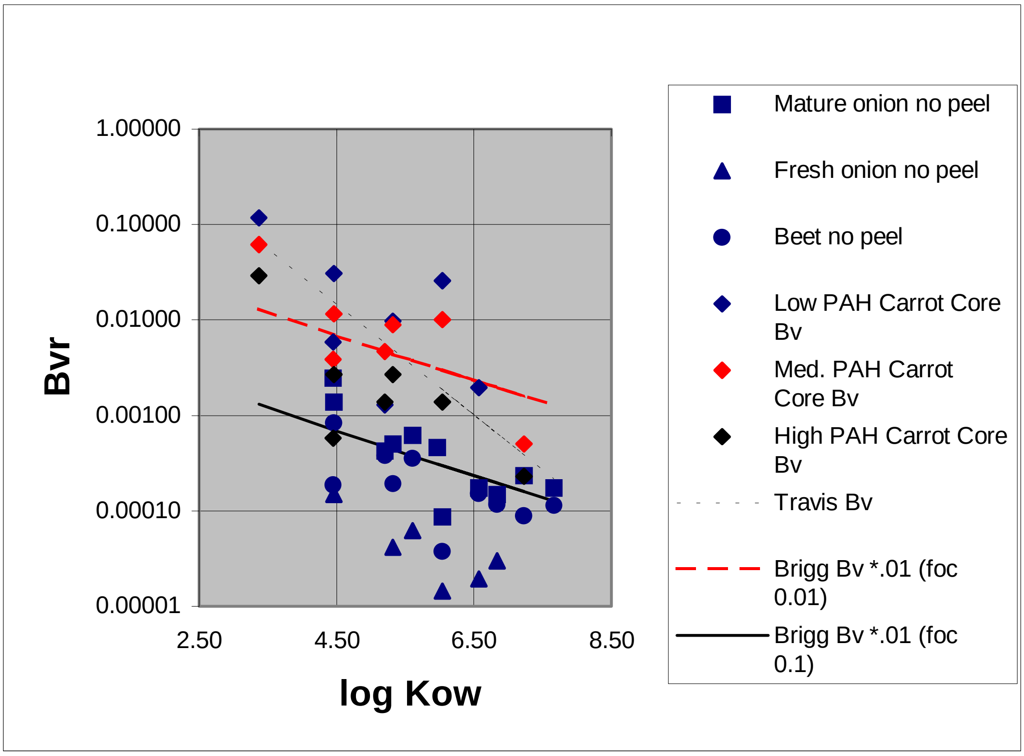

Figure O-1. Wild and Jones (1983) Carrot Core Data For Three Different PAH Concentrations, and Wang and Meresz Peeled Root Vegetable Data as a Function of K_{ow}

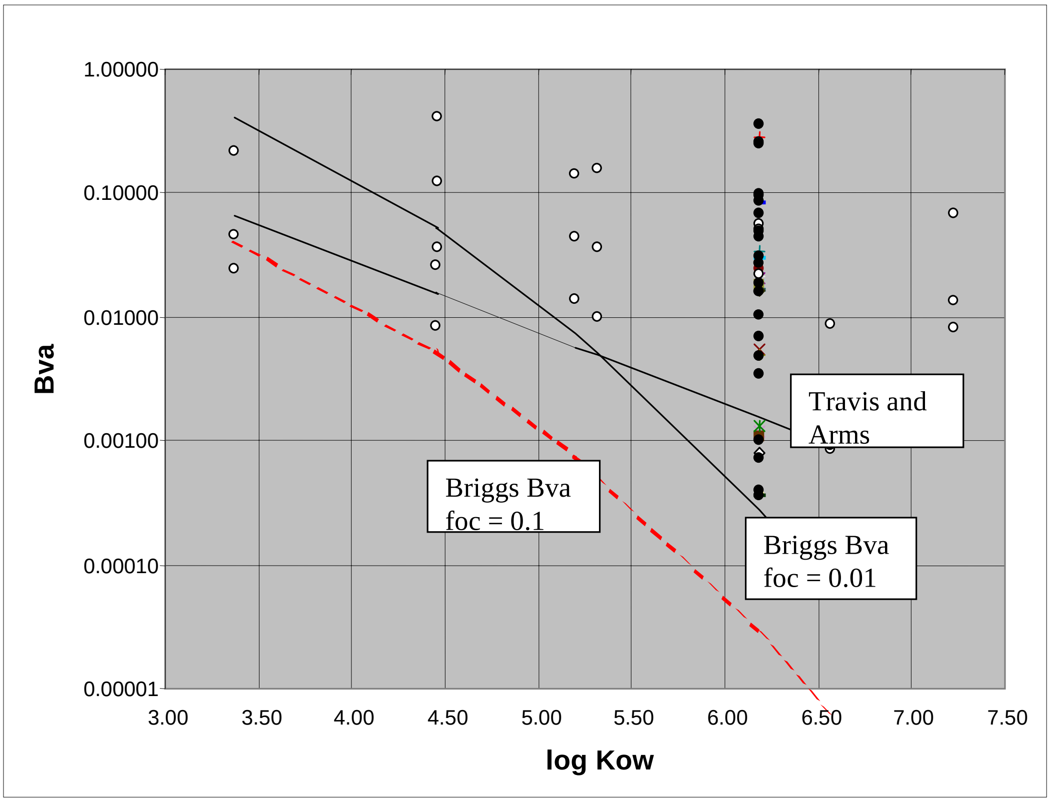

Figure O-2. Comparison of Above Ground Uptake Factors, B_{va}

The B_v results from the literature for a variety of PAHs has also been plotted. The sources for this information include:

- A paper by Wild and Jones (1992) on uptake of PAH into carrot parts (skin, core, and tops) grown in sludge-amended soil.
- A report on PAH in several root vegetables grown near highways (Wang and Meresz, 1981). Two things are important to note concerning this report. First, other plant parts were included in the study, but not used in the figures, because of concern that the nature of the study (PAH from automobile deposition) was such that PAH in above-ground portions of the plant would be more likely be due to air deposition than soil uptake. Second, the data for this study was obtained from a secondary citation on the results (Edwards, 1983) rather than from the original study. However, it was felt that the information was important even as a secondary source, because the paper reports concentrations of PAH in peeled root vegetables and thus represents optimal data for evaluating the 0.01 adjustment factor suggested by USEPA to account for poor transport of highly lipid soluble compounds.
- A literature review of benzo(a)pyrene concentration in various plants (Edwards, 1983).

While the last study relates only to benzo(a)pyrene, the previous sources report on a variety of polynuclear aromatic compounds, so that comparison across a wide range of K_{ow} is possible.

B_v values were calculated by dividing wet weight plant concentrations by dry weight soil concentrations as reported in the empirical observations. Note that no correction was made for soil organic carbon content, because F_{oc} was not reported in all cases. As such, the calculated B_v should be considered rough approximations.

Figure O-1 shows the B_{vr} calculations for the Wild and Jones (1992) carrot core data as well as the Wang and Meresz (1981) peeled root vegetable data as a function of K_{ow}, which were obtained from the USEPA Drinking Water Criteria Document for PAHs. The Travis and Arms equation (O-3) adjusted to calculate wet weight vegetable concentrations, and two values for the Briggs root equation, as modified by USEPA (1993), based on assumed F_{oc} values of 0.01 and 0.1 were also included in Figure O-1. A statistical analysis of the equation fits to the data was not performed, however, visual inspection suggests the following:

- In contrast to the USEPA concerns, it would appear that at high K_{ow}, the Travis and Arms equations would over-estimate rather than under-estimate plant root uptake, at least for peeled vegetables.
- The Briggs B_{vr} equations seem to fit the data reasonably well, but the assumed F_{oc} is extremely important. It is of interest that the Wild and Jones report on carrots (symbolized by diamonds) indicate that F_{oc} was in the 1 to 4% range and the Briggs B_{vr}, using an assumed 1%, fits these data well. Unfortunately the F_{oc} from other reports used here is not available, so it is not clear whether the generally lower B_{vr} for these data is a result of higher F_{oc}.

In view of these observations, the adjusted Briggs root uptake equation (O-6) is used in the RISC model for root vegetables. It is recommended that F_{oc} measurements be taken during site investigations.

Figure O-2 plots B_{va} calculated for carrot tops from the Wild and Jones experiment (several different polynuclear aromatic compounds are reported), as well as B_{va} from the review data on benzo(a)pyrene, as reported by Edwards. All data are reported as a function of K_{ow}. Additionally, the Travis and Arms equation, adjusted to wet weight, and two values for the Briggs/Ryan stem equation, assuming F_{oc} as 0.01 and 0.1, are included in the figure. In this figure, it appears that all models perform poorly. This may be due to model failure (remembering Travis and Arms fit few data at high K_{ow} and Briggs fit none), or, equally possibly, because the PAH measured in above-ground vegetables resulted from other uptake mechanisms (e.g. air-to-leaf uptake, particulate deposition). Because of these observations, the Travis and Arms model is chosen to estimate B_{va} in RISC because it fits "least poorly."

O.4 PRODUCE INGESTION RATES

Two separate uptake factors are used in RISC, one to determine plant uptake in roots and the other for above-ground plants. This means that the exposure calculations use separate ingestion rate values for each plant "type".

