RISK-INTEGRATED
RISC5
SOFTWARE FOR CLEAN-UPS

RISC5 User's Guide

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RISC5 User’s Guide

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INTRODUCTION

The *Risk-Integrated Software for Cleanups* version 5 (RISC5), formerly known as “BP RISC”, is designed to calculate human health and ecological risk from contaminants in the environment. It contains contaminant fate and transport models for predicting exposure point concentrations, a wide range of exposure pathways and a large chemical database with toxicological, fate and transport, and regulatory standards. RISC was developed to be a user-friendly tool that both helps teach about risk assessment for the novice user, and has fairly complex capabilities for the experienced risk assessor.

The fifth version of the RISC software, RISC5, was released publically in December 2010. This version is the culmination of a many-year upgrade process in which the software interface was reprogrammed in a new computer language to better run on the wide variety of computer configurations.

As of this writing (April 2011), there are over 1000 users of RISC worldwide. RISC has been evaluated by the UK Environment Agency (2003), the New Zealand Landcare Research Company (2002), and Europe’s Network for Industrially Contaminated Land in Europe (NICOLE), Industrial Sub-Group (Geraghty and Miller, 2004). The US State of Colorado (Oil Inspection Section) uses RISC5 internally to check all risk assessments submitted to the state by external consultants. Regulatory petroleum site managers in numerous states also use the RISC software.

BACKGROUND

In 1993, British Petroleum (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*.

While BP supported its development, there is no computed-coded bias in the software reflecting how BP feels risk assessments should be performed. All fate and transport models are externally developed, and the modules allow the user to choose how subjective issues like pathway/compound additivity, acceptable risk levels or degradation are to be handled. In fact there are no locked cells or other limitations on user inputs. The 'BP' name was dropped from the RISC title when Version 4 was released in October, 2001 to avoid any misunderstanding in this regard.

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. Paul C. Johnson provided the technical peer review of version 3 (including the Johnson and Ettinger model). In versions 4.0, and now, "RISC5" (RISC version 5), several new models were added including a plant uptake model, two vapor intrusion models that consider degradation (for petroleum hydrocarbons), a simple surface water mixing model and a simple ecological food web model. Version 4.0 was peer-reviewed by Arcadis, Geraghty and Miller in Cambridge, UK. Their review is included in Appendix R. Version 5 was tested by over 20 beta testers in two separate beta tests – the focus of the beta tests were the new interface with Excel capabilities and getting the software to work in various international settings, including those with different decimal separators and number formats from the US.

Some of the key features of the RISC5 software are::

- RISC has an intuitive graphical interface; it was developed with teaching principles of risk assessment and fate and transport as a primary goal.
- RISC allows for pathway, compound and receptor additivity both when calculating risk and in calculating clean-up levels.
- All of the fate and transport models that start with a soil source can be used in the presence of phase-separated product (Raoult's Law is considered for all soil source models).
- There is a transient vadose zone leaching model in RISC than can also be used to predict volatile emissions.
- The soil source models consider mass balance (that is, they can model depleting sources).
- The groundwater models are transient (i.e. they can handle time varying input).
- RISC includes several exposure pathways not considered in other risk assessment software (to date) such as dermal exposure and inhalation during indoor showering, irrigation pathways and surface water and sediment intake pathways (both for humans and ecological receptors).
- RISC has a large internationally derived surface water criteria and sediment criteria database for comparing modeled results with these environmental criteria.

TECHNICAL SUPPORT

The RISC5 software is supported by the primary software developer, Lynn Spence. Her details are as follows:

Phone: +01 925 846 4721
E-mail: lynnspence@RISC5.com or lynnspence@comcast.net

Tutorials (hands-on example problems) are available from www.RISC5.com (coming soon). Several FAQ documents will also be available from that web page covering various RISC5 topics.

REFERENCES

Geraghty and Miller International, Inc., 2004. Final Report of NICOLE Project to Evaluate Human Health Risk Assessment Models - Executive Summary -- Risk Assessment Comparison Study. Available from: http://www.nicole.org/documents/DocumentList.aspx?w=n&L=4, April 2004.

New Zealand Landcare Trust, Review of BP RISC. Available from http://contamsites.landcareresearch.co.nz/review_models.htm.

United Kingdom (UK) Environment Agency, 2003. Fact Sheet for RISC. Available from www.environment-agency.gov.uk, April 2003.

RISC5: Frequently Asked Questions

Are there tutorials or examples available?

Yes. There are a number of tutorials available for download (as PDFs) on the web site where RISC5 was purchased or from www.RISC5.com (coming soon).   These tutorials cover many different types of risk assessment scenarios and are designed to be worked through step-by-step in the software.

What are the system (computer) requirements?

The system requirements for RISC5 are:

- A minimum of 15MB of free hard disk space
- Windows XP/Vista/Windows 7
- A Pentium class chip
- 1024 * 768 pixel monitor minimum
- Excel 2003 or higher

RISC5 has been designed to run on an individual computer, that is, it can not be run over a network.

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Installation Instructions

To install RISC5, double-click on the file called “UIRISC5.msi”. This will start the installation process. It is highly encouraged to install the software in the default directory (i.e. under your Windows Program Files directory). If you have a previous version of RISC5 installed, you will need to uninstall it using the “Add/Remove Programs” option under Windows Control Panel.

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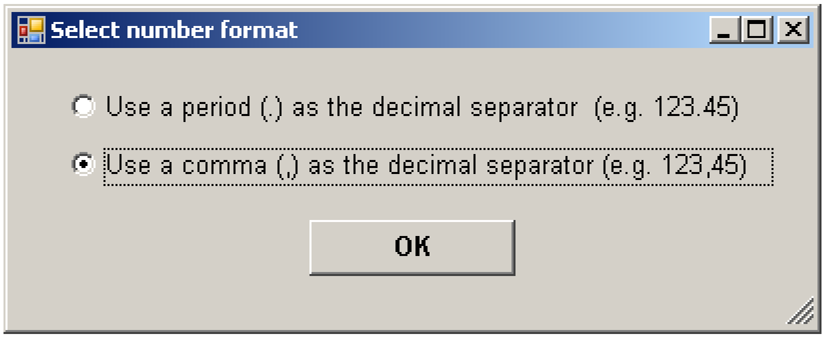
How do I use a comma (,) as a decimal separator?

Select the "Options" drop down menu from the menu bar on the main screen. Then click on "Select Number Format". This will bring up the following screen:



○ Use a period (.) as the decimal separator (e.g. 123.45)

● Use a comma (,) as the decimal separator (e.g. 123,45)

Choosing to Use Commas for Decimal Separators

Then select the comma option from the "Select number format" window.

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How many computers can I run the software on?

The license for the software is similar to Microsoft's license for Office. That is, it is licensed one per user. If you have both a desktop computer and a laptop, and the same person uses the laptop occasionally, you may ask for an additional license for the laptop computer. Note, the two computers must belong to the same user.

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How does RISC5 differ from RISC v. 4?

Installation

The RISC5 software was designed to be installed in the "C:\Program Files" directory (or equivalent directory depending on your version of Windows.) The installation will create a directory called "RISC5UserDir" under the C:\ drive. This means that the user must have permission to write to the C:\ drive. To uninstall the software, use "Add/Remove Programs" option under the Windows Control Panel.

Interface and Saved Project Files

The user interface of the RISC5 software was developed in Windows Visual Basic.Net. This version was developed in a new programming language (from the one used in previous versions of RISC) because the programming language used for RISC versions 1 through 4 is no longer supported and will not run properly under Windows 7. This means that the saved project files from version 4 will not work in RISC5.

Use of Excel for Output

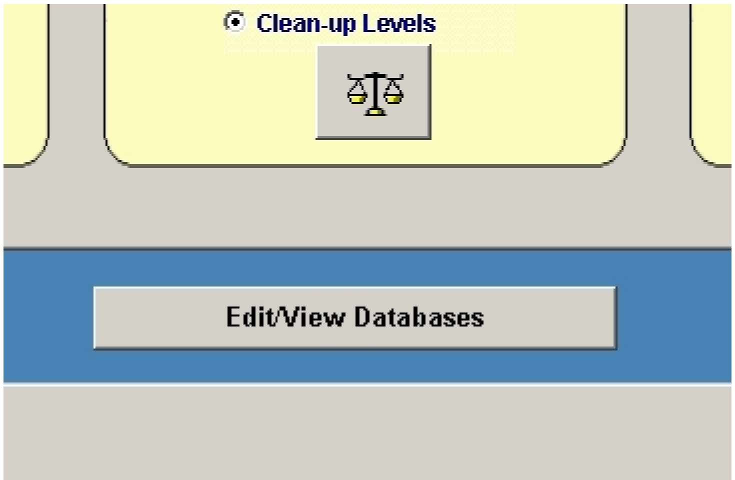
One very important new feature of the model is the use of Excel to view the model outputs, the model input summaries and to create plots of concentration vs. time. The use of Excel allows the user to easily customize the tables and charts to fit different printers and report requirements. Note, you must enable macros in Excel in order to view RISC5 results.

Master Database Editor

In RISC5, the databases and the interface to the databases have been completely redesigned in an attempt to make them easier to maintain and update. There are five main databases:

- chemical properties
- soil properties
- human receptor exposure parameters (deterministic)
- human receptor exposure parameters (Monte Carlo)
- ecological receptor exposure parameters

These databases are modified using the Master Database Editor (accessed from the bottom of the main screen of RISC5 "Edit/Modify Databases").



Accessing the Master Database Editor

You can add new profiles (such as a new receptor, a new chemical, etc.) or you may change the default values associated with the existing profiles.

The following tasks can be performed in the master database editor (accessed through "Edit/View Databases"):

- Add or remove chemicals from the database.
- Change default chemical properties permanently (rather than just changing the properties for a specific project file.)
- Add or remove receptor profiles from the database.

- Permanently change default values of exposure parameters in the receptor profiles database (rather than just modifying exposure parameters for the specific project in Step 4).
- Add or remove soil types.
- Change default soil property values permanently (rather than just in the project file).
- Add or remove ecological receptors.
- Permanently change default exposure values for the ecological receptors.

Project-Specific Data vs. Modifying the Permanent Databases

One thing that is different about the chemical database is that you may modify any of the chemical parameters used in your project from Steps 1, 3 or 4 directly. When the values are modified outside of the Master Database Editor, then the values are stored with the project file, not in the permanent databases. This allows you to evaluate sensitivity of the chemical parameter values without changing the permanent databases.

The human receptor database is new in RISC5 in that you can define your own default receptor scenarios that will then be available to choose in Step 4 (exposure). To do this, use the Master Database Editor. The same goes for soil profiles and ecological receptors (i.e. you can add new profiles for each of these).

To restore (reinstall) the original database(s) you will need to delete the Excel file containing the database that you want to replace. The Excel database files are located in “C:\RISC5UserDir\InputFiles”.

Computational Models

As in version 4, the computational models were written in FORTRAN and are run automatically by the user interface.