The USEPA recently updated their *Exposure Factors Handbook* (1998). This document uses the most recent market basket survey of the U.S. population (conducted by the U.S. Department of Agriculture in 1990) and is therefore more up to date than other sources for U.S. intake rates. Additionally, the data in this document are presented in percentiles, so that an empirical distribution can be obtained for probabilistic risk assessment. As such, the use of data from this source for ingestion rates is recommended. It should be noted however that the data are not without problems. These include:

- The data are for U.S. populations and they may not represent habits of other countries. It is recommended that the U.S. data be used only until it can be determined if relevant country market basket studies are available from which to derive more pertinent data.
- The total vegetable intake reported in this document (4.3 g vegetable/kg body weight or about 300 g/day for a 70 kg adult) is substantially higher than that reported by other sources including the *AIHC Exposure Factors Handbook* (200 g/d), *Estimating Exposure to Dioxin Like Compounds* (140 g/d), the *Methodology for Assessing Health Risks Associated with Indirect Exposure to Combustor Emissions* (200 g/d) and a review of Canadian vegetable ingestion rates (200 g/d) (Davies). This might be explained based on the newer data

> used in the 1996 *Exposure Factors Handbook*. However, no increase is reported in fruit intake between older market basket surveys and the 1990 USDA data, which makes one question if the upward trend in vegetable intakes is real. Additionally, the vegetable data are internally inconsistent. The Handbook reports intake rates for different vegetable types (root vegetables, unprotected above-ground vegetables and protected above-ground vegetables). The sum of the mean intakes for these three types, which should be inclusive of total vegetable intake, is 3.1g/kg day (approximately 215 g/d), or 25% lower than the new value suggested for total intake (but a number that is more consistent with the other studies).

"Unprotected" above-ground vegetables are those eaten without peeling (e.g. lettuce), while protected vegetables require peeling or hulling (e.g., peas). This distinction is of no consequence in a RISC evaluation, but is important in risk assessments of vegetables contaminated by deposition from the air.

In view of the latter difficulty, the data from the *Handbook* was used, but it was grouped by vegetable type. These data are better suited to the separate evaluation of above- ground and root vegetables.

It may be necessary to evaluate the plant ingestion exposure pathway for children as well. The *Handbook* only provides a total vegetable intake for children, but it is notable that this value is much higher than that for adults on a gram per kilogram basis. Total mass intake is lower in a child, but because toxicity values are on a unit body weight basis, children would be more at risk than adults. Under the assumption that total vegetable intake would be distributed in proportions equal to that consumed by adults, the intake rates for small children (1-2 years of age) can be calculated. The values suggested are presented in Table O-1.

Table O-1. Vegetable Ingestion Rates

	Mean Adult Ingestion Rate (g wet weight/kg body weight day)	**Mean Small Child Ingestion Rate** (g wet weight/kg body weight day)[2]
Above-ground vegetables[1]	1.82	3.72
Root vegetables	1.25	3.23
Fruit	3.40	11.84

Notes:
(1) above-ground vegetables calculated as the sum of protected and unprotected vegetables
(2) 1-2 year old child. Rates calculated from total vegetable ingestion rate multiplied by proportions of vegetable types in adults.

If intake rates of particular vegetables are required, they are available in the *Exposure Factors Handbook.*

All values provided here are means. The mean values are used rather than some upper confidence level because the data underlying the estimates are based on reports of short-term (3-day menus) reports of intake, but are being extrapolated to long-term daily intake. The mean value of such reports should be stable, but extreme confidence limits will be very much "wider" for this type of data than would be the case if long-term data were available.

Note: Food-type intake is sporadic so that even a commonly eaten food might be missing from the diet during a three-day period. Alternatively, ingestion of a very large portion of a food type may occur during the reporting period, but never eaten again during the year. These possibilities are balanced in the mean estimate, but result in make for very wide ranges at the extreme of distributions.

O.5 SUMMARY OF RECOMMENDATIONS

In summary, equations O-1 and O-2 are used to calculate the concentration of contaminants in vegetables. These equations are actually incorporated into Equations 7-10 and 7-11 in the main part of this manual. Separate uptake factors are calculated for above-ground and root vegetables. The Briggs approach as modified by USEPA (Equation O-6) is used to calculate B_{vr} for root vegetables and Travis and Arms (equation O-3) is used to calculate B_{va} for above-ground vegetables. A concise summary of the approach used in RISC is presented in the next section.

In view of the major uncertainties discussed for any of these models and the wide range of PAH concentrations reported in vegetation, direct measurement should be considered as an alternative to modeling. Also, it is important to consider that specially amended garden soils will have higher F_{oc} than typical soils and current field measurements of F_{oc} may not reflect this value.

For inorganic compounds, the default values provided by Baes, et al (1984) for uptake factors are used. If available, site-specific vegetation data would be more appropriate.

The vegetable ingestion rates from the USEPA Exposure Factors *Handbook* are used as default values. As additional information (e.g., other country market basket surveys) become available, these ingestion rates should be modified to reflect country-specific rates.

It is worth noting certain issues associated with other equation parameters:

- The fraction ingested from impacted soil (the FI term) is extremely important and highly contentious. One way of obtaining a value for FI is to ask what percent of produce is home grown. The USEPA has generally set this at 25%, but it is probably too high for U.S. gardening habits. European customs may be quite different from the U.S.
- The soil concentration is assumed to be a constant. However, much risk modeling underway at the USEPA currently involves calculation of dynamic environmental contaminant concentrations (e.g. risk assessment models for evaluation of combustion sources to support the Clean Air Act MACT standards, and underlying the Hazardous Waste Identification Rule). As such, it would be perfectly consistent with USEPA approaches to use a value for soil concentration that reflects the time-weighted average concentration over a period where loss mechanisms such as volatilization or biodegradation are active. (This is currently not an option in RISC).
- Note that the soil "compartment" for plant uptake is quite small. The USEPA generally considers a root zone that is approximately 15 cm deep from the surface and, given the slow diffusion rate of many compounds, the horizontal dimensions of the compartment are expected to be only a few centimeters from the plant root. As such, it may be important to treat the source as finite. (This is currently not an option in RISC).

O.6 SUMMARY OF APPROACH

This section presents a concise summary of the methodology used in RISC for calculating the vegetable uptake factors from soil and water. These uptake factors are then used to calculate the exposure (or dose) as part of the risk calculation.

Briefly, the rules used to calculate the B_v's used in RISC are as follows:

1. If the chemical has a vegetable uptake factor explicitly entered in the chemical database, then this value is used for both above-ground and root vegetables.
2. A non-zero partitioning coefficient, K_d, is required for the calculation of all uptake factors except for the case of uptake from soil where the uptake factor, B_v, is explicitly specified in the RISC chemical database (for non-organics). If the chemical has a K_d value in the chemical database, this value is used; otherwise the K_d is calculated from the product of F_{oc} and K_{oc}.
3. If the chemical has a value for K_{ow} entered in the chemical database, then the vegetable uptake factor is calculated from K_{ow}.
4. If the chemical has neither a value for B_v nor a value for K_{ow}, then the vegetable uptake factors are assumed to be equal to zero.

O.6.1 Chemicals With B_v Values Entered In The Chemical Database

The Baes, et al (1984) report presents soil-to-plant concentration factors (called B_v by Baes) for the elements of the periodic table. (Note, the Baes uptake factors are from **soil**-to-plant.) Eleven chemicals in RISC have values for B_v entered in the database (Table 11-2). Both the B_{vr} and B_{va} values are assumed to equal the B_v value for these chemicals. The following relationships are used if the uptake factor is entered in the chemical database.

For soil:

$$B_{va} = B_{vBaes} \times (1 - 0.85) \quad \textbf{(O-10)}$$

$$B_{vr} = B_{vBaes} \times (1 - 0.85) \quad \textbf{(O-11)}$$

For water:

$$RCF = B_{vBaes} \times (1 - 0.85) \times K_d \qquad \textbf{(O-12)}$$

$$ABCF = B_{vBaes} \times (1 - 0.85) \times K_d \qquad \textbf{(O-13)}$$

where:

B_{vr} = soil-to-root uptake factor [mg chemical/kg **wet weight** root vegetable per mg chemical/kg soil]

B_{va} = soil-to-above-ground vegetable uptake factor [mg chemical/kg **wet weight** above-ground vegetable per mg chemical/kg soil]

B_{vBaes} = soil-to-plant concentration factor [mg chemical/kg **dry weight** vegetable per mg chemical/kg dry soil]

$(1 - 0.85)$ = adjustment from dry weight to wet weight vegetable where 0.85 is the assumed moisture content of the vegetable

RCF = root concentration factor [mg chemical/kg produce per mg chemical/l water]

$ABCF$ = above-ground concentration factor [mg chemical/kg vegetable per mg chemical/l water]

K_d = equilibrium partitioning coefficient [l/kg or ml/g]

The chemicals that have B_v's entered in the database are inorganic, (i.e. they are not expected to have K_{ow} or K_{oc} values). If a chemical does not have a K_d, K_{oc}, or a K_{ow} value entered in the database, the uptake factors from water are assumed to be equal to zero.

O.6.2 Organic Chemicals

If the chemical has a non-zero value entered for K_{ow}, then the root concentration factor, RCF, is calculated from Equation O-5, repeated here (Briggs, 1982):

$$RCF = 10^{0.778 \log K_{ow} - 1.52} + 0.82 \qquad \textbf{(O-5 repeated)}$$

where:

RCF = the root concentration factor [mg chemical/kg produce per mg chemical/l water]

$\log K_{ow}$ = chemical-specific log octanol/water partitioning coefficient [(l/kg) (see Chapter 11 of the main text for definition)]

Equation O-5 presents the uptake factor that is used to estimate the dose from ingestion of root vegetables irrigated with contaminated water. The soil-to-root uptake factor is estimated using the *RCF* calculated in equation O-6 and an adjustment factor as proposed by USEPA (1993):

$$B_{vr} = \frac{0.01 RCF}{K_d} \qquad \textbf{(O-6 repeated)}$$

where:

B_{vr} = soil-to-root uptake factor [mg chemical/kg **wet weight** root vegetable per mg chemical/kg soil]

The partitioning coefficient, K_d, is calculated as the product of K_{oc} and F_{oc} if not explicitly entered in the chemical database:

$$K_d = K_{oc} \times F_{oc} \qquad \textbf{(O-14)}$$

where:

K_d = equilibrium partitioning coefficient [l/kg or ml/g]

K_{oc} = chemical-specific organic carbon partition coefficient [kg/l or ml/g]

F_{oc} = fraction organic carbon [g oc/g soil]

The soil-to-above-ground vegetable concentration factor, B_{va}, is calculated from Equation O-3 (Travis and Arms, 1988):

$$B_{va} = 10^{1.588-0.578\ \log K_{ow}} \times (1 - 0.85) \qquad \textbf{(O-3 repeated)}$$

where:

B_{va} = soil-to-above-ground vegetable uptake factor [mg chemical/kg **wet weight** above-ground vegetable per mg chemical/kg soil]

$\log K_{ow}$ = chemical-specific log octanol/water partitioning coefficient [l/kg] (see Chapter 11 of the main text for definition)

(1 - 0.85) = adjustment from dry weight to wet weight vegetable where 0.85 is the assumed moisture content of the vegetable

Finally, the water-to-above-ground vegetable concentration factor, *ABCF*, is calculated from equation O-3 assuming equilibrium partitioning:

$$ABCF = B_{va} \times K_d = 10^{1.588-0.578\ \log K_{ow}} \times (1 - 0.85) \times K_d \qquad \textbf{(O-15)}$$

where:

ABCF = above-ground concentration factor [mg chemical/kg vegetable per mg chemical/l water]

O.7 ACKNOWLEDGEMENTS

This appendix was researched and written by Ogden Environmental and Energy Services (Brad Schwab and Allison Yuhas) of Westford, Massachusetts, under contract to BP.

O.8 REFERENCES

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Appendix
P

Irrigation Water Model

P.1 MODEL DESCRIPTION

The irrigation water pathway refers to the use of a backyard private well to irrigate a garden whereas the primary water supply for the household is provided by municipally-supplied water. This is a common scenario in Europe, South Africa, Australia/New Zealand and parts of the US. A paper by the authors of RISC (Walden and Spence, 1997) provides more background and explanation on this risk scenario.

There are four potential pathways by which human health risk could be impacted by use of contaminated groundwater for irrigation:

- Ingestion of the water by children playing in a sprinkler connected to the irrigation well or by adults gardening near the sprinkler or by residents in a swimming pool filled with the well water
- Dermal contact with the water by the above receptors
- Inhalation of the spray by the above receptors
- Consumption of vegetables grown in a garden irrigated by the well water

The method by which the receptor concentrations and risks are calculated by these pathways have been developed in previous chapters. The following briefly references these sections.

P.2 INGESTION OF IRRIGATION WATER

The amount of water ingested is a function of the way in which the irrigation water contacts the receptor. The highest intake is likely if the irrigation water is used to fill a swimming pool, followed by children playing in a sprinkler and then by an adult gardening near a sprinkler. Equations 7.8a and 7.8b in the main text are the risk calculations for non-carcinogens and carcinogens, respectively.

P.3 DERMAL CONTACT WITH IRRIGATION WATER

The degree of dermal contact follows the same trend as ingestion of irrigation water above. Equations 7.9a and 7.9b in the main text are the risk calculations for non-carcinogens and carcinogens, respectively.

P.4 INHALATION OF SPRINKLER SPRAY

Volatile compounds in a sprinkler spray can be released to the atmosphere and potentially inhaled by nearby receptors, such as children playing in the sprinkler or adults gardening downwind. Section G.3 in the appendices describes the way this is modelled in RISC, while Equations 7.14a and 7.14b are the risk calculations for non-carcinogens and carcinogens, respectively.

P.5 VEGETABLES IRRIGATED IN CONTAMINATED GROUNDWATER

Vegetables grown and consumed by a household having a contaminated irrigation well are the fourth pathway in this risk scenario. The concentrations in the vegetables are calculated from Equations O.9 to O.11 in Appendix O, while the risks are calculated from Equations 7.11a and 7.11b for non-carcinogens and carcinogens, respectively.

P.6 REFERENCES

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Appendix Q

Calculating Clean-up Levels for TPH Mixtures

This appendix describes how RISC calculates a site-specific target level (SSTL) for a TPH mixture. These calculations use the SSTLs calculated for the individual TPH carbon range fractions and the site-specific measured concentrations of the TPH fractions detected in the soil to estimate a unique SSTL that is protective for the TPH mixture at that site. Chapter 8 of this manual describes how clean-up levels are calculated for individual chemicals both for an individual chemical target and a cumulative target summed across all chemicals of concern. The approach presented in this appendix has some similarities with the cumulative option presented in Chapter 8, however, the algorithms presented here apply solely to the cumulative effects of the TPH fractions and the calculation of a total TPH clean-up level.

TPH Fractions Used in the Calculations

If the user has chosen to calculate clean-up levels in Step 5 of RISC and the chemicals of concern contain more than one of the TPH fractions, then a site-specific clean-up level for the total TPH mixture will be calculated. The model checks the names of the chemicals of concern and any name containing the letters "TPH" will be included in TPH calculations. This allows the user to define new fractions for different regulatory or site-specific needs and still calculate SSTLs for the TPH mixture.

Q.1 SOIL SOURCES IN RISC WHERE THE TPH SSTLS CAN BE CALCULATED

The RISC model has four different potential soil sources. When any of these sources have been chosen, the TPH SSTL is calculated automatically if more than one of the chemicals of concern contains the phrase "TPH" in its chemical name. The four soil sources are as follows:

- surface soil (for direct pathways)
- vadose zone model source
- saturated soil model source
- vapor model source from soil (rather than soil gas)

For fate and transport modeling, solubility limits are checked explicitly when back-calculating the source term, as described in each of their respective model appendix (Appendices A, C, and D, J or K). Solubility limits are not checked (i.e. SSTLs are not limited due to residual levels) for the surface soil source.

Q.2 APPROACH USED TO CALCULATE TPH SSTLS

The first step in calculating the TPH SSTL is to calculate the mass fraction for each individual carbon range. The following algorithm is used

$$MF_i = \frac{C_{soil\ i}}{C_{TPH}} \qquad \textbf{Q-1}$$

where

MF_i = mass fraction of TPH carbon range fraction i in the total mixture [(mg/kg TPH fraction i)/(mg/kg total TPH)]

$C_{soil\ i}$ = concentration of the TPH carbon range fraction in soil [(mg/kg TPH fraction i)/(mg/kg soil]

C_{TPH} = concentration of the TPH mixture in soil [(mg/kg TPH)/(mg/kg soil]

If the concentration of the TPH mixture, C_{TPH}, is not entered by the user, it is calculated from the sum of the concentrations of all of the TPH fractions. Note: if the user enters a TPH concentration (for the modeled sources), the sum of all of the mass fractions may not equal 1 (but the entered TPH concentration is still used). This is the usual scenario encountered when using field data because there are losses during sampling and not all of the ranges can be quantified. There is no option to enter a TPH concentration for the direct soil exposure pathways in this version of RISC.

Q.2.1 Calculating TPH SSTLS FOR DIRECT EXPOSURE PATHWAYS

The approach used to calculate the TPH SSTL is based on an inverse weighted average of the contribution towards the overall risk from all of the fractions:

$$HI = \sum_{i=1}^{13} HQ_i = \sum MF_i \frac{SSTL_{TPH}}{SSTL_i} \qquad \textbf{Q-2}$$

where

HI = hazard index for total TPH [-]

HQ_i = hazard quotient contributed by TPH fraction i [-]

$SSTL_{TPH}$ = site-specific target level for total TPH [mg/kg]

$SSTL_i$ = site-specific target level for TPH fraction i [mg/kg]

MF_i = mass fraction of TPH carbon range fraction i in the total mixture [(mg/kg TPH fraction i)/(mg/kg total TPH)]

Equation Q-2 can be rearranged to solve for $SSTL_{TPH}$

$$SSTL_{TPH} = \frac{HI}{\sum \frac{MF_i}{SSTL_i}} \qquad \textbf{Q-3}$$

Equation Q-3 is solved by choosing a target hazard index (HI) for the exposure pathway(s) of interest. In RISC, the target hazard index entered in Step 5 for the cumulative option is used as the value for HI in equation Q-3. Note that this equation requires the SSTLs for the individual TPH fractions as if they were not part of the TPH mixture.

This approach conservatively assumes that each TPH fraction acts cumulatively on the same organ system. Volume 5 of the TPH Criteria Working Group (TPHCWG) documentation (Vorhees et al, 1999) and the Texas Risk Reduction Program Draft Guidance for Development of PCLs for TPH Mixtures (TRRP 2000) describe calculating TPH SSTLs in more detail.

Q.2.2 Calculating TPH SSTLs for in Soil for Cross-Media Exposure Pathways

For cross-media exposure pathways, such as leaching from soil to groundwater, solubility limitations must be checked and utilized. The fate and transport models in RISC check for solubility limitations explicitly, i.e., if the model equilibrium partitioning equation predicts a dissolved-phase concentration that exceeds the estimated effective solubility for the TPH fraction being modeled, the dissolved-phase concentration is limited to the effective solubility *by the source term*.

Both the TPHCWG (Vorhees et al, 1999) and the Texas Risk Reduction Program (2000) present the following modification to the additive fraction approach for situations when the models being used to predict partitioning do not account for solubility limitations :

$$HI = \sum_{i=1}^{13} HQ_i = \sum MIN\left[SSTL_{TPH} \frac{MF_i}{SSTL_i}, \frac{C_{sat\,i}}{SSTL_i} \right] \qquad \textbf{Q-4}$$

$C_{sat\,i}$ = fraction-specific saturated soil concentration of TPH fraction i [mg/kg]

The equation to use for calculating saturated soil concentration, C_{sati}, is presented in Table H-4 of Appendix H. The second term in the brackets in Equation Q-4 reflects the limits of dissolved or vapor concentrations when in the presence of residual product. Note: Equation 4 is not used in RISC because the models account for solubility limitations explicitly.