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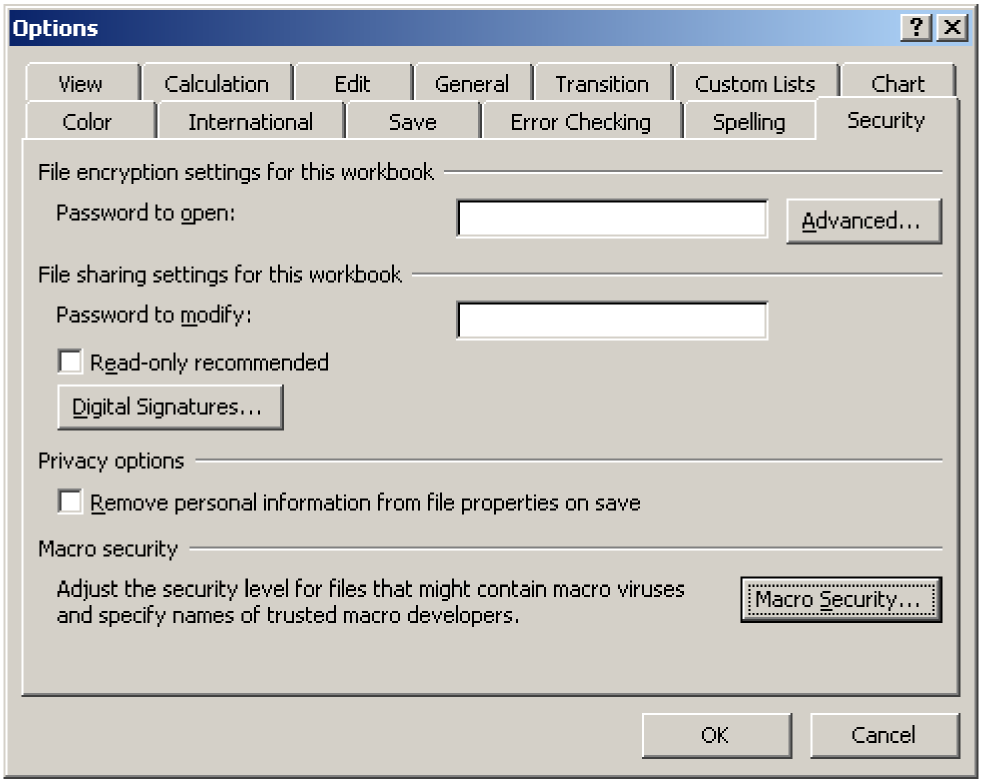
Running the Excel Macros

The Excel portions of the software use macros to display the results of the calculations. As such, the macros must be enabled on your Excel version. Usually, this involves changing the security settings to “medium”. Under Windows XP, you would select “Options” under the “Tools” menu. From the tabbed headers choose “Security”. This will bring up a screen like this:



File encryption settings for this workbook

Password to open:

File sharing settings for this workbook

Password to modify:

☐ Read-only recommended

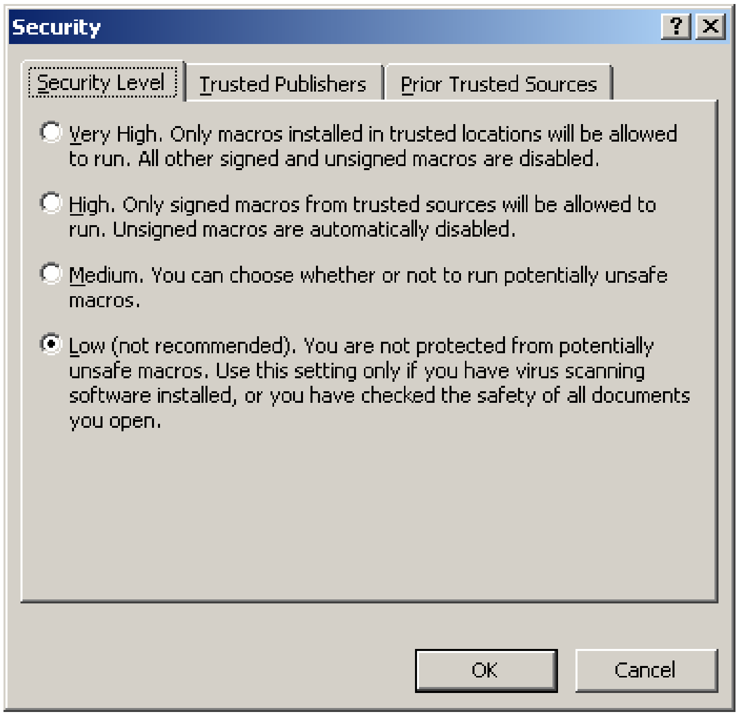
Privacy options

☐ Remove personal information from file properties on save

Macro security

Adjust the security level for files that might contain macro viruses and specify names of trusted macro developers.

Choose the “Macro Security...” button and select “Medium” or “Low” as your macro security setting as shown in the following screen shot.



○ Very High. Only macros installed in trusted locations will be allowed to run. All other signed and unsigned macros are disabled.

○ High. Only signed macros from trusted sources will be allowed to run. Unsigned macros are automatically disabled.

○ Medium. You can choose whether or not to run potentially unsafe macros.

● Low (not recommended). You are not protected from potentially unsafe macros. Use this setting only if you have virus scanning software installed, or you have checked the safety of all documents you open.

On some company intranets, the software will need to be installed in a “trusted directory”. That is, if your company computers do not allow macros to be run (or Visual Basic programs to be run) outside of a special directory, then RISC5 will need to be installed in the protected directory. Another option is to consult your IT person to help you run the software given your computer security settings.

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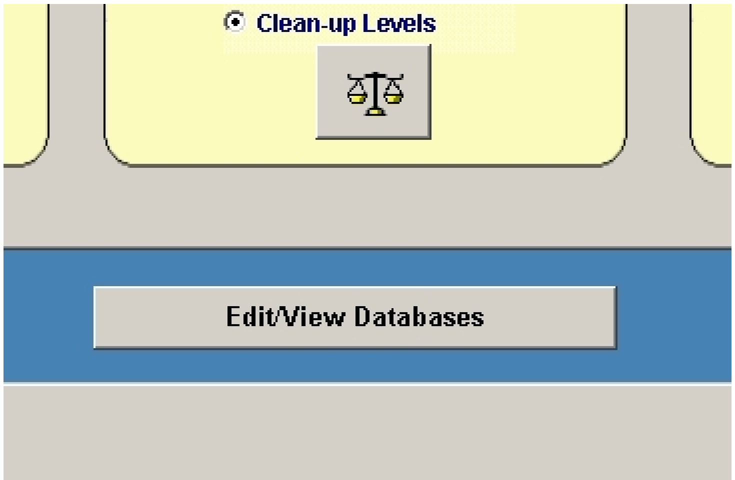
How do I add a new chemical?

New chemicals are added in the Master Database Editor.

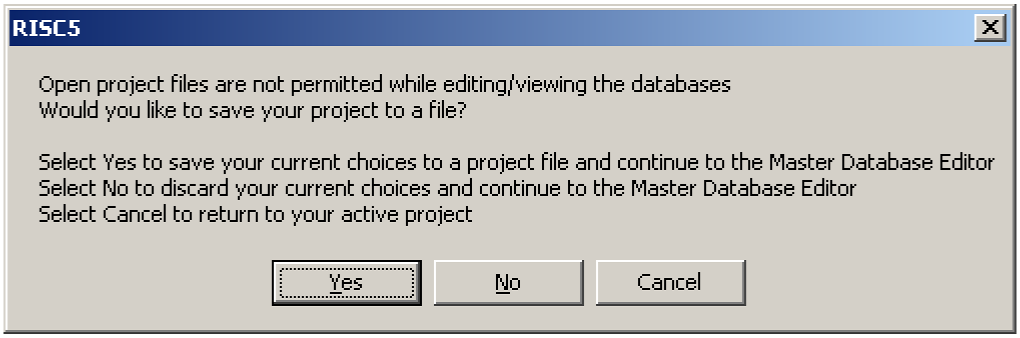
By choosing to “Edit/View Databases” you will enter the master database editor for RISC5. Note, you cannot have data entered into the software (Steps 1 through 6) when you modify (or view) the databases.

First click on the “Edit/View Databases” button from the bottom of the main screen:



Lower Part of Main Screen of RISC5

If you have data entered in any of Steps 1 through 6 at this point, you will get a dialog box that indicates you should save or cancel your entries so far:



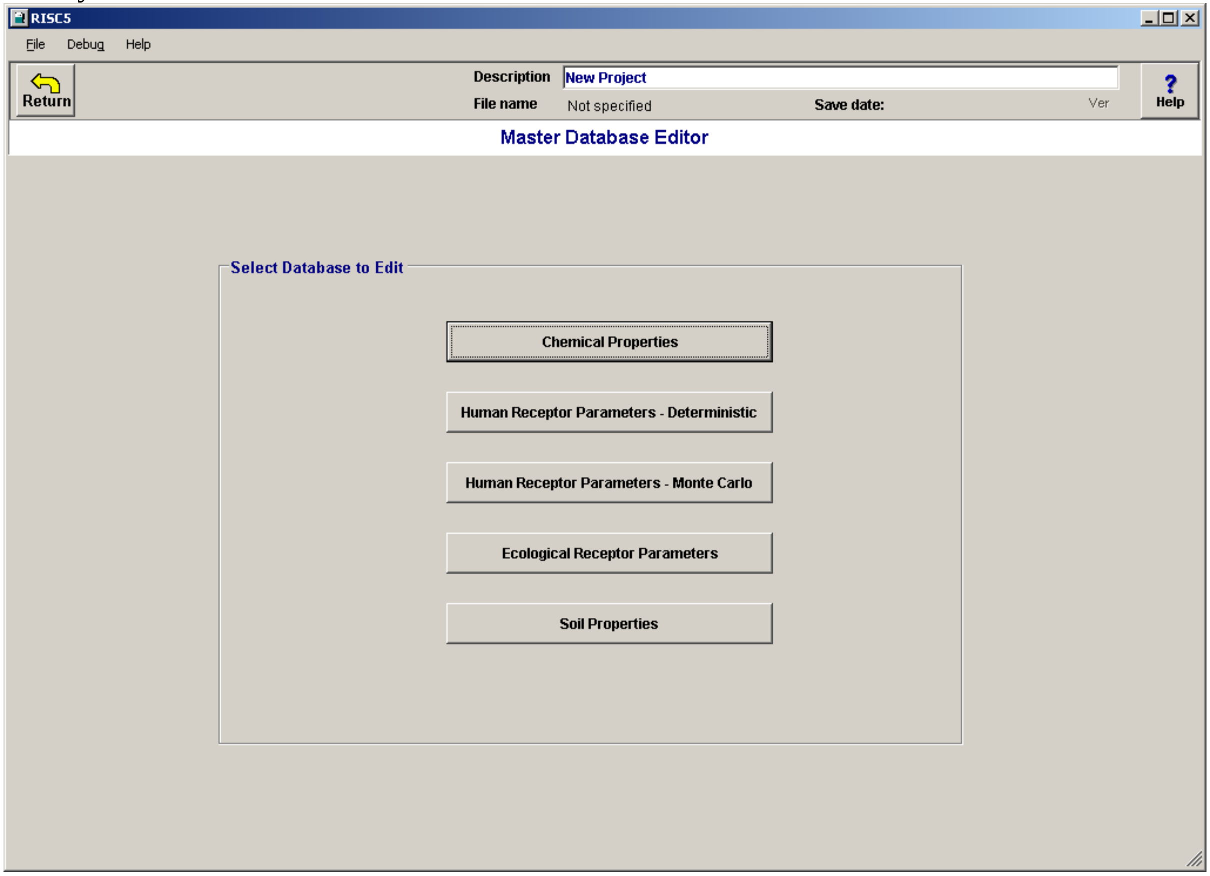
Open project files are not permitted while editing/viewing the databases
Would you like to save your project to a file?

Select Yes to save your current choices to a project file and continue to the Master Database Editor
Select No to discard your current choices and continue to the Master Database Editor
Select Cancel to return to your active project

Select “Yes” to save your data to a project file and then provide a project file name. Select “No” to discard your current data (or choices) and proceed directly to the Master Database Editor.

This section will show you how to add a chemical to the chemical database.

Then you should be at the first screen for the master database editor.

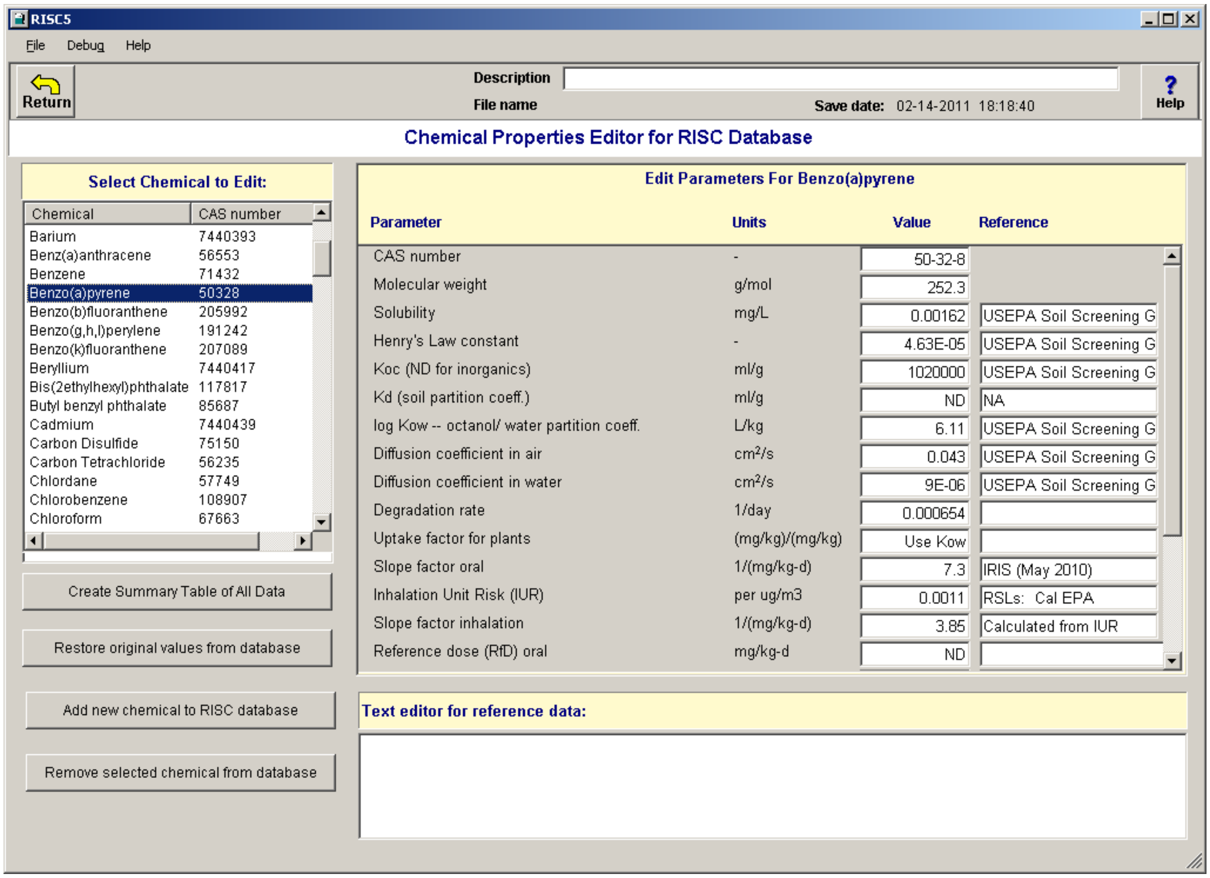


Master Database Editor

Description: New Project
File name: Not specified
Save date:

Master Database Editor Interface (Screen)

For this example (adding a new chemical to the database), select the first button, “Chemical Properties”. This will bring up the following screen:



Description:

File name

Save date: 02-14-2011 18:18:40

Chemical Properties Editor for RISC Database

Select Chemical to Edit:

Chemical	CAS number
Barium	7440393
Benz(a)anthracene	56553
Benzene	71432
Benzo(a)pyrene	50328
Benzo(b)fluoranthene	205992
Benzo(g,h,l)perylene	191242
Benzo(k)fluoranthene	207089
Beryllium	7440417
Bis(2ethylhexyl)phthalate	117817
Butyl benzyl phthalate	85687
Cadmium	7440439
Carbon Disulfide	75150
Carbon Tetrachloride	56235
Chlordane	57749
Chlorobenzene	108907
Chloroform	67663

Edit Parameters For Benzo(a)pyrene

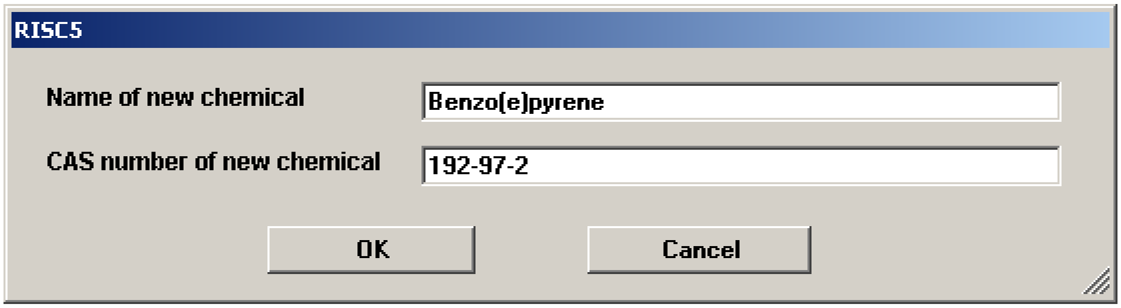
Parameter	Units	Value	Reference
CAS number	-	50-32-8	
Molecular weight	g/mol	252.3	
Solubility	mg/L	0.00162	USEPA Soil Screening G
Henry's Law constant	-	4.63E-05	USEPA Soil Screening G
Koc (ND for inorganics)	ml/g	1020000	USEPA Soil Screening G
Kd (soil partition coeff.)	ml/g	ND	NA
log Kow -- octanol/ water partition coeff.	L/kg	6.11	USEPA Soil Screening G
Diffusion coefficient in air	cm²/s	0.043	USEPA Soil Screening G
Diffusion coefficient in water	cm²/s	9E-06	USEPA Soil Screening G
Degradation rate	1/day	0.000654	
Uptake factor for plants	(mg/kg)/(mg/kg)	Use Kow	
Slope factor oral	1/(mg/kg-d)	7.3	IRIS (May 2010)
Inhalation Unit Risk (IUR)	per ug/m3	0.0011	RSLs: Cal EPA
Slope factor inhalation	1/(mg/kg-d)	3.85	Calculated from IUR
Reference dose (RfD) oral	mg/kg-d	ND	

Text editor for reference data:

The Chemical Database Editor

When you add a new chemical to the database, the software makes a copy of the chemical that you are currently viewing. The reason for this is that there are times when you might want to add a chemical that is very similar to one already in the database. It is important that you change the chemical parameters for the new chemical for those properties that are different than the original chemical.

For this example, we will be adding the chemical "Benzo(e)pyrene" (a Polyaromatic Hydrocarbon [PAH] that is not currently in the database). Click on the button called "Add new chemical to RISC database" and enter the new chemical name and its Chemical Abstract Number (CAS).

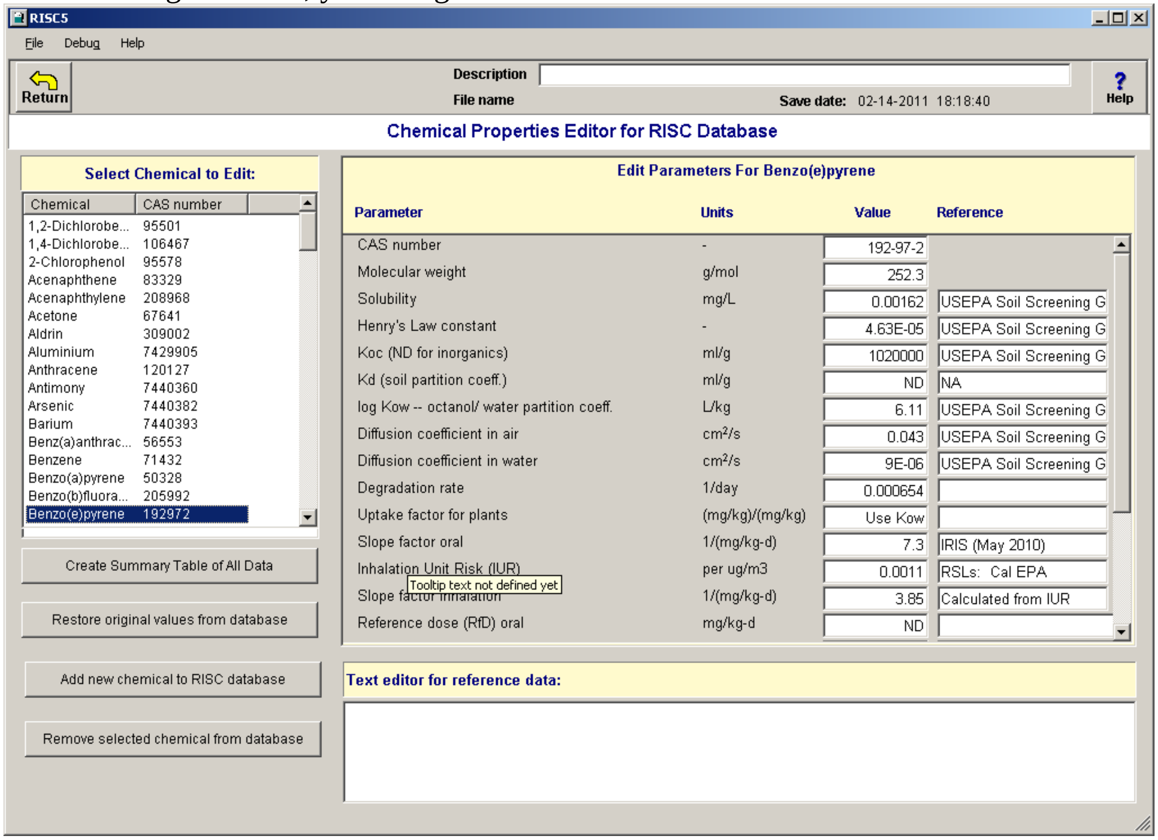


Name of new chemical: Benzo(e)pyrene

CAS number of new chemical: 192-97-2

Adding a New Chemical

After clicking on “OK”, you will get this screen:



Chemical	CAS number
1,2-Dichlorobe...	95501
1,4-Dichlorobe...	106467
2-Chlorophenol	95578
Acenaphthene	83329
Acenaphthylene	208968
Acetone	67641
Aldrin	309002
Aluminium	7429905
Anthracene	120127
Antimony	7440360
Arsenic	7440382
Barium	7440393
Benz(a)anthrac...	56553
Benzene	71432
Benzo(a)pyrene	50328
Benzo(b)fluora...	205992
Benzo(e)pyrene	192972

Edit Parameters For Benzo(e)pyrene

Parameter	Units	Value	Reference
CAS number	-	192-97-2	
Molecular weight	g/mol	252.3	
Solubility	mg/L	0.00162	USEPA Soil Screening G
Henry's Law constant	-	4.63E-05	USEPA Soil Screening G
Koc (ND for inorganics)	ml/g	1020000	USEPA Soil Screening G
Kd (soil partition coeff.)	ml/g	ND	NA
log Kow -- octanol/ water partition coeff.	L/kg	6.11	USEPA Soil Screening G
Diffusion coefficient in air	cm^2/s	0.043	USEPA Soil Screening G
Diffusion coefficient in water	cm^2/s	9E-06	USEPA Soil Screening G
Degradation rate	1/day	0.000654	
Uptake factor for plants	(mg/kg)/(mg/kg)	Use Kow	
Slope factor oral	1/(mg/kg-d)	7.3	IRIS (May 2010)
Inhalation Unit Risk (IUR)	per ug/m3	0.0011	RSLs: Cal EPA
Slope factor inhalation	1/(mg/kg-d)	3.85	Calculated from IUR
Reference dose (RfD) oral	mg/kg-d	ND	

Chemical Properties for the New Chemical

Note, all of the chemical properties, with the exception of the CAS number, have been copied from benzo(a)pyrene. Now, you need to modify the chemical parameters for benzo(e)pyrene to be appropriate for that chemical (rather than benzo(a)pyrene). Use the “Reference” column to add a description of the source reference for the chemical property. When you click on one of the reference boxes, the contents of the box will be displayed in the “Text editor for reference data” box. This is to provide more room to enter the reference information, if necessary.

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How do I restore the original database(s)?

You **can not** restore the original databases by reinstalling RISC5. The reason for this is that, occasionally, there may be updates to the software that need to be installed. When these updates are installed it is important to not overwrite any of the databases that the user may have modified.

The “C:\RISC5UserDir” contains a sub folder called “InputFiles”. This is where the Excel files containing the RISC 5 databases are located. There are four database files, as follows:

1. Chemical database: “*RISC Chemical DB.xls*”
2. Human receptor database: “*Human receptor database.xls*”
3. Soil properties database: “*Soil properties database.xls*”

4. Ecological (food web) receptor database: "*Eco receptor calculations.xls*"

If you would like to restore one or all of the original databases that were shipped with RISC5, you must delete the appropriate Excel file from the C:\RISC5UserDir\InputFiles directory. You do not need to reinstall the software. Then when you run the software, it will detect a missing database and will copy the original database file into the InputFiles directory.

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What is the RISC5UserDir (located on my C:\ drive)?

The installation of the software will create a directory on your C: drive called "RISC5UserDir" which will contain three sub-directories. These are "For_temp", "InputFiles", and "Project Files". The "For_temp" directory is used to save interim model results that are used by the software to generate the Excel output. The "Project Files" directory is the default location used by RISC5 to save project files to. You may save the project files in other locations, however.

The "InputFiles" directory is used to store the system databases (as Excel files) that the user may edit using the interface in RISC5. These databases are (1) the chemical database, (2) the human receptors database (of exposure parameters), (3) the soil properties database, and (4) the ecological receptors database. These files are kept separate from the installed software (under "Program Files") because it is anticipated that the user may modify the databases and would like to retain those changes even if a software update is installed.

If you would like to reinstall the default databases supplied with the software, you should delete the Excel files in the "C:\RISC5UserDir\InputFiles". When you run RISC5, the software will automatically copy the databases from "Program Files" to the user directory.

It is highly recommended that you do not edit the Excel files in this directory directly. That is, if you would like to change some of the defaults permanently, the databases should be modified through the RISC5 interface (specifically from the Master Database Editor). The spreadsheet files have not been protected, however, so you are free to view them and print out sheets if you like. Do not modify any rows or columns in these files. It is suggested that you make a copy of the Excel spreadsheet before viewing them.

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1.0

Overview and Getting Started

1.1 INTRODUCTION

Risk-Integrated Software for Cleanups, version 5, (RISC5) was been developed to assist in the evaluation of potential human health risks from contaminated sites. RISC5 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 a simple ecological food web model, risk from particulate emissions, and volatilization to indoor air using user-specified attenuation factors. The software contains vadose zone, saturated zone, and air fate and transport models for estimating receptor point concentrations.

There are at least five broad applications for the RISC5 software. RISC5 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, (4) evaluate potential ecological impacts to surface water and sediment, and (5) evaluate ecological risk at a screening model level. These five different applications are discussed in the following sections.

1.1.1 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 RISC5 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 (or by using a “Tier 1 spreadsheet” to screen out chemicals [see “Risk-Based Clean-up Levels”]). 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 RISC5 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 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 RISC5 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.

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.

1.1.3 Fate and Transport Modeling

The fate and transport models in RISC5 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 also simulate degradation and three-dimensional dispersion. These type of models are generally 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 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?
- 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.

RISC5 includes the following embedded chemical fate and transport models:

- Unsaturated Zone Model for leaching from vadose zone soil source to groundwater;
- Groundwater Model for dispersion, advection, retardation and degradation of groundwater as it moves in an aquifer;
- Saturated Soil Source Model for modeling a soil source (such as non-aqueous phase liquid, NAPL) at the water table impacting groundwater;
- Vapor Emission Models (3) from soil to outdoor and indoor air (including models considering biodegradation);
- Vapor Emission Model from groundwater to indoor air; and
- Sediment Partitioning and Surface Water Mixing Model that can be linked with the groundwater model;
- Outdoor Air Model to estimate concentrations in outdoor air due to volatilization from soil or groundwater; and
- Particulate Emissions Model to estimate concentrations in outdoor air due to volatilization from soil or groundwater and soil particulates in the air.

The models listed above may be linked together in a risk analysis. 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 at a point downgradient of the source.

1.1.4 Surface Water and Sediment Quality Criteria

RISC5 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 RISC5, potential surface water concentrations can be estimated using the models and then the concentrations can be compared with the criteria listed above.

1.1.5 Screening Level Ecological Risk Assessment

RISC5 has the option to perform a screening level ecological risk assessment using a food web model. The model can be run for aquatic or for terrestrial environments. Standard ecological wildlife receptors (from USEPA guidance) have been included in the model and the user has the option to add new receptors, if desired.

1.2 OVERVIEW OF FEATURES

The RISC5 software includes many features to assist in performing and presenting risk assessments or the results of fate and transport models. RISC5 allows the user to:

- Choose chemicals of concern from a standard library of 128 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 human exposure scenarios (with up to seventeen 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;
- Print or save tables, charts, and figures.

New features that were included in Version 4.0 of RISC5 included:

- 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).

New features in Version 5 of RISC include:

- Tables and charts of model results are displayed directly in Excel for easier printing and incorporation in risk assessment reports;
- Expanded chemical database, including the references for all chemical property values;

- Saved project file names may exceed 8 characters;
- A particulate emission (dust emissions) model has been added;
- An updated vegetable uptake model based on Trapp and Mathis ();
- For volatilization to outdoor air from soil, the soil source term is allowed to deplete over time, if desired; and
- Default receptor profiles may be added, or modified, by the user.
- Screening level food web model for evaluating ecological risk;

1.3 ORGANIZATION AND SCOPE OF THIS REPORT

This User's Guide gives instructions on how to use RISC5 and presents the equations used to estimate risk. The Technical Background Document (the appendices) present the technical details including the fate and transport models, the databases, and outside review of the software.

The organization of this User’s Guide mimics the organization and flow of the RISC5 software. Chapter 2 guides the user through software installation, system requirements, and general operating instructions. Chapters 3 through 8 discuss the six main steps (shown on the Main Menu) showing how the software can be used to perform risk assessment calculations and determine cleanup levels.

2.0

Getting Started

2.1 OVERVIEW AND SYSTEM REQUIREMENTS

The system requirements for RISC5 are:

- A minimum of 15MB of free hard disk space
- Windows XP/Vista/Windows 7 or higher
- A Pentium class chip
- 1024 * 768 pixel monitor minimum
- Excel 2003 or higher

The user interface of the RISC5 software was developed in Windows Visual Basic.Net. This version was developed in a new programming language (from the one used in previous versions of RISC) because the programming language used for RISC versions 1 through 4 is no longer supported and will not run properly under Windows 7. This means that the saved project files from version 4 will not work in RISC5.

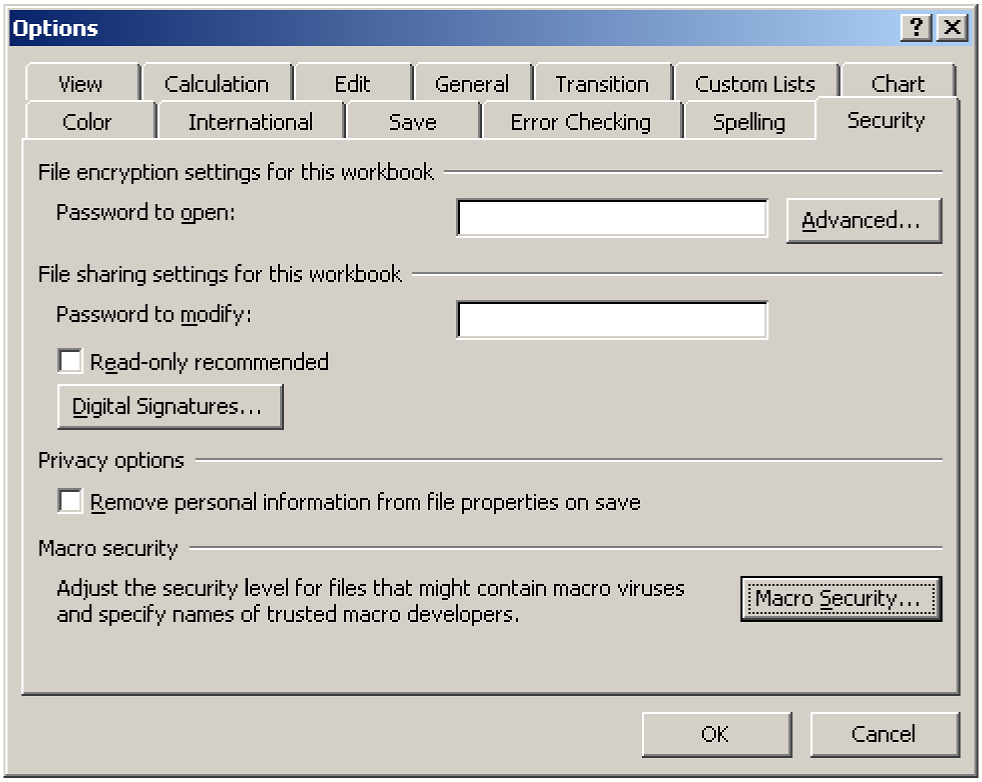
As in version 4, the computational models were written in FORTRAN and are run automatically by the user interface. One very important new feature of the model is the use of Excel to view the model outputs, the model input summaries and to create plots of concentration vs. time. The use of Excel allows the user to easily customize the tables and charts to fit different printers and report requirements.

2.2 INSTALLATION INSTRUCTIONS

To install RISC5, double-click on the file called “UIRISC5.msi”. This will start the installation process. It is highly encouraged to install the software in the default directory (i.e. under your Windows Program Files directory). If you have a previous version of RISC5 installed, you will need to uninstall it using the “Add/Remove Programs” option under Windows Control Panel.

2.2.1 Running the Excel Macros

RISC5 has been designed to run on an individual computer, that is, it can not be run over a network. The Excel portions of the software use macros to display the results of the calculations. As such, the macros must be enabled on your Excel version. Usually, this involves changing the security settings to “medium”. Under Windows XP, you would select “Options” under the “Tools” menu. From the tabbed headers choose “Security”. This will bring up a screen like this:



File encryption settings for this workbook

Password to open:

File sharing settings for this workbook

Password to modify:

☐ Read-only recommended

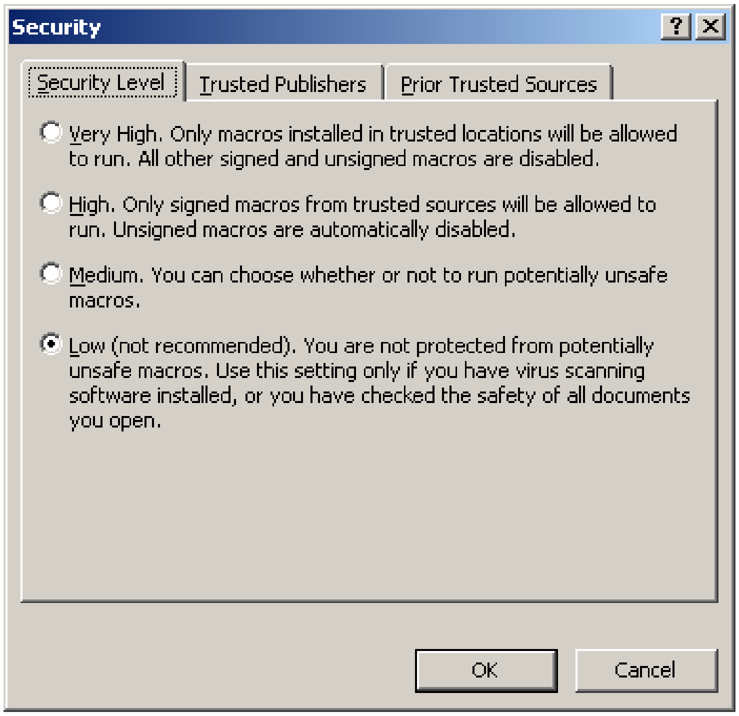
Privacy options

☐ Remove personal information from file properties on save

Macro security

Adjust the security level for files that might contain macro viruses and specify names of trusted macro developers.

Choose the “Macro Security...” button and select “Medium” or “Low” as your macro security setting as shown in the following screen shot.



○ Very High. Only macros installed in trusted locations will be allowed to run. All other signed and unsigned macros are disabled.

○ High. Only signed macros from trusted sources will be allowed to run. Unsigned macros are automatically disabled.

○ Medium. You can choose whether or not to run potentially unsafe macros.

● Low (not recommended). You are not protected from potentially unsafe macros. Use this setting only if you have virus scanning software installed, or you have checked the safety of all documents you open.

On some company intranets, the software will need to be installed in a “trusted directory”. That is, if your company computers do not allow macros to be run (or Visual Basic programs to be run) outside of a special directory, then RISC5 will need to be installed in the protected directory. Another option is to consult your IT person to help you run the software given your computer security settings.

2.2.2 RISC5 User Directory

The installation of the software will create a directory on your C: drive called “RISC5UserDir” which will contain three sub-directories. These are “For_temp”, “InputFiles”, and “Project Files”. The “For_temp” directory is used to save interim model results that are used by the software to generate the Excel output. The “Project Files” directory is the default location used by RISC5 to save project files to. You may save the project files in other locations, however.

The “InputFiles” directory is used to store the system databases (as Excel files) that the user may edit using the interface in RISC5. These databases are (1) the chemical database, (2) the human receptors database (of exposure parameters), (3) the soil properties database, and (4) the ecological receptors database. These files are kept separate from the installed software (under “Program Files”) because it is anticipated that the user may modify the databases and would like to retain those changes even if a software update is installed.

If you would like to reinstall the default databases supplied with the software, you should delete the Excel files in the “C:\RISC5UserDir\InputFiles”. When you run RISC5, the software will automatically copy the databases from “Program Files” to the user directory.