Q.2.3 Approach Used in RISC to Calculate TPH SSTLs

For direct soil exposure pathways (i.e. the case where the fate and transport models are not used), RISC uses equations Q-1 and Q-3 to calculate the TPH SSTLs. The approach used for the modeled pathways with a soil source is different than equation Q-4 presented above. When calculating clean-up levels, RISC already is calculating SSTLs for each chemical to meet the overall risk target. That is, if the hazard from the individual fractions is summed, the total should equal the target hazard index entered by the user. Therefore, the TPH SSTL is the sum of all of the individual SSTLs. Since the soil source terms in all of the models check for the solubility limitations, equation Q-4 does not need to be applied.

Q.3 EXAMPLE PROBLEM

In this example problem, an SSTL for a TPH mixture is calculated for surficial soil. Note that RISC performs these calculations automatically, this example is provided to show the exact process used. The exposure pathways of concern are dermal exposure to soil and ingestion of soil for a residential scenario. Because this is a direct exposure scenario, solubility constraints do not need to be considered so equation Q-3 may be used. If solubility constraints apply, Equation Q-4 (which is already accounted for in the RISC model) would apply.

The steps required to calculate the SSTL for the TPH are as follows:

1. Measure total TPH concentration (or choose to have TPH be the sum of the individual measured fractions).
2. Measure concentrations of each TPH fraction. Determine mass fraction by dividing the TPH fraction concentration by the total TPH concentration.
3. Determine appropriate SSTLs for each TPH fraction.
4. Choose the target hazard index.
5. Calculate the SSTL for TPH using Equation Q-3 or Q-4, whichever is appropriate.

The total TPH concentration for this example will be assumed to equal the sum of the concentrations of the individual fractions, 2.1E4 mg/kg. The TPH fraction concentrations are shown in Table Q-1. The mass fractions, MF_i, shown in the third column of Table Q-1 are the quotient of the TPH fraction concentration and the total TPH concentration.

The SSTLi's may be obtained several ways. For a unique exposure situation they should be calculated. For a "standard" exposure scenario, some regulatory programs have SSTLs for the TPH fractions listed in their Tier 1 guidance. In this example, the SSTLs were obtained by running RISC with the "Individual Constituent Levels" target option in Step 5. There, an individual target of HI=1 was entered for each TPH fraction. The results are then presented in Step 6 under the table option entitled "Clean-up Levels". These values are entered in the fourth column of Table Q-1.

The last column contains the quotients, $MF_i/SSTL_i$, the sum of these (3.15E-04) form the denominator of the calculation for the $SSTL_{TPH}$ equation (Equation Q-3). The target hazard index is chosen to be equal to one and the total TPH concentration is calculated to be equal to 3.2E+03 mg/kg (1/3.15E-04).

Table Q-1. Example Calculation of a Surficial Soil TPH SSTL.

Carbon Range	TPH Fraction Conc. (mg/kg)	Mass Fraction, MF_i (-)	$SSTL_i$ for Direct Exposure Pathways (mg/kg)	$MF_i/SSTL_i$
>5-6 C aliphatics	**0.0E+00**	0.0E+00	**2.8E+05**	0.0E+00
>6-8 C aliphatics	**8.5E+00**	4.3E-04	**2.8E+05**	1.5E-09
>8-10 C aliphatics	**9.0E+01**	4.5E-03	**5.6E+03**	8.1E-07
>10-12 C aliphatics	**1.1E+02**	5.3E-03	**5.6E+03**	9.4E-07
>12-16 C aliphatics	**2.0E+03**	9.8E-02	**5.6E+03**	1.7E-05
>16-21 C aliphatics	**2.7E+00**	1.4E-04	**1.1E+05**	1.2E-09
>5-7 C aromatics	**1.6E-01**	8.1E-06	**1.1E+04**	7.3E-10
>7-8 C aromatics	**1.0E+02**	5.2E-03	**1.1E+04**	4.7E-07
>8-10 C aromatics	**7.5E+02**	3.8E-02	**2.2E+03**	1.7E-05
>10-12 C aromatics	**9.9E+02**	4.9E-02	**2.2E+03**	2.2E-05
> 12-16 C aromatics	**3.4E+03**	1.7E-01	**2.2E+03**	7.7E-05
> 16-21 C aromatics	**8.9E+01**	4.5E-03	**1.7E+03**	2.6E-06
> 21-35 C aromatics	**1.3E+04**	6.5E-01	**5.6E+04**	1.2E-05
Totals	**2.0E+04**	**1.0E+00**		**1.50E-04**

$SSTL_{TPH}$ **6.7E+03**

Q.4 REFERENCES

Texas Risk Reduction Program. June 2000. Development of Human Health PCLs for Total Petroleum Hydrocarbon Mixtures. TNRCC Regulatory Guidance. RG-366/TRRP-27

This guidance is available from:

http://www.tnrcc.state.tx.us/permitting/trrp.htm

by going to TRRP Guidance and Forms and then searching for the above referenced document.

Vorhees, Donna, Weisman, Wade and Gustafson, John. June 1999. Total Petroleum Hydrocarbon Criteria Working Group Series, Volume 5: Human Health Risk-Based Evaluation of Petroleum Release Sites: Implementing the Working Group Approach.

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Appendix R

Review of Risk Integrated Software for Cleanups (RISC) v4.0

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R.1 INTRODUCTION

R.1.1 Introduction to RISC

RISC *v*4.0 is a software package for integrated risk evaluation of contaminated sites, providing a tool for quantitative assessment of the potential effects of site contaminants on human health and environmental receptors.

The increasing awareness of the need to manage contaminated land has led to the development by various national agencies, industry groups and others of framework systems for risk assessment of contaminated sites. Examples include US EPA Superfund Guidance (US EPA 1989), American Society for Testing and Material's Risk-Based Corrective Action Guidance (ASTM 1995, 1998), American Petroleum Institute's Decision Support System (API 1994), CONCAWE 1997, the Norwegian risk assessment guidance (SFT 1999), and the UK Environment Agency guidance on risk assessment (Environment Agency 1999a).

A number of software systems have been developed which provide a software implementation of a quantitative risk assessment approach. Examples include Groundwater Services International' "RBCA Toolkit for Petroleum Release Sites" and "RBCA Toolkit for Chemical Release Sites" both of which implement the ASTM RBCA systems; Human Exposure to Soil Pollutants (HESP) developed by Shell

International Petroleum in The Netherlands; the German UMS model (Hempfling et al 1997); and the UK CLEA (DoE 1995) and CONSIM (Environment Agency 1999b) models.

RISC *v*4.0 is a development of earlier versions of RISC. The first versions, *v*1.0 and *v*2.0 were released in 1994 and 1995 respectively, but were only used internally by BP. These versions were broadly similar to later versions, but allowed for *forward* risk calculations only. The major development in *v*3.0, which was released in 1997, was the inclusion of a facility to calculate cleanup target concentrations by *backward* calculations. RISC *v*3.0 was peer reviewed by Johnson 1997.

R.1.2 Arcadis GMI

RISC *v*3.0 is a key software tool used by Arcadis GMI. Our in depth knowledge and experience using this package placed us an ideal position to run an extensive program of testing and validation work on *v*4.0. Beginning with a single compound and a single pathway, complex scenarios were built up with comprehensive checking carried out at each level of complexity. At each stage input and output results were examined and parameters varied to verify that the expected results were achieved. Many interface and programming problems were uncovered and communicated to the authors on a regular basis; each solution was rigorously tested and the software checked for any knock-on effects of the changes.

R.1.3 Organisation of Review

The organisation of this review adheres to the following structure:

Enhancements in RISC *v*4.0
Overview of Functional Capabilities
RISC User Interface and User’s Manual
RISC Source Partitioning Algorithms
Back Calculation and Clean-up Targets For Soil and Groundwater
Comparison of RISC with Independent Calculations

R.2 ENHANCEMENTS IN RISC V4.0

RISC *v*4.0 has been substantially extended and improved from *v*3.0. New exposure pathways and fate and transport models for existing supported pathways have been added. Improvements have been made to the fate and transport models and presentation of results

R.2.1 Additional Pathways and Models

The following new human health exposure pathways have been added to *v*4.0:

“Irrigation pathways”. The pathways that can be evaluated in this option are (i) ingestion of vegetables irrigated with contaminated groundwater, (ii) ingestion of irrigation water either directly from irrigation sprinklers or from a swimming pool filled with irrigation water, (iii) dermal contact with ingestion water and (iv) inhalation of irrigation water applied by spray irrigation.

Vegetables grown in contaminated soil. This pathway evaluates the intake of contaminants from ingestion of root and above-ground vegetables grown in contaminated soil.

The following new modelling options have been added to *v*4.0:

Surface Water Mixing and Sediment Partitioning Model. This model is used to estimate surface water and sediment concentrations arising from mixing between the surface water and a groundwater plume. The following pathways that can be evaluated in this option: (i) ingestion of surface water and (ii) dermal contact with surface water, while playing or swimming in a surface water course impacted by site-derived groundwater.

Ecological/Water Quality Option. This option utilises the surface water mixing and sediment partitioning models to estimate the concentration in either rivers or lakes from groundwater contaminant influx. The predicted concentrations may be compared to a selection of quality criteria, which are tabulated within this option. Clean-up levels can be calculated based on target surface water concentrations.

Two new vapour intrusion models have been included for simulation of vapour phase transport from soil to indoor and outdoor air. These are:

Dominant Layer Model, Johnson, Kemblowski and Johnson 1998. This model divides the unsaturated zone into three layers, with first order aerobic degradation allowed in the middle layer only. The model is based a conceptual model developed from field observations. The lower layer contains zero oxygen and therefore no degradation is allowed while diffusion dominates. The middle layer contains both oxygen and contaminant, and degradation and diffusion transport occur. The upper layer contains oxygen but lower contaminant concentration and negligible degradation is assumed, thus diffusion dominates.

Oxygen-Limited Model, (Johnson, unpublished). This model determines the rate of aerobic degradation in a system where degradation is limited by the availability of oxygen from a surface source.

Soil gas can be used as the source term for vapour models from soil.

R.2.2 Alterations Within Existing Models

The following sections outline the main alterations in *v*4.0:

Database and Input Options

Many of the default exposure parameters have been changed to reflect new data presented by the US EPA in the updated Exposure Factors Handbook (August, 1997).

Several of the toxicity parameters in the chemical database have been changed, some of which reflect updates to the IRIS database.

Within the site properties there are some additional parameters that must be specified, for example, the porosity and water content in foundation cracks can now be specified rather than being fixed within the software. The lithology of the source zone can now be specified as a different lithology to the unsaturated zone.

Groundwater Transport Models

Modifications have been made to the internal calculation of dispersivity in the groundwater transport models. Dispersivity is calculated as a function of groundwater flowpath length in both versions. However, in *v*4.0 the flowpath distance used to calculate longitudinal dispersivity is the distance from the downgradient edge of the source to the receptor or compliance point. In *v*3.0, the flowpath distance was calculated from the x-coordinate of the compliance point, which was equivalent to the distance from the centre of the user-defined source to the compliance point.

All three source dimensions input by the user are now used to define the source zone in the groundwater models. In *v*3.0 it was assumed that the source area was a vertical planar source at the down gradient edge of the actual source area. Therefore in *v*3.0 all of the contaminant loading was assumed to enter groundwater at the down gradient edge of the source. In *v*4.0 the contaminant loading is distributed over the specified source area. This will lead to reduced concentrations at the receptor, relative to *v*3.0, because the contaminant will be more dispersed since some of it has started further back from than the down gradient edge.

Vapour Phase Transport Models

In *v*4.0 it is assumed that one of the indoor or outdoor air pathways will be dominant (usually the indoor air pathway). These models may not now be run at the same time.

Additional Changes

In RISC *v*3.0 the hazard quotients for adult and child receptors were reported separately, but also as a combined total assuming that the hazard quotient was additive for a child that becomes an adult and remains at the same residence. This additive approach is not appropriate for non-carcinogenic effects or hazard quotients and has been discontinued in *v*4.0. Note that the additive receptor option is still applicable and functional in *v*4.0 for carcinogens.

For depleting sources (in the vadose zone and saturated soil models) in *v*4.0 the clean-up level may lie somewhere between the residual concentration (the concentration at which a fourth phase is present) and complete soil saturation (which is arbitrarily cut-off at 1 x 10^6 mg/kg for all contaminants for modelling purposes). This is possible since the additional mass in the source can increase the risk as the exposure may last longer than just a source at the residual level. In *v*4.0 these actual clean-up levels are reported with the residual saturation values also usefully reported alongside each SSTL, so that it is immediately apparent if the SSTL exceeds the residual saturation value. For steady state models and the dissolved groundwater model, if the risk cannot be exceeded at the point at which residual phase begins to form, the SSTL will be reported as RES to represent the residual concentration. In *v*3.0, all SSTLs in excess of the residual saturation value were reported as the residual saturation value (which was incorrect for a finite mass soil source).

In RISC *v*3.0 the soil to outdoor air vapour transport pathway was evaluated using the same soil zone model used to estimate contaminant loading to the groundwater model; the volatile emission rate calculated by the Vadose Zone Model (described in Appendix A) was required as the input to a “box” model. This model incorporated a depleting source term i.e. mass was conserved, with depletion due to the combined effects of leaching to groundwater and volatilisation to the overlying atmosphere. However, in RISC *v*4.0 leaching to groundwater and volatilisation to atmosphere are out using separate models. The method used for volatilisation from soil to outdoor air is now a steady state, non-depleting, soil model based on the Johnson and Ettinger 1991 model. This model was already used in the soil to indoor air model and has the advantage that the results can be compared to those from the dominant layer and oxygen-limited models. A second, compatible model must be run to calculate the leachate losses, if required.

An overall TPH SSTL can now be calculated using the cumulative risk option (see section 6.0 for further detail).

SSTLs can now be calculated to target concentrations such as MCLs (see section 6.0 for further detail).

The interface has been structured within *v*4.0 to include food chain pathways and ecological receptor impacts. However, these options are not yet active but will become so when *v*5.0 is released.

R.3 OVERVIEW OF THE FUNCTIONAL CAPABILITIES OF RISC

RISC *v*4.0 provides one of the most comprehensive quantitative risk evaluation capabilities of all the risk software packages available. Table R-1 provides a summary of the features supported in RISC *v*4.0, with the capabilities of GSI's RBCA Tier 2 Toolkit shown for comparison.

Table R-1. Summary of Features in RISC *v*4.0.
(Page 1 of 2)

Function/ F&T Models	**RISC *v*4.0**	**GSI Tier 2 Toolkit**
General Features:		
Internal Chemical Database	✔	✔
Sample database	✔	✘
Monte Carlo uncertainty analysis	✔	✘
Backward calculation for cleanup targets	✔	✔
Tier 1 Look up Tables	✔	✔
Forward Calculations	✔	✔
Source Conceptualisation:		
Free product solubility corrections	✔	✔
Fate & Transport Models:		
Outdoor air	✔	✔
Indoor air	✔	✔
Unsaturated zone model to Groundwater Model	✔	✘
Groundwater – saturated soil leaching to groundwater	✔	✘
Groundwater – dissolved phase source	✔	✔
Groundwater - Surface water	✔	✘
Soil – surface	✔	✔
Soil – subsurface	✔	✔

Table R-1. Summary of Features in RISC *v*4.0.
(Page 2 of 2)

Function/ F&T Models	**RISC *v*4.0**	**GSI Tier 2 Toolkit**
Intake routes supported:		
Ingestion of soil	✔	✔
Dermal contact with soil	✔	✔
Ingestion of groundwater	✔	✔
Dermal intake and inhalation in shower	✔	✘
Inhalation of indoor and outdoor air	✔	✔
Ingestion and dermal contact with impacted surface water	✔	✔
Ingestion of fish from impacted surface water	✘	✔
Ingestion of home-grown vegetables	✔	✘
Ingestion/dermal contact with irrigation water	✔	✘
Inhalation of irrigation water spray	✔	✘

Most of the fate & transport models are widely used in the industry and in many cases are also used in other software systems.

R.4 RISC USER INTERFACE AND USER’S MANUAL

RISC is predominantly a point-and-click program. The interface leads the user through six steps, which must be completed sequentially in order to progress to the choice of two end-points - calculating risk or calculating clean-up levels.

The user interface has undergone some significant changes since *v*3.0. Step 2, Choosing Exposure Pathways, is now a divided screen, which highlights the distinction between Environmental Pathways (Selecting Contaminated Media and Fate and Transport Models) and Human Health Exposure Pathways (Exposure Pathways). The inclusion of a visual representation of the selected fate and transport models will assist more novice users in visualising the conceptual model being modelled in RISC. A further improvement is the division of the main data entry screen (Step 3a) into two screens, distinguishing between the data required for groundwater models and the data required for volatilisation models.

An on-line help system and a user's manual accompany the RISC software. The on-line help system has undergone some development and now has a structure similar to that of the user's manual, and is therefore more easily navigated. However, this system primarily contains definitions and descriptions and does not refer to the algorithms or models, which are contained in the user's manual. In order to gain an insight into the operations being performed by the RISC software, the user should read the user's manual, and particularly those appendices that give a detailed description of the models being used. In addition to reflecting updates to the software, the manual has been generally revised. The appendices in particular have been expanded and contain further descriptions into the workings and assumptions intrinsic to the fate and transport models.

As with *v*3.0, a range of output options is available to the user. The user may still find that the output tables do not always print out well in A4 portrait or landscape format.

R.5 RISC SOURCE PARTITIONING ALGORITHMS

RISC partitions the chemicals between vapor, sorbed and dissolved phases using conventional partitioning algorithms based on Henry's Law (liquid to vapor phase) and the organic carbon partition coefficient, K_{oc}, or inorganic partition coefficient, K_d, (solid to liquid phase).

An important feature in RISC *v*4.0, which was also in *v*3.0, is the inclusion of facilities that simulate some of the effects of the presence of residual free phase hydrocarbon. In common with all comparable software tools, RISC cannot simulate the fate and transport of mobile residual phase hydrocarbons. Separate stand-alone models are available that simulate the fate and transport of mobile residual phase e.g. ARMOS (ES&T) or MOFAT (RASI), although these models do not provide a quantitative evaluation of risk. RISC accounts for the effects of *immobile* residual phase on the solubility of individual compounds within multiple-constituent hydrocarbon mixtures.

RISC carries out a calculation to determine whether residual phase hydrocarbon is present. This applies in the following fate and transport models:

Vadose zone model – leaching to groundwater / volatilisation to outdoor air
Saturated soil groundwater model
Vapor transport from soil to indoor air

Where residual phase is calculated to be present, RISC uses Raoult's Law to calculate the effective solubility or effective vapour pressures. Where residual phase is calculated not to be present, RISC calculates the concentration in each phase (sorbed, dissolved and vapor) based on the relevant equilibrium partitioning equations.

RISC uses different source term assumptions for the Vadose Zone model and the Vapor Transport to Indoor Air model. The Vadose Zone model uses a depleting source, where depletion occurs due to volatilisation, leaching and / or degradation loses. The Vapor Transport model uses a steady state non-depleting source.