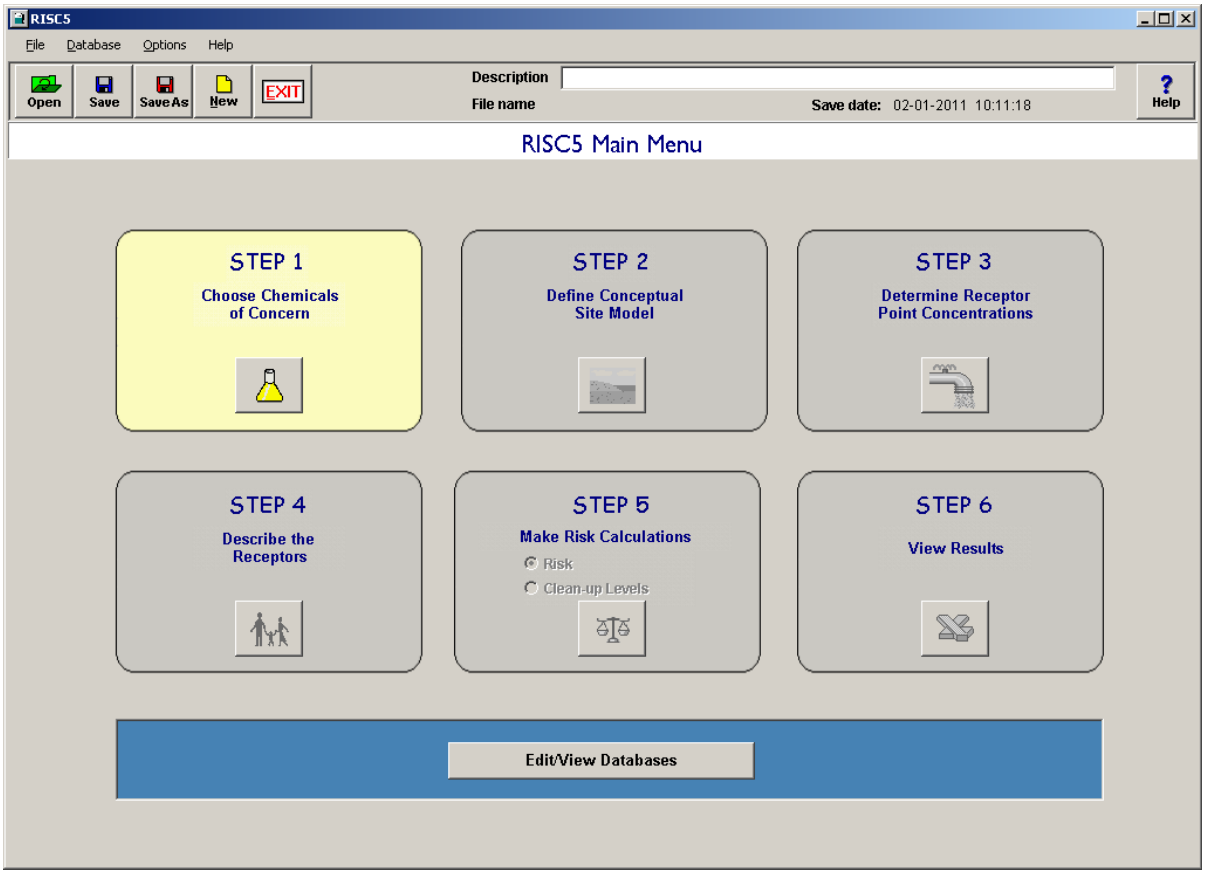
It is highly recommended that you do not edit the Excel files in this directory directly. That is, if you would like to change some of the defaults permanently, the databases should be modified through the RISC5 interface (specifically the database editor).

2.3 GENERAL INSTRUCTIONS (HOW TO USE RISC)

To start RISC5, either double-click on the “RISC5” icon on the Windows desktop or use the “Start” button and then choose “RISC5”. The user is encouraged to start the software and use it while reading the instructions in this chapter.

2.3.1 Main Screen Layout

The main screen of RISC5 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 “Edit/View Databases” button (at the bottom of the screen) is used to change default values in the softwares databases.



Save date: 02-01-2011 10:11:18

● Risk
○ Clean-up Levels

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.

2.3.1.2 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.

2.3.1.3 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. The project file name will be shown on the top tool bar along with the time and date that the file was saved last.

SaveAs

2.3.1.4 Save As

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

2.3.1.5 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

2.3.1.6 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.

? Help

2.3.1.7 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.

2.4 EDIT/VIEW DATABASES

To modify or view any of the RISC5 databases, choose to “Edit/View Databases” (from the bottom center of the main screen).

This will open the "Master Database Editor." Note, you cannot have project data entered or have an open project file when you modify (or view) the databases. If you do have data entered, the software will ask you if you would like to save your project file before continuing.

The following tasks can be performed in the master database editor (accessed through "Edit/View Databases"):

- Add or remove chemicals (permanently) from the database.
- Change default chemical properties permanently (rather than just changing the properties for a specific project file.)
- Add or remove receptor profiles (permanently) from the database.
- Permanently change default values of exposure parameters in the receptor profiles database.
- Add or remove soil types.
- Change default soil property values permanently (rather than just in the project file).
- Add or remove ecological receptors.
- Permanently change default exposure values for the ecological receptors.

2.5 RESTORING ORIGINAL DATABASE(S)

You **can not** restore the original databases by reinstalling RISC5. The reason for this is that, occasionally, there may be updates to the software that need to be installed. When these updates are installed it is important to not overwrite any of the databases that the user may have modified.

The "C:\RISC5UserDir" contains a sub folder called "InputFiles". This is where the Excel files containing the RISC 5 databases are located. There are four database files, as follows:

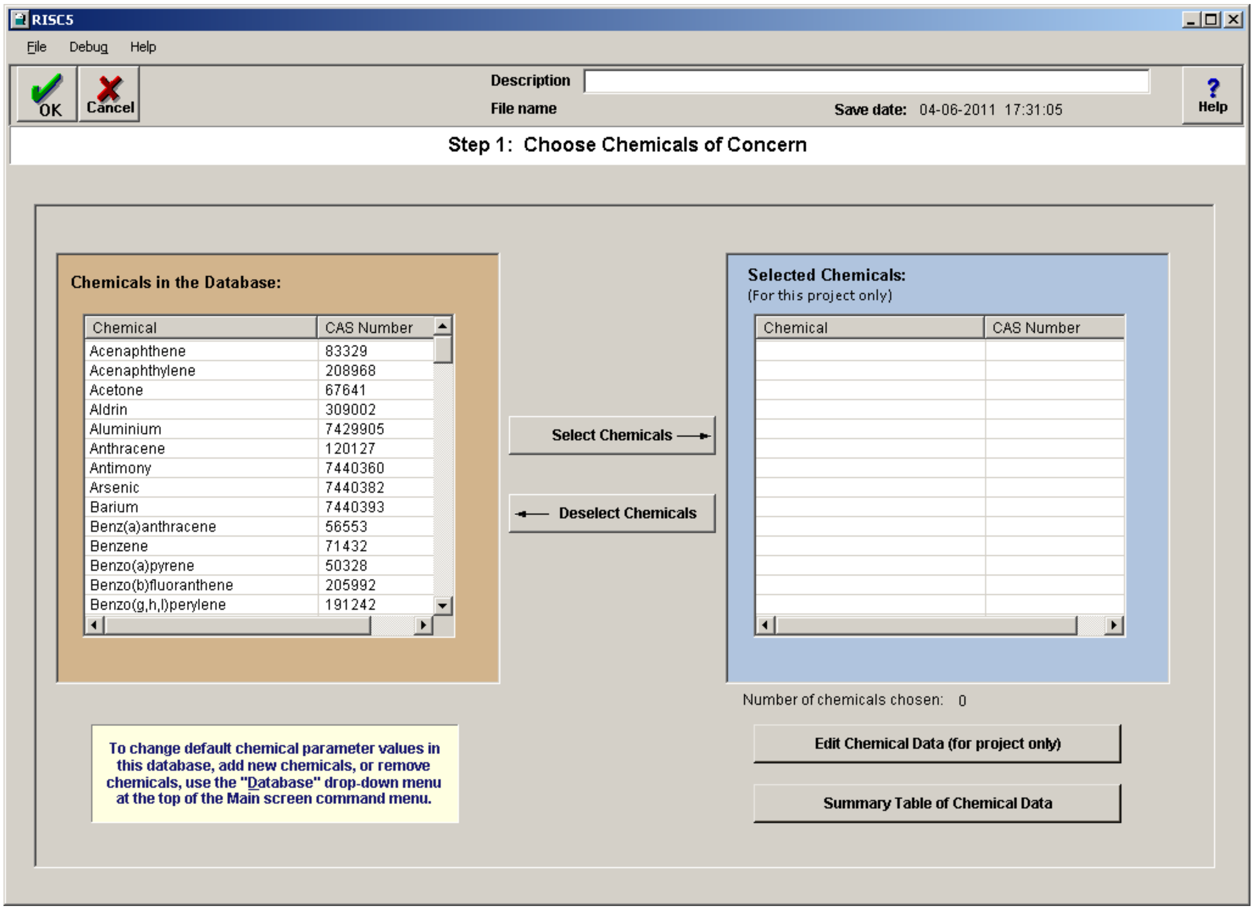
1. Chemical database: "*RISC Chemical DB.xls*"
2. Human receptor database: "*Human receptor database.xls*"
3. Soil properties database: "*Soil properties database.xls*"
4. Ecological (food web) receptor database: "*Eco receptor calculations.xls*"

If you would like to restore one or all of the original databases that were shipped with RISC5, you must delete the appropriate Excel file from the C:\RISC5UserDir\InputFiles directory. You do not need to reinstall the software. Then when you run the software, it will detect a missing database and will copy the original database file into the "InputFiles" directory.

3.0

Step 1:
Choose Chemicals of Concern

In step 1, users identify chemicals that are of concern for their analysis. The RISC software contains a database with 128 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.



Save date: 04-06-2011 17:31:05

Chemicals in the Database:

Chemical	CAS Number
Acenaphthene	83329
Acenaphthylene	208968
Acetone	67641
Aldrin	309002
Aluminium	7429905
Anthracene	120127
Antimony	7440360
Arsenic	7440382
Barium	7440393
Benz(a)anthracene	56553
Benzene	71432
Benzo(a)pyrene	50328
Benzo(b)fluoranthene	205992
Benzo(g,h,l)perylene	191242

Selected Chemicals:
(For this project only)

Chemical	CAS Number

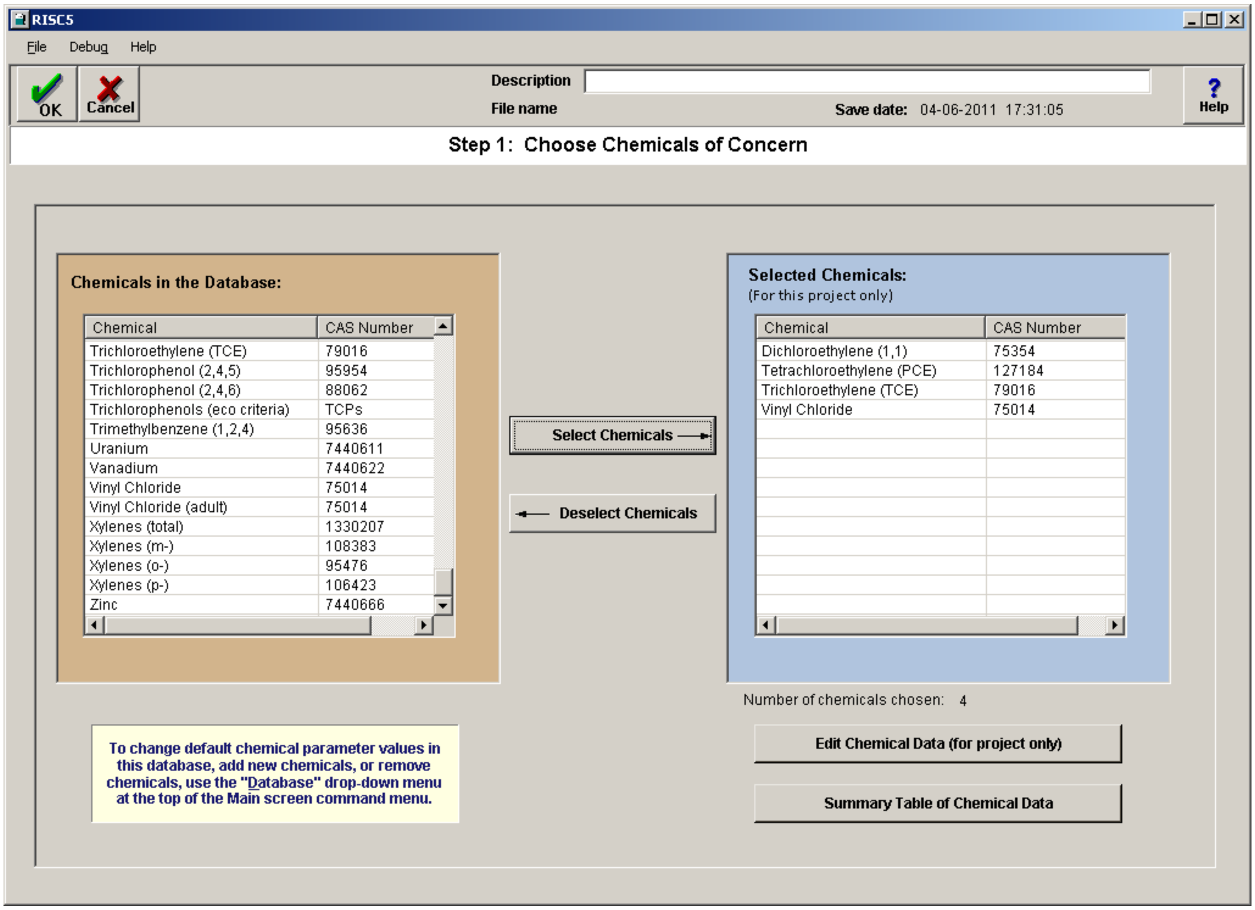
Number of chemicals chosen: 0

To change default chemical parameter values in this database, add new chemicals, or remove chemicals, use the "Database" drop-down menu at the top of the Main screen command menu.