R.6 BACK-CALCULATION OF CLEANUP TARGETS FOR SOIL AND GROUNDWATER

RISC allows the user to calculate site specific clean-up target levels for deterministic scenarios. For scenarios involving transport models, clean-up levels can only be calculated for one receptor at a time, though it should be noted that this receptor may be defined as the "additive" child + adult case.

There are two options for calculating clean-up targets:

If the "Individual Constituent Levels" option is chosen, each individual chemical source concentration is reduced or increased to achieve the selected target level. If groundwater or surface water is a receptor media, a target concentration such as Maximum Contaminant Levels (MCLs) may be specified instead of the target risk. This back calculation does not depend on the original source concentration.

If the "Cumulative Risk" option is chosen, the concentrations of each chemical are increased or reduced proportionately to each other until the specified target is reached. This back calculation does not depend on the magnitude of the original source concentrations but does depend on the relative proportions of the source concentrations. The clean-up levels will be of the same proportions as the original source concentrations. This cumulative option can also be used in RISC to calculate a site-specific target level for a TPH mixture. The model recognises chemical names containing the letters "TPH" and automatically uses the SSTLs calculated for each individual TPH fraction and the site specific measured concentrations of the TPH fractions to estimate a unique SSTL that is protective for the TPH mixture at the site.

The second approach may lead to the conclusion that remediation is required for compounds present at low concentrations as all SSTLs would decrease in the same proportion as the compound that is in the risk driver. The first approach should guard against this as compounds present at low concentrations will have target clean-up levels greater than the current concentrations on site.

R.7 COMPARISON OF RISC WITH INDEPENDENT CALCULATIONS

The output from RISC was compared to the output from a number of independent calculations using the equations described in the user's manual.

R.7.1 Direct Exposure Pathways

Good or perfect agreement was obtained for all contaminants and exposure pathways evaluated. The results of this comparison can be seen in the tables at the end of this peer review.

R.7.2 Validation of Monte Carlo Simulations

The Monte-Carlo option in RISC was used to generate a probability distribution of risks for exposure to benzene in drinking water. Default adult RME exposure data were used, with exposure to a constant concentration of 0.005mg/l benzene.

The RISC output was compared to the results of similar calculations carried out using Crystal Ball software package. The output from both are shown in the table below. The agreement is very good in the centre of the range, with a consistent difference between the two estimates at the extreme ends of the range. This was demonstrated using five hundred model runs.

Table R-2. Comparison of Monte Carlo Results from RISC *v*4.0 and Crystal Ball.

Summary Statistics	Cancer Risk (RISC)	Cancer Risk (Crystal Ball)
minimum	$4.19x10^{-9}$	$5.6x10^{-9}$
5%	$4.02x10^{-8}$	$3.9x10^{-8}$
50%	$3.83x10^{-7}$	$2.3x10^{-7}$
75%	$4.73x10^{-7}$	$4.7x10^{-7}$
90%	$8.88x10^{-7}$	$8.7x10^{-7}$
95%	$1.23x10^{-6}$	$1.2x10^{-6}$
maximum	$5.59x10^{-6}$	$7.4x10^{-6}$

R.7.3 Indoor and Outdoor Air Fate and Transport Models

Johnson & Ettinger – Soil – Indoor Air Model

The Johnson & Ettinger model is used to estimate the emissions from a soil source, either into buildings or to the atmosphere. The indoor air case has been used to validate the model against an independent solution of the Johnson & Ettinger equations. The input data and the results are presented in the following table:

Table R-3. Input Data Used and Results from the Johnson and Ettinger Model Comparison Runs.

Soil Properties			
Parameter	Vadose Zone	Lens	Foundation
Thickness of Transport Zone [m]	2.60	0.2	0.15
Total Porosity [m^3/m^3]	0.35	0.35	0.25
Moisture Content [m^3/m^3]	0.05	0.15	0.00
Soil Bulk Density [g/cm^3]	1.7	1.7	1.7
Building Properties			
Volume [m3]	400		
Air Exchange Rate [changes/d]	12		
Total Infiltration Area [m^2]	150		
Fraction of Area with Cracks	0.001		
Depth Below Ground Surface [m]	2.0		
Length of Foundation Perimeter [m]	50.0		
Pressure Gradient [g/cm^2-s]	10.0		
Permeability of Soil to Vapours [cm^2]	1x10^{-9}		
Soil Concentrations	**Case A**	**Case B**	
Benzene [mg/kg]	1000	10	
Total Hydrocarbons [mg/kg]	0	1000	
Output–Indoor Air Concentrations			
Benzene [mg/m^3]	8.57x10^{0}	8.57x10^{-2}	
Independent calculation [mg/m^3]	8.59x10^{0}	8.59x10^{-2}	

Dominant Layer Model

The Dominant Layer model was also validated against independent solutions of the equations. In addition this model has been used to validate the use of soil gas, rather than soil, as the source term. The input data and results are presented in the following table:

Table R-4. Input Data Used and Results from the Dominant Layer Model Comparison Runs.

Soil Properties	**Layer 1**	**Layer 2 (Dominant)**	**Layer 3**
Total Porosity [-]	0.35	0.35	0.35
Water Content [-]	0.05	0.15	0.05
Air Content [-]	0.30	0.20	0.30
Thickness [m]	1.3	0.2	1.3
Soil Source			
Porosity [-]	0.35		
Water Content [-]	0.15		
Soil Bulk Density [g/cm^3]	1.7		
F_{oc}	0.01		
Degradation Rate Vapour Phase	0.09		
Chemical-Specific Parameters			
Source Benzene Concentration [mg/kg]	1000		
Initial Source Vapour Concentration [mg/m^3]	3.23×10^5		
Calculated Value [mg/m^3]	3.23×10^5		
Concentration in Building [mg/m^3]	7.28		
Calculated Value [mg/m^3]	7.28		
Concentration in Building using Initial Source Vapour Concentration as Soil Gas Source Term [mg/m^3]	7.27		

Oxygen Limited Model

The output from this model has not been validated.

R.7.4 Groundwater Fate and Transport Models

Groundwater – Indoor Air

The modelling of vapour transport from groundwater into buildings has been validated against independent calculations. The input data and results are presented in the following table:

Table R-5. Input Data Used and Results from Groundwater Vapour to Indoor Air Model Comparison Runs.

Soil Properties				
Parameter	**Vadose Zone**	**Lens**	**Capillary Fringe**	**Foundation**
Thickness of Zone [m]	1.2	0.2	0.2	0.1
Total Porosity [-]	0.35	0.35	0.35	0.25
Moisture Content [-]	0.05	0.15	0.345	0.00
Soil Bulk Density [g/cm^3]	1.7	1.7	1.7	1.7
Building Properties				
Volume [m^3]	400			
Air Exchange Rate [changes/d]	12			
Total Infiltration Area [m^2]	150			
Fraction of Area with Cracks [-]	0.001			
Groundwater Source				
Groundwater Concentration [mg/l]	1.00			
Output – Indoor Concentrations				
Benzene [mg/m^3]	2.27x10^{-3}			
Independent calculation [mg/m^3]	2.27x10^{-3}			

Groundwater – Outdoor Air

The modelling of vapour transport from groundwater into buildings has been validated against independent calculations. The input data and results are presented in the following table:

Table R-6. Input Data Used and Results from Groundwater Vapour to Outdoor Air Model Comparison Runs.

Soil Properties			
Parameter	**Vadose Zone**	**Lens**	**Capillary Fringe**
Thickness of Zone [m]	1.2	0.2	0.2
Total Porosity [-]	0.35	0.35	0.35
Moisture Content [-]	0.05	0.15	0.345
Soil Bulk Density [g/cm^3]	1.7	1.7	1.7
Outdoor Air Parameters			
Height of Box [m]	2.00		
Length of Box [m]	10.00		
Wind Speed [m/s]	2.25		
Groundwater Source			
Groundwater Concentration [mg/l]	1.00		
Output – Outdoor Concentrations			
Benzene [mg/m^3]	2.27x10^{-3}		
Independent calculation [mg/m^3]	2.27x10^{-3}		

Vadose Zone Leaching to Groundwater Model

The Vadose Zone Model has been validated against independent solutions of the equations. The input data and results are presented in the table and graphs below:

Table R-7. Input Data Used and Results from Vadose Zone Leaching to Groundwater Model Comparison Runs.

Soil Properties			
Parameter	**Vadose Zone**	**Lens**	**Source**
Thickness of Zone [m]	4.0m above source 2.8m below source	0.2	3.0
Total Porosity [-]	0.35	0.35	0.35
Soil Bulk Density [g/cm^3]	1.7	1.7	1.7
Infiltration Rate [cm/yr]	20	20	20
Van Genuchten's N [-]	2.68	2.00	2.68
Residual Moisture Content [-]	0.05	0.15	0.05
Saturated Hydraulic Conductivity [m/d]	10	1.00	10
Moisture Content [-]	Calculated	Calculated	Calculated
F_{oc} [-]	0.01	0.01	0.01
Source Zone Parameters			
Source Length [m]	10.0		
Source Width [m]	10.0		
Chemical-Specific Parameters			
First-order decay coefficient in the source zone [1/day]	0.00		
First-order decay coefficient in the vadose zone [1/day]	0.001		
Soil Concentration (Benzene) [mg/kg]	500		
Soil TPH Concentration [mg/kg]	5000		
TPH Molecular Weight [mg/kg]	100		
Output – Groundwater Concentrations			
Benzene at Source [mg/l]	224		
Independent Calculation [mg/1]	224		
Concentration at Water Table at t=10yrs [mg/l]	10.8		
Independent Calculation at t=10yrs [mg/l]	11.0		

Shown below is a graph of the concentration of benzene at the source vs time, for the Vadose Zone Model, to compare the RISC model outputs to the independent hand calculations. In general the agreement is good with small differences arising because the concentration displayed for each year is an average for that year based on the concentration at each of the monthly time steps. This explains why the difference is most notable early in the simulation.