FIGURE 3-1. Chemical Selection Screen

3.1 SELECTING CHEMICALS OF CONCERN

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

File name

Save date: 04-06-2011 17:31:05

Step 1: Choose Chemicals of Concern

Chemicals in the Database:

Chemical	CAS Number
Trichloroethylene (TCE)	79016
Trichlorophenol (2,4,5)	95954
Trichlorophenol (2,4,6)	88062
Trichlorophenols (eco criteria)	TCPs
Trimethylbenzene (1,2,4)	95636
Uranium	7440611
Vanadium	7440622
Vinyl Chloride	75014
Vinyl Chloride (adult)	75014
Xylenes (total)	1330207
Xylenes (m-)	108383
Xylenes (o-)	95476
Xylenes (p-)	106423
Zinc	7440666

Selected Chemicals:
(For this project only)

Chemical	CAS Number
Dichloroethylene (1,1)	75354
Tetrachloroethylene (PCE)	127184
Trichloroethylene (TCE)	79016
Vinyl Chloride	75014

Number of chemicals chosen: 4

To change default chemical parameter values in this database, add new chemicals, or remove chemicals, use the "Database" drop-down menu at the top of the Main screen command menu.

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 50.

3.2 EDIT CHEMICAL DATA

In Step 1, the user may modify the chemical data for the current project. There are times when a user may need to use different toxicity parameters than are in the master database, however they do not want to modify the default chemical parameters. In this case, the chemical parameters may be modified in Step 1. The toxicity parameters may also be modified in Step 4c and the fate and transport properties may be modified in Step 3c. All of these processes are equivalent. For example, if the oral slope factor is changed in Step 1, when the user reaches Step 4c (project-specific chemical toxicity data), the change will be shown. Alternatively, the user can choose to change the toxicity factor in Step 4c and the change will be shown in Step 1. The difference between these two options is that in Step 1, all of the chemical parameter values can be viewed or edited. In Steps 3c and 4c, only the chemical parameters that are needed for the current scenario (chosen in Step 2) will be shown.

This will not modify or affect the master chemical database. Any changes made in Step 1 are retained for the project only. To modify the chemical parameters permanently, i.e. to update the values that will be used for defaults, the master chemical database editor is used. This is discussed in *RISC5 Frequently Asked Questions* at the beginning of this manual.

3.3 VIEW SUMMARY TABLE OF CHEMICAL DATA

By choosing this button (on the lower right of the Step 1 screen), an Excel table is created with the chemicals that have been selected. There will be two sheets in the table. One sheet contains the chemical data in a simple table, the other sheet contains all of the references for the chemical parameters. Note, this step just summarizes the chemicals of concern, to view the entire chemical database, go to the *Master Database Editor* (see *RISC5 Frequently Asked Questions* at the beginning of this manual.

4.0

Step 2:
Define Initial
Conceptual Site Model

4.1 CONCEPTUAL SITE MODEL (CSM)

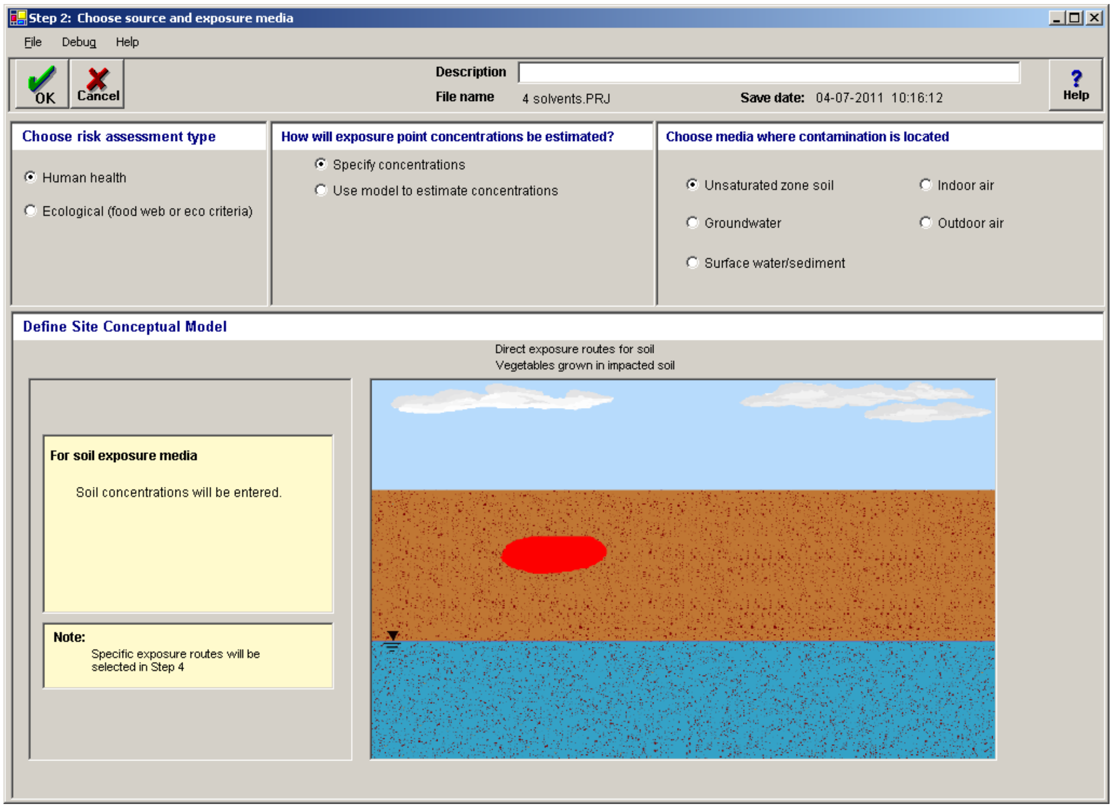
Conceptual site models (CSMs) are used to describe the location of the contaminated media, any potential transport pathways, location of exposure points and types of receptors and exposure pathways that could occur. In Step 2, the user will be asked to define the location of the contaminated media and potential fate and transport pathways to be considered for the risk scenario being evaluated. This is the first part of the CSM. The second part of the CSM is defined in Step 4 where the exposure pathways (such as ingestion of water and dermal contact with soil) and types of receptors to be evaluated will be chosen.

In Step 2 the user first choose whether to evaluate human or ecological risk. Next, the user will choose the location of contaminated media, the location of the exposure point(s), and the fate and transport models to be used (if any) to estimate receptor point concentrations.

RISC5 is set up so that a single source media (contaminated media) is evaluated at one time. There may, however, be a number of different exposure routes that could potentially occur as a result of contaminant transfer or transport. For example, if the source is "unsaturated zone soil," this source media may be contacted directly by a receptor (for dermal and ingestion exposure pathways), the contaminants may leach to groundwater and then onsite groundwater may be ingested, and/or the contaminants may volatilize to outdoor air and be inhaled.

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.

Figure 4-1 shows the initial setup of the Step 2 screen.



Description

File name 4 solvents.PRJ

Save date: 04-07-2011 10:16:12

Choose risk assessment type

● Human health
○ Ecological (food web or eco criteria)

How will exposure point concentrations be estimated?

● Specify concentrations
○ Use model to estimate concentrations

Choose media where contamination is located

● Unsaturated zone soil
○ Indoor air
○ Groundwater
○ Outdoor air
○ Surface water/sediment

Define Site Conceptual Model

Direct exposure routes for soil
Vegetables grown in impacted soil

For soil exposure media

Soil concentrations will be entered.

Note:
Specific exposure routes will be selected in Step 4

Figure 4-1. Step 2 Initial Screen

The first choice to be made (top left panel) is whether to evaluate human health risk or ecological risk. Next, for both the human and ecological options, the choice is made of whether or not to use a model to estimate receptor point concentrations.

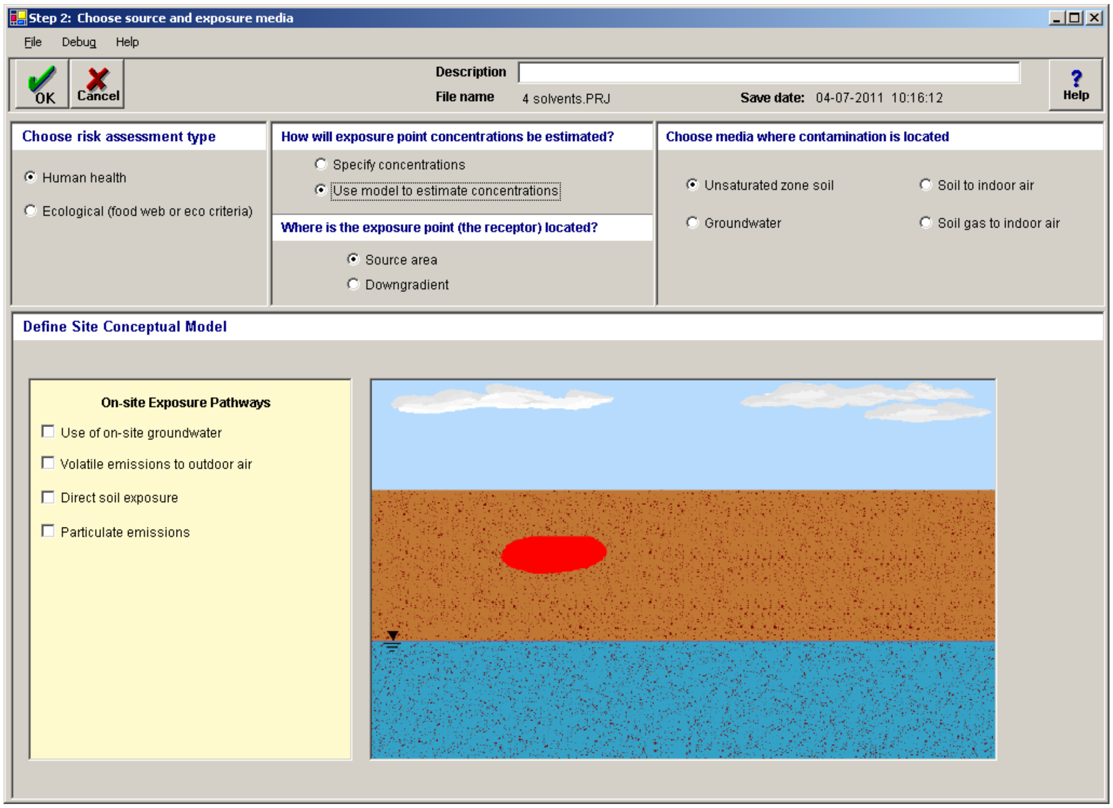
4.2 HUMAN HEALTH RISK ASSESSMENT

4.2.1 Directly Specify Exposure Point Concentrations

For the human health option (top left panel), if the user selects “Specify concentrations”, then one of five contaminated medium may be selected (top right panel). When the “specify concentrations” option is chosen, the exposure point concentrations will be need to be specified directly by the user in Step 3, i.e., the “source” media (for purposes of the risk evaluation) and exposure point media are assumed to be the same.

4.2.1 Use Model to Estimate Exposure Point Concentrations

If the choice to use fate and transport models is made (top center panel), then the options for source media change slightly. Figure 4-2 shows the Step 2 Screen for a human health evaluation using fate and transport models.



Description

File name 4 solvents.PRJ

Save date: 04-07-2011 10:16:12

Choose risk assessment type

● Human health
○ Ecological (food web or eco criteria)

How will exposure point concentrations be estimated?

○ Specify concentrations
● Use model to estimate concentrations

Where is the exposure point (the receptor) located?

● Source area
○ Downgradient

Choose media where contamination is located

● Unsaturated zone soil
○ Soil to indoor air
○ Groundwater
○ Soil gas to indoor air

Define Site Conceptual Model

On-site Exposure Pathways

☐ Use of on-site groundwater
☐ Volatile emissions to outdoor air
☐ Direct soil exposure
☐ Particulate emissions

Figure 4-2. Step 2 Screen for Human Health Evaluation Using Fate and Transport Models.