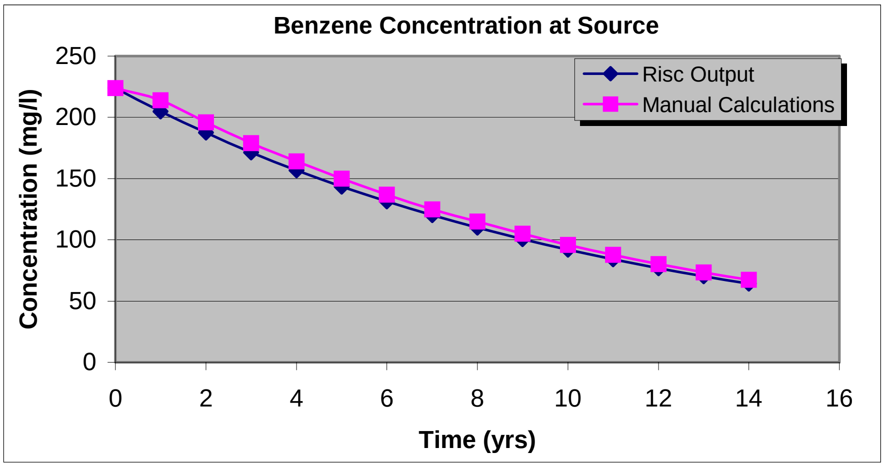

Figure R-1. Benzene Concentration vs Time in the Vadose Zone Source.

The Graph of concentration at the water table (2.8m below the base of the source) indicates good agreement between the RISC output and independent calculations. The slight discrepancy as time increases is likely to be due to the fact that for the independent calculations the error function values were calculated empirically using the formula erf (x) = $(1- \exp(-4x^2/\text{pi}))^{1/2}$, which can have an error of up to 0.7%.

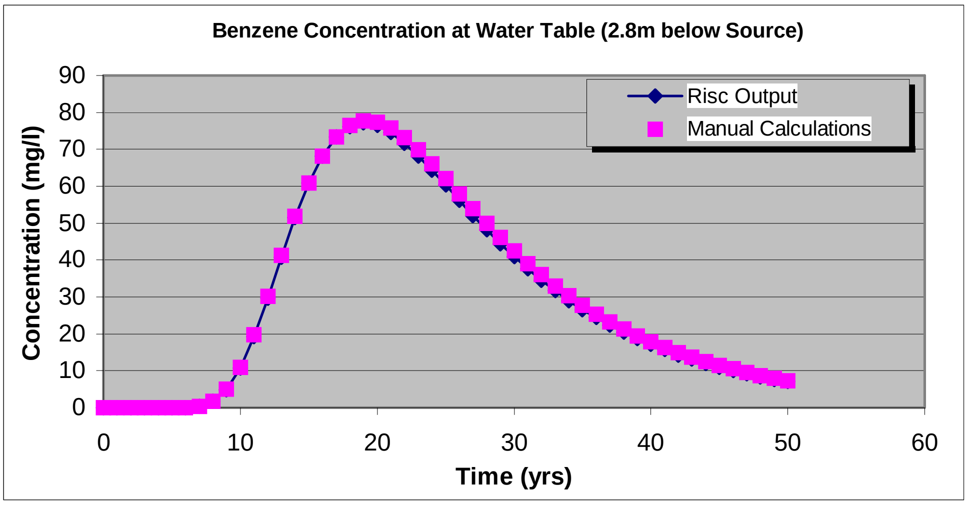

Figure R-2. Benzene Concentration vs Time at the Water Table.

R.7.5 Surface Water Mixing Models

The RISC output was compared with manual calculations, as shown in the table below. For the conditions modelled the RISC output and the manual calculation were in exact agreement.

Table R-8. Input Data Used and Results from the Surface Water Model Comparison Runs.

Surface water	**River**	**Lake**
Hydraulic Conductivity of SW bed [m/d]	10	10
Foc in sediment [g/g]	0.01	0.01
Depth of SW [m]	5	5
Length of reach [m]	100	100
Hydraulic gradient between GW and SW [m/m]	0.05	0.05
Cross Sectional Area of River [m^2]	5	
Lake Volume [m^3]		100000
Fraction available for mixing [-]	1	0.1
SW flow rate [m^3/day]	180	180
Degradation rate in SW [1/d]	0.00	0.005
Groundwater Concentration		
Benzene (mg/l)	5	5
Chemical Parameters		
Mass Flux from GW to SW [mg/d]	1.25×10^6	1.25×10^6
Manual Calculation	1.25×10^6	1.25×10^6
Surface water concentration [mg/l]	2.91	3.93
Manual Calculation	2.91	3.93
Sediment Concentration [mg/kg]	2.95	2.95
Manual Calculation	2.95	2.95

DECLARATION

This peer review was carried out by the following Arcadis staff:

Helen Tighe
Clair Smith
Matt Gardner
Stephen Swift
Jonathon Rigby
Lawrence Houlden

We declare that the review was completed as described above:

Signed			
Name	Lawrence Houlden	Matt Gardner	Helen Tighe
Date	24th September 2001		

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Table R-9. Verification Calculations for the Direct Exposure Pathways.
(Page 1 of 3)

Exposure Pathway/Results	Arsenic	Benzene	Benzo(a)pyrene	TPH Aliphatic C12-C16
Ingestion of Soil				
Concentration (mg/kg-soil)	5.00	5.00	5.00	5.00
CDI (RISC) [mg/kg-d] CDI (calculated) [mg/kg-d]	$6.85x10^{-6}$ $6.85x10^{-6}$	$6.85x10^{-6}$ $6.85x10^{-6}$	$6.85x10^{-6}$ $6.85x10^{-6}$	$6.85x10^{-6}$ $6.85x10^{-6}$
Cancer Risk (RISC) Cancer Risk (calculated)	$4.4x10^{-6}$ $4.4x10^{-6}$	$8.5x10^{-8}$ $8.51x10^{-8}$	$2.1x10^{-5}$ $2.14x10^{-5}$	0.00 NQ
Hazard Index (RISC) Hazard Index (calculated)	$2.3x10^{-2}$ $2.28x10^{-2}$	0.00 NQ	0.00 NQ	$6.8x10^{-5}$ $6.85x10^{-5}$
Dermal Contact with Soil				
Concentration (mg/kg-soil)	5.00	5.00	5.00	5.00
CDI (RISC) [mg/kg-d] CDI (calculated) [mg/kg-d]	$1.18x10^{-5}$ $1.18x10^{-5}$	$3.94x10^{-5}$ $3.94x10^{-5}$	$3.94x10^{-5}$ $3.94x10^{-5}$	$3.94x10^{-5}$ $3.94x10^{-5}$
Cancer Risk (RISC) Cancer Risk (calculated)	$7.6x10^{-6}$ $7.60x10^{-6}$	$4.9x10^{-7}$ $4.9x10^{-7}$	$1.2x10^{-4}$ $1.2x10^{-4}$	0.00 NQ
Hazard Index (RISC) Hazard Index (calculated)	$3.9x10^{-2}$ $3.94x10^{-2}$	0.00 NQ	0.00 NQ	$3.9x10^{-4}$ $3.9x10^{-4}$
Ingestion of Groundwater				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d] CDI (calculated) [mg/kg-d]	$5.48x10^{-2}$ $5.48x10^{-2}$	$5.48x10^{-2}$ $5.48x10^{-2}$	$5.48x10^{-2}$ $5.48x10^{-2}$	$5.48x10^{-2}$ $5.48x10^{-2}$
Cancer Risk (RISC) Cancer Risk (calculated)	$3.5x10^{-2}$ $3.52x10^{-2}$	$6.8x10^{-4}$ $6.81x10^{-4}$	$1.7x10^{-1}$ $1.71x10^{-1}$	0.00 NQ
Hazard Index (RISC) Hazard Index (calculated)	$1.8x10^{2}$ $1.83x10^{2}$	0.00 NQ	0.00 NQ	$5.5x10^{-1}$ $5.48x10^{-1}$
Dermal Contact in Shower				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d] CDI (calculated) [mg/kg-d]	$1.26x10^{-4}$ $1.26x10^{-4}$	$2.65x10^{-3}$ $2.65x10^{-3}$	$1.51x10^{-1}$ $1.51x10^{-1}$	$1.03x10^{0}$ $1.03x10^{0}$
Cancer Risk (RISC) Cancer Risk (calculated)	$8.1x10^{-5}$ $8.10x10^{-5}$	$3.3x10^{-5}$ $3.29x10^{-5}$	$4.7x10^{-1}$ $4.73x10^{-1}$	0.00 NQ
Hazard Index (RISC) Hazard Index (calculated)	$4.2x10^{-1}$ $4.20x10^{-1}$	0.00 NQ	0.00 NQ	$1.0x10^{1}$ $1.03x10^{1}$
Inhalation in Shower				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d] CDI (calculated) [mg/kg-d]	$0.00x10^{0}$ $0.00x10^{0}$	$6.67x10^{-2}$ $6.67x10^{-2}$	$2.34x10^{-4}$ $2.34x10^{-4}$	$4.84x10^{-2}$ $4.84x10^{-2}$
Cancer Risk (RISC) Cancer Risk (calculated)	$0.00x10^{0}$ $0.00x10^{0}$	$7.7x10^{-4}$ $7.7x10^{-4}$	$3.1x10^{-4}$ $3.1x10^{-4}$	0.00 NQ
Hazard Index (RISC) Hazard Index (calculated)	$0.00x10^{0}$ $0.00x10^{0}$	0.00 NQ	0.00 NQ	$1.8x10^{-1}$ $1.8x10^{-1}$
Ingestion of Root Vegetables (Soil)				
Concentration (mg/kg)	5.00	5.00	5.00	5.00
CDI (RISC) [mg/kg-d] CDI (calculated) [mg/kg-d]	$1.08x10^{-5}$ $1.08x10^{-5}$	$1.29x10^{-5}$ $1.29x10^{-5}$	$6.05x10^{-7}$ $6.05x10^{-7}$	$4.24x10^{-7}$ $4.24x10^{-7}$
Cancer Risk (RISC) Cancer Risk (calculated)	$6.93x10^{-6}$ $6.93x10^{-6}$	$1.61x10^{-1}$ $1.61x10^{-1}$	$1.89x10^{-6}$ $1.89x10^{-6}$	0.00 NQ
Hazard Index (RISC) Hazard Index (calculated)	$3.60x10^{-2}$ $3.60x10^{-2}$	0.00 NQ	0.00 NQ	$4.24x10^{-6}$ $4.24x10^{-6}$

Table R-9. Verification Calculations for the Direct Exposure Pathways.