The exposure point may be located at the source area (e.g. onsite) or downgradient from the source area. If there are potential exposure pathways for both onsite and downgradient then the two scenarios will be evaluated separately.

With the modeling option, there are four potential source media: unsaturated zone soil, groundwater, soil to indoor air and soil gas to indoor air. The unsaturated zone source and soil to indoor air source are considered separately because the conditions in the unsaturated zone are expected to be different for these two scenarios. That is, for the soil to indoor air scenario, the saturated zone is assumed to not be subject to infiltration (i.e. the soil to indoor air models do not consider infiltration and leaching to groundwater.)

There are a few assumptions and/or limitations for a given analysis:

- The exposure location are assumed to be either at the source area (onsite), or downgradient, but not both for a single scenario. Both of these options (onsite and downgradient) may involve using a fate and transport model to estimate exposure point concentrations. For example, for a source area exposure location, the exposure points may include the unsaturated zone soil and outdoor air impacted by volatile emissions.
- 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 (downgradient well location) are used as the “source term” for the vapor model.

- Exposure from vegetable ingestion can be evaluated for surface soil or for groundwater but not from both during the same analysis.
- Indoor air concentrations may be estimated using one of three vapor intrusion models. The source for these models may be soil, groundwater or soil gas. Only one source is considered at a time. For example, if both the unsaturated zone and groundwater are impacted with contamination, and soil gas data is available, then it should be assumed that the soil gas is the appropriate source since it is assumed to account for the contribution from groundwater already. Similarly, soil concentration data (if available) is assumed to account for the contribution from groundwater. However, it should be noted that soil data can be “spotty” and the best source term to use for the volatilization to indoor air models is soil gas concentrations.

Use of the fate and transport models is described in more detail in Chapter 5 (Step 3: Determine Receptor Point Concentrations) and the equations and assumptions of the models are detailed in the Appendices.

4.3 ECOLOGICAL RISK ASSESSMENT

The ecological food web model is presented in Appendix T. Setting up the ecological risk assessment in Step 2 will be forthcoming in the next User’s Guide revision.

5.0

Step 3.0: Determine Receptor Point Concentrations

The third step in RISC5 is to determine receptor point concentrations for the various exposure media identified in Step 2. The Step 3 interface will appear differently depending on the choices made in Step 2. There are two methods available for “determining” receptor point concentrations: the user can enter receptor point concentrations directly, or fate and transport models can be used to estimate the receptor point concentrations. The method(s) to be used in Step 3 are determined by the choices made in Step 2. This chapter will describe how to use both the direct option and the modeling options for estimating receptor point concentrations.

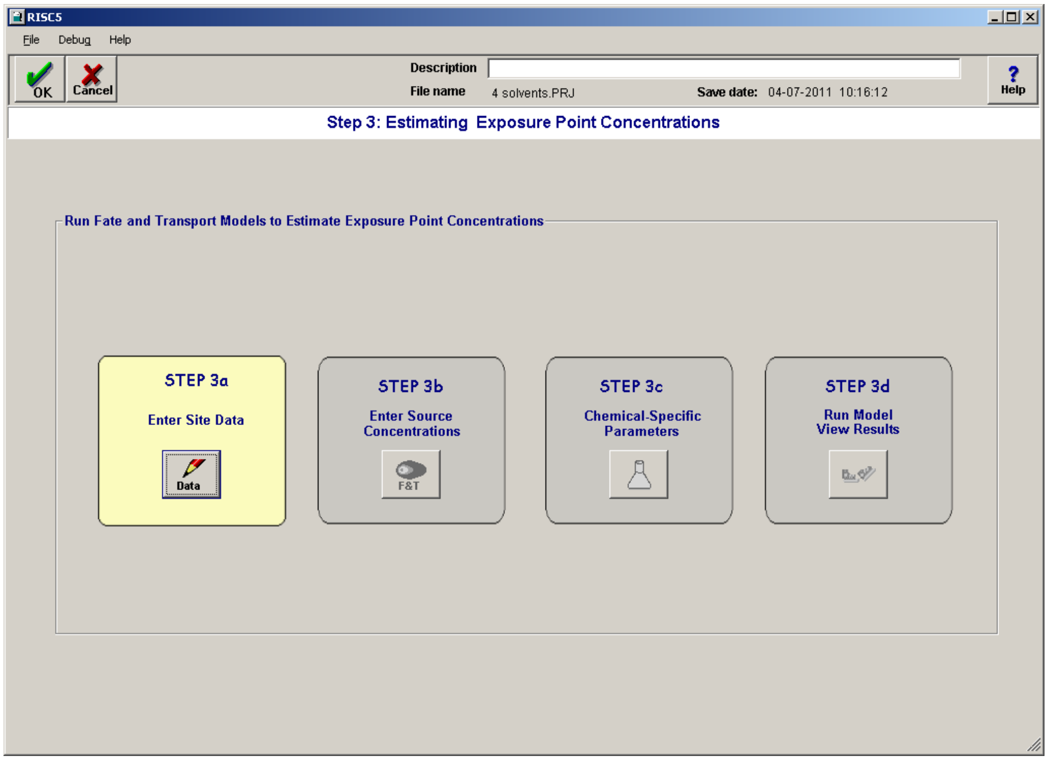
5.1 USER-SPECIFIED CONCENTRATIONS

Receptor point concentrations can be specified directly by the user (as opposed to using fate and transport models) for any receptor media. The concentration values entered here will only be used for ingestion of soil, dermal contact with soil, and/or vegetable ingestion exposure pathways; that is, the concentrations entered in this scenario are not the source term for any fate and transport models.

The direct exposure concentrations should be appropriate for the exposure pathways. For example, if soil concentrations are being specified for direct contact pathways with soil (ingestion and dermal contact), then the soil concentrations should be appropriate for the soil that receptors are likely to come in contact with - usually the top few centimeters to possibly a meter of soil for residential and no deeper than typical excavation depths for a construction scenario.

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, sediment, outdoor air, and/or indoor air. The models to be used in this step are determined by the choices made in Step 2. Figure 5-1 shows the four basic steps in using the fate and transport models.



Description

File name 4 solvents.PRJ

Save date: 04-07-2011 10:16:12

Step 3: Estimating Exposure Point Concentrations

Run Fate and Transport Models to Estimate Exposure Point Concentrations

STEP 3a Enter Site Data

STEP 3b Enter Source Concentrations

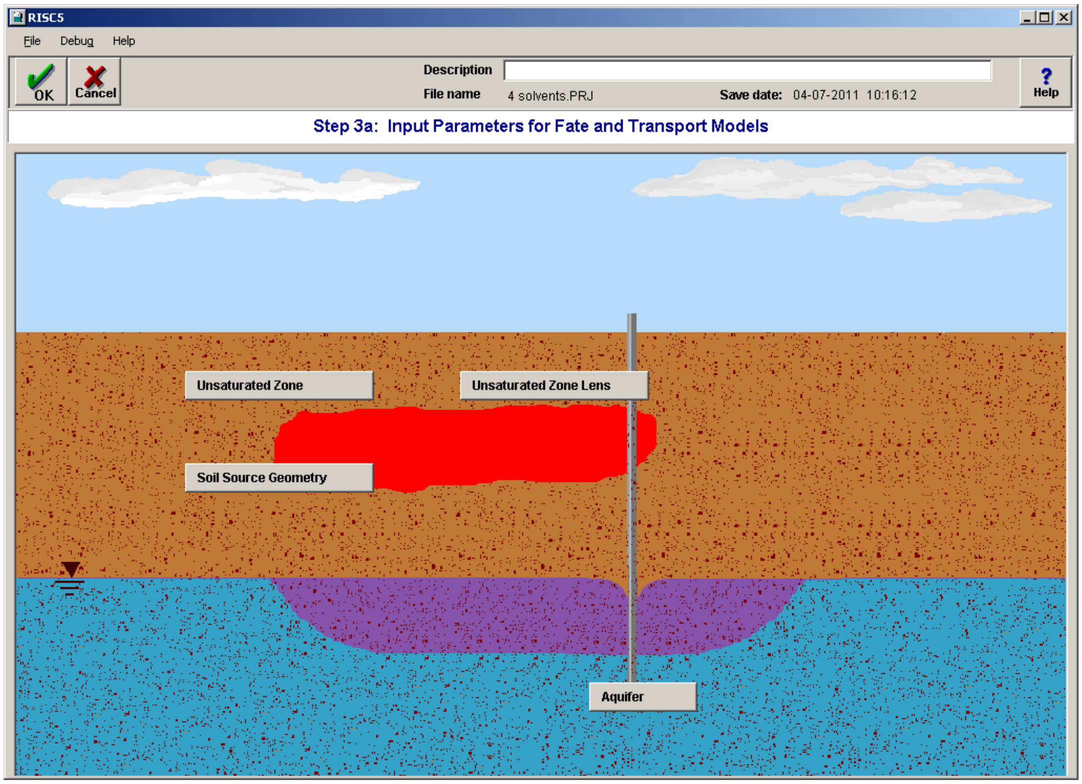
STEP 3c Chemical-Specific Parameters

STEP 3d Run Model View Results

Figure 5-1. The Four Main Steps for Using Fate and Transport Models.

5.2.1 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 5-2 shows the input screen that appears when the source is “unsaturated zone soil” and leaching to groundwater is being modeled with exposure concentrations in onsite groundwater being estimated.



Description

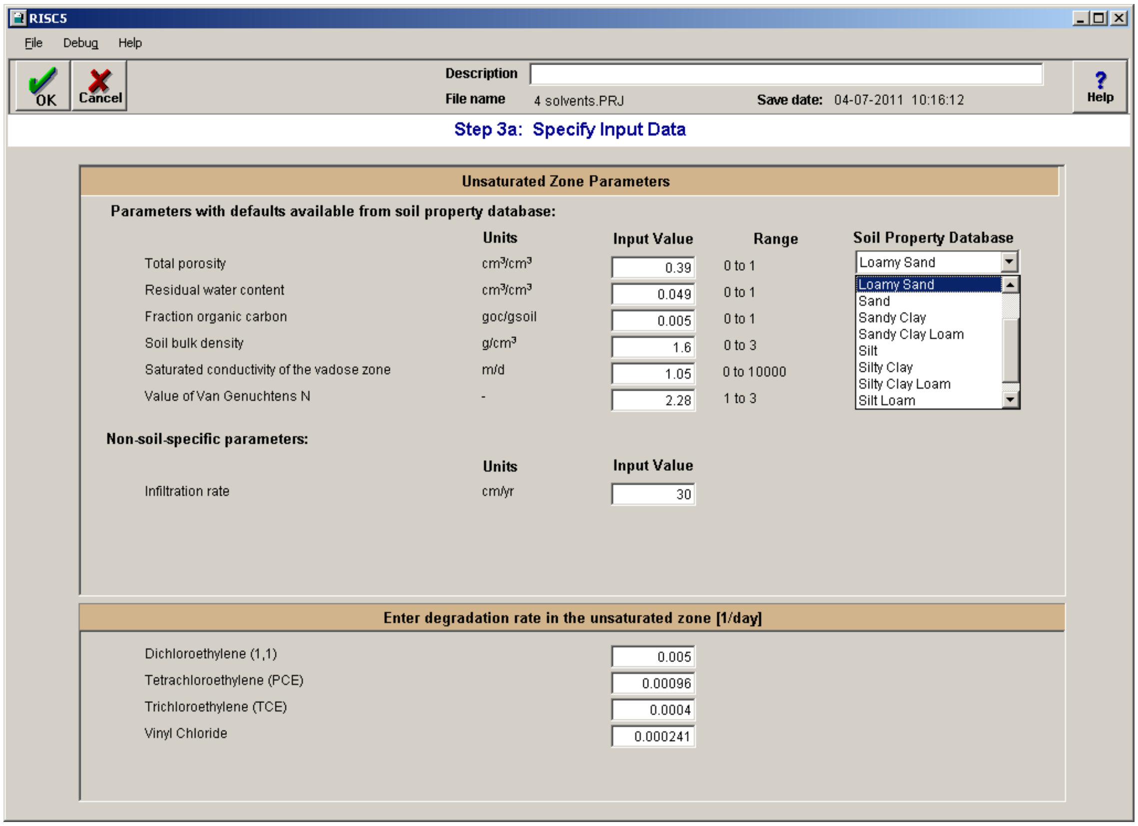
File name 4 solvents.PRJ

Save date: 04-07-2011 10:16:12

Step 3a: Input Parameters for Fate and Transport Models

Figure 5-2. Entering Site Data for an Unsaturated Zone Source Leaching to Groundwater.