(Page 2 of 3)

Exposure Pathway/Results	Arsenic	Benzene	Benzo(a)pyrene	TPH Aliphatic C12-C16
Ingestion of Above Ground Vegetables (Soil)				
Concentration (mg/kg)	5.00	5.00	5.00	5.00
CDI (RISC) [mg/kg-d]	1.57x10^{-5}	9.27x10^{-4}	4.52x10^{-6}	1.78x10^{-6}
CDI (calculated) [mg/kg-d]	1.57x10^{-5}	9.27x10^{-4}	4.52x10^{-6}	1.78x10^{-6}
Cancer Risk (RISC)	1.01x10^{-5}	1.15x10^{-5}	1.41x10^{-5}	0.00
Cancer Risk (calculated)	1.01x10^{-5}	1.15x10^{-5}	1.41x10^{-5}	NQ
Hazard Index (RISC)	5.22x10^{-2}	0.00	0.00	1.78x10^{-5}
Hazard Index (calculated)	5.22x10^{-2}	NQ	NQ	1.78x10^{-5}
Ingestion of Root Vegetables (Groundwater)				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d]	1.25x10^{-4}	1.52x10^{-3}	1.21x10^{0}	4.24x10^{0}
CDI (calculated) [mg/kg-d]	1.26x10^{-4}	1.53x10^{-3}	1.21x10^{0}	4.26x10^{0}
Cancer Risk (RISC)	8.1x10^{-5}	1.9x10^{-5}	3.8x10^{-1}	0.00
Cancer Risk (calculated)	8.0x10^{-5}	1.9x10^{-5}	3.8x10^{-1}	NQ
Hazard Index (RISC)	4.2x10^{-1}	0.00	0.00	4.2x10^{1}
Hazard Index (calculated)	4.2x10^{-1}	NQ	NQ	4.2x10^{1}
Ingestion of Above Ground Vegetables (Groundwater)				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d]	1.82x10^{-4}	1.09x10^{-3}	9.03x10^{-2}	1.78x10^{-1}
CDI (calculated) [mg/kg-d]	1.82x10^{-4}	1.09x10^{-3}	9.03x10^{-2}	1.78x10^{-1}
Cancer Risk (RISC)	1.17x10^{-4}	1.36x10^{-5}	2.83x10^{-1}	0.00
Cancer Risk (calculated)	1.17x10^{-4}	1.35x10^{-5}	2.82x10^{-1}	NQ
Hazard Index (RISC)	6.05x10^{-1}	0.00	0.00	1.78x10^{0}
Hazard Index (calculated)	6.05x10^{-1}	NQ	NQ	1.78x10^{0}
Inhalation of Groundwater Spray				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d]	0.00	6.7x10^{-2}	2.4x10^{-4}	4.8x10^{-2}
CDI (calculated) [mg/kg-d]	0.00	6.7x10^{-2}	2.4x10^{-4}	4.9x10^{-2}
Cancer Risk (RISC)	0.00	7.8x10^{-4}	3.1x10^{-4}	0.00
Cancer Risk (calculated)	0.00	7.8x10^{-4}	3.1x10^{-4}	NQ
Hazard Index (RISC)	0.00	0.00	0.00	1.8x10^{-1}
Hazard Index (calculated)	0.00	NQ	NQ	1.8x10^{-1}
Dermal Contact with Irrigation Water				
Concentration (mg/l-H$_2$0)	2.0	2.0	2.0	2.0
CDI (RISC) [mg/kg-d]	2.70x10^{-4}	5.67x10^{-3}	3.24x10^{-1}	2.21x10^{0}
CDI (calculated) [mg/kg-d]	2.70x10^{-4}	5.67x10^{-3}	3.24x10^{-1}	2.21x10^{0}
Cancer Risk (RISC)	1.74x10^{-4}	7.05x10^{-5}	1.01x10^{0}	0.00
Cancer Risk (calculated)	1.74x10^{-4}	7.05x10^{-5}	1.01x10^{0}	NQ
Hazard Index (RISC)	9.00x10^{-1}	0.00	0.00	2.21x10^{1}
Hazard Index (calculated)	9.00x10^{-1}	NQ	NQ	2.21x10^{1}
Ingestion of Irrigation Water				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d]	1.17x10^{-3}	1.17x10^{-3}	1.17x10^{-3}	1.17x10^{-3}
CDI (calculated) [mg/kg-d]	1.17x10^{-3}	1.17x10^{-3}	1.17x10^{-3}	1.17x10^{-3}
Cancer Risk (RISC)	7.55x10^{-4}	1.46x10^{-5}	3.67x10^{-3}	0.00
Cancer Risk (calculated)	7.55x10^{-4}	1.46x10^{-5}	3.67x10^{-3}	NQ
Hazard Index (RISC)	3.91x10^{0}	0.00	0.00	1.17x10^{-2}
Hazard Index (calculated)	3.91x10^{0}	NQ	NQ	1.17x10^{-2}

Table R-9. Verification Calculations for the Direct Exposure Pathways.

(Page 3 of 3)

Exposure Pathway/Results	Arsenic	Benzene	Benzo(a)pyrene	TPH Aliphatic C12-C16
Inhalation of Outdoor Air				
Concentration (mg/m^3-air)	4.00	4.00	4.00	4.00
CDI (RISC) [mg/kg-d]	$2.73x10^{-1}$	$2.73x10^{-1}$	$2.73x10^{-1}$	$2.73x10^{-1}$
CDI (calculated) [mg/kg-d]	$2.73x10^{-1}$	$2.73x10^{-1}$	$2.73x10^{-1}$	$2.73x10^{-1}$
Cancer Risk (RISC)	$1.8x10^{0}$	3.2x10-3	3.6x10-1	0.00
Cancer Risk (calculated)	$1.8x10^{0}$	3.2x10-3	3.6x10-1	NQ
Hazard Index (RISC)	0.00	0.00	0.00	$1.0x10^{0}$
Hazard Index (calculated)	NQ	NQ	NQ	$1.0x10^{0}$
Inhalation of Indoor Air				
Concentration (mg/m^3-air)	3.00	3.00	3.00	3.00
CDI (RISC) [mg/kg-d]	$4.11x10^{-1}$	$4.11x10^{-1}$	$4.11x10^{-1}$	$4.11x10^{-1}$
CDI (calculated) [mg/kg-d]	$4.11x10^{-1}$	$4.11x10^{-1}$	$4.11x10^{-1}$	$4.11x10^{-1}$
Cancer Risk (RISC)	$2.6x10^{0}$	$4.8x10^{-3}$	$5.5x10^{-1}$	0.00
Cancer Risk (calculated)	$2.6x10^{0}$	$4.8x10^{-3}$	$5.5x10^{-1}$	NQ
Hazard Index (RISC)	0.00	0.00	0.00	$1.5x10^{0}$
Hazard Index (calculated)	NQ	NQ	NQ	$1.5x10^{0}$
Ingestion while Swimming				
Concentration (mg/l-H_20)	6.00	6.00	6.00	6.00
CDI (RISC) [mg/kg-d]	$1.10x10^{-3}$	$1.10x10^{-3}$	$1.10x10^{-3}$	$1.10x10^{-3}$
CDI (calculated) [mg/kg-d]	$1.10x10^{-3}$	$1.10x10^{-3}$	$1.10x10^{-3}$	$1.10x10^{-3}$
Cancer Risk (RISC)	$7.1x10^{-4}$	$1.4x10^{-5}$	$3.4x10^{-3}$	0.00
Cancer Risk (calculated)	$7.1x10^{-4}$	$1.4x10^{-5}$	$3.4x10^{-3}$	NQ
Hazard Index (RISC)	$3.7x10^{0}$	0.00	0.00	$1.1x10^{-2}$
Hazard Index (calculated)	$3.7x10^{0}$	NQ	NQ	$1.1x10^{-2}$
Dermal – Swimming				
Concentration (mg/l-H_20)	6.00	6.00	6.00	6.00
CDI (RISC) [mg/kg-d]	$5.06x10^{-4}$	$1.06x10^{-2}$	$6.07x10^{-1}$	$4.15x10^{0}$
CDI (calculated) [mg/kg-d]	$5.06x10^{-4}$	$1.06x10^{-2}$	$6.07x10^{-1}$	$4.17x10^{0}$
Cancer Risk (RISC)	$3.2x10^{-4}$	$1.3x10^{-4}$	$1.9x10^{0}$	0.00
Cancer Risk (calculated)	$3.2x10^{-4}$	$1.3x10^{-4}$	$1.9x10^{0}$	NQ
Hazard Index (RISC)	$1.7x10^{0}$	0.00	0.00	$4.1x10^{1}$
Hazard Index (calculated)	$1.7x10^{0}$	NQ	NQ	$4.1x10^{1}$

NQ- Toxicological information not available