In this example there are only four groups of data that need be entered: Soil Source Geometry, Aquifer properties, Unsaturated Zone properties and the Unsaturated Zone Lens properties. Depending on the model(s) chosen, the screen in Figure 5-2 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 12 soil types, ranging from gravel to clay. An example of the unsaturated zone parameter input screen is shown in Figure 5-3. The drop-down list (with "Loamy sand" shown) allows the user to select a different default soil type. The default values for the soil types in the soil parameter database may be modified using the *Master Database Editor* (discussed in Section 2.4 and 2.5 of this guide). New soil types may be added as well using the *Master Database Editor*.



Description

File name 4 solvents.PRJ **Save date:** 04-07-2011 10:16:12

Step 3a: Specify Input Data

Unsaturated Zone Parameters

Parameters with defaults available from soil property database:

	Units	Input Value	Range	Soil Property Database
Total porosity	cm^3/cm^3	0.39	0 to 1	Loamy Sand
Residual water content	cm^3/cm^3	0.049	0 to 1	
Fraction organic carbon	goc/gsoil	0.005	0 to 1	
Soil bulk density	g/cm^3	1.6	0 to 3	
Saturated conductivity of the vadose zone	m/d	1.05	0 to 10000	
Value of Van Genuchtens N	-	2.28	1 to 3	

Non-soil-specific parameters:

	Units	Input Value
Infiltration rate	cm/yr	30

Enter degradation rate in the unsaturated zone [1/day]

Dichloroethylene (1,1)	0.005
Tetrachloroethylene (PCE)	0.00096
Trichloroethylene (TCE)	0.0004
Vinyl Chloride	0.000241

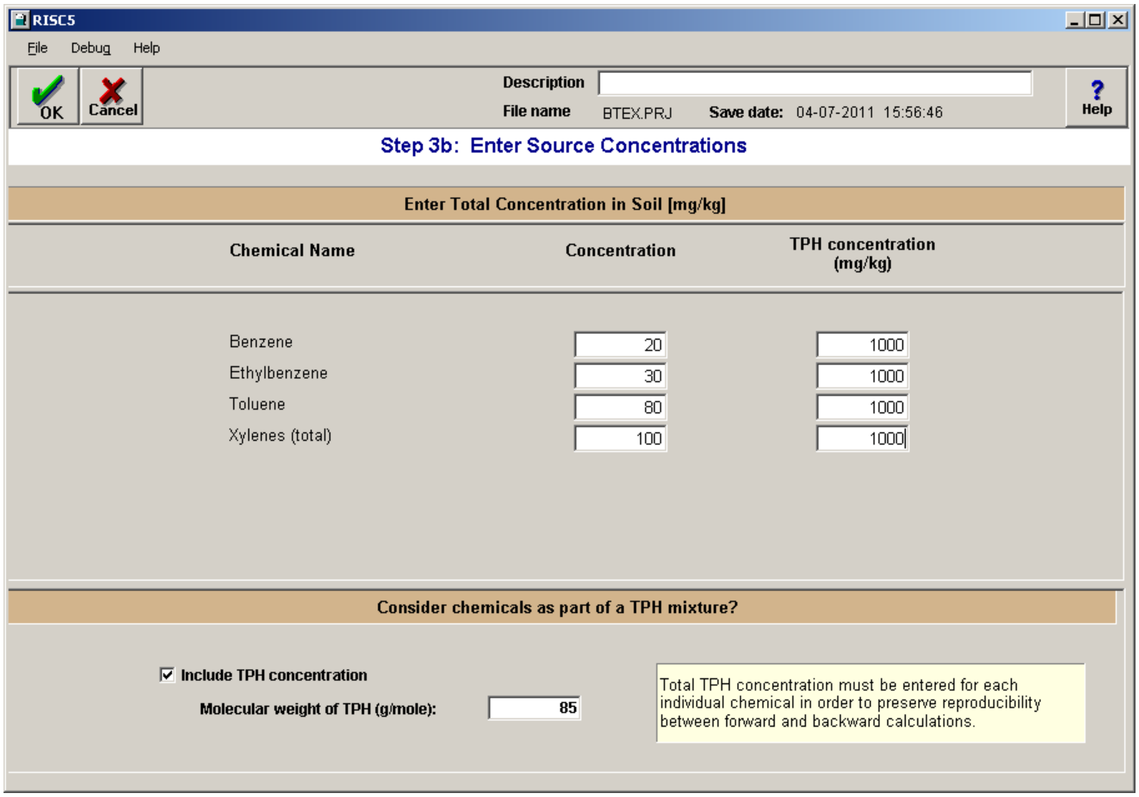
Figure 5-3. Specifying Input Data for Unsaturated Zone Soil.

These soil properties 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.

5.2.2 Step 3b: Enter 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 concentrations in soil, groundwater, or soil gas.

For the soil concentration sources, total petroleum hydrocarbon (TPH) concentrations may also be entered. To use this option, check the “Include TPH Concentrations” box in the lower panel of the screen. Figure 5-4 shows the TPH concentration box checked and TPH concentrations entered for each chemical of concern. This option is used when the chemicals of concern are individual petroleum hydrocarbons or individual TPH fractions that are part of a larger mixture of chemicals. The TPH concentration is used to calculate effective solubility for the chemicals of concern. The presence of a TPH mixture can greatly reduce the chemical’s solubility in water, thereby limiting its leaching rate from the source. This means that the source may last longer than if the TPH present was ignored. In other words, depending on the scenario being evaluated, it may or may not, be conservative to ignore the presence of TPH.



Description

File name BTEX.PRJ Save date: 04-07-2011 15:56:46

Step 3b: Enter Source Concentrations

Enter Total Concentration in Soil [mg/kg]

Chemical Name	Concentration	TPH concentration (mg/kg)
Benzene	20	1000
Ethylbenzene	30	1000
Toluene	80	1000
Xylenes (total)	100	1000

Consider chemicals as part of a TPH mixture?

☑ Include TPH concentration

Molecular weight of TPH (g/mole): 85

Total TPH concentration must be entered for each individual chemical in order to preserve reproducibility between forward and backward calculations.

Figure 5-4. Entering Source Concentrations with TPH.

TPH concentrations must be entered for each chemical separately although it is expected that initially all of the TPH concentrations will be equal. The reason separate TPH values are entered for each chemical is that after calculating individual site-specific clean-up levels in Step 5, if the TPH at the clean-up level could be different for each chemical. In this case, the fraction of the chemical of concern in the TPH is assumed to be fixed. That is, if benzene is 2% (by mass) of the original mixture of TPH, then the TPH will be decreased or increased so that at the clean-up level for benzene, the TPH is still 50 times the benzene concentration (i.e. benzene is 2% of the TPH). If the cumulative clean-up level option is used in Step 5, then all of the chemical concentrations will be scaled relative to the original relationships and the overall TPH concentration will be the same for each chemical.

5.2.3 Step 3c: Chemical-Specific Parameters

In Step 3c, the chemical-specific parameter values may be reviewed and/or changed. Any changes made in this screen will not be stored in the master database, they will just be retained for this project scenario. To change chemical parameter values in the permanent database, discussed in Section 2.4 and 2.5 of this guide.

5.2.4 Step 3d: Run Model/View Results

In Step 3d, the fate and transport model(s) are run and the results can be viewed in the Excel results tables. Excel may also be used to create charts of concentration vs. time for the sources and exposure media.

In this step, the simulation time and time step length are entered. If the dissolved phase groundwater model is being used, then the source pulse length, the time the source is active, is also entered. For the non-depleting source indoor air models, the model is steady-state, i.e. it does not matter how long the model is run. For transient models, if is important to make sure the simulation time includes the potential exposure period. When viewing the results in Excel, the breakthrough curves (concentration vs. time) for the exposure points may be viewed to make sure that the model was run for a long enough simulation time.

In the Excel results file, a RISC5 menu is brought up automatically when the file opens. This menu must be used to view the model output. The tables and charts shown in Excel will vary depending on the model(s) run. There is always a “Model Input Summary” listing all of the input parameter values and chemical-specific model results summaries showing the intermediate model calculations and results. 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. If the RISC5 menu is closed, it can be reopened by selecting “RISC5” from the main menu of Excel (Excel 2003).

6.0

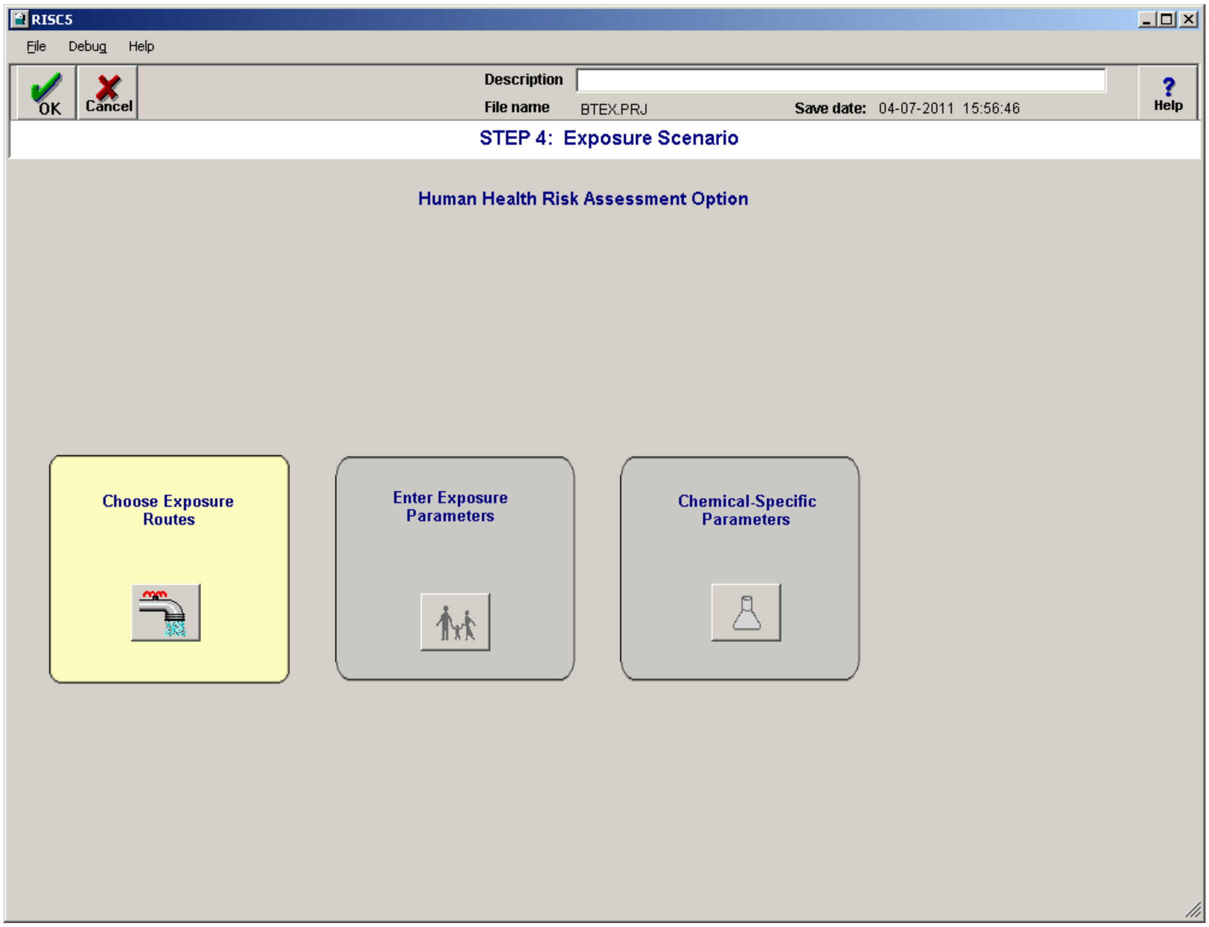
Step 4:
Describe The Receptors

The screens in this step appear differently depending on the type of analysis chosen in Step 2 (human health or ecological). The first of these two options is described in the following sections. The ecological food web model is presented in Appendix T.

Note, if a back-calculation is to be performed where the targets are groundwater or surface water concentrations, then the data entered in Step 4 will not be used in the calculations since the clean-up levels will be based on target concentrations rather than target risk levels. In that case, you still need to go through all of the sub-steps in Step 4: choose an exposure pathway, view exposure parameters, and view chemical-specific parameters. These values will not be used in the clean-up level calculation, however.

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 default exposure parameters 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 or regulatory preferences. Figure 6-1 shows the main screen for Step 4.



Description

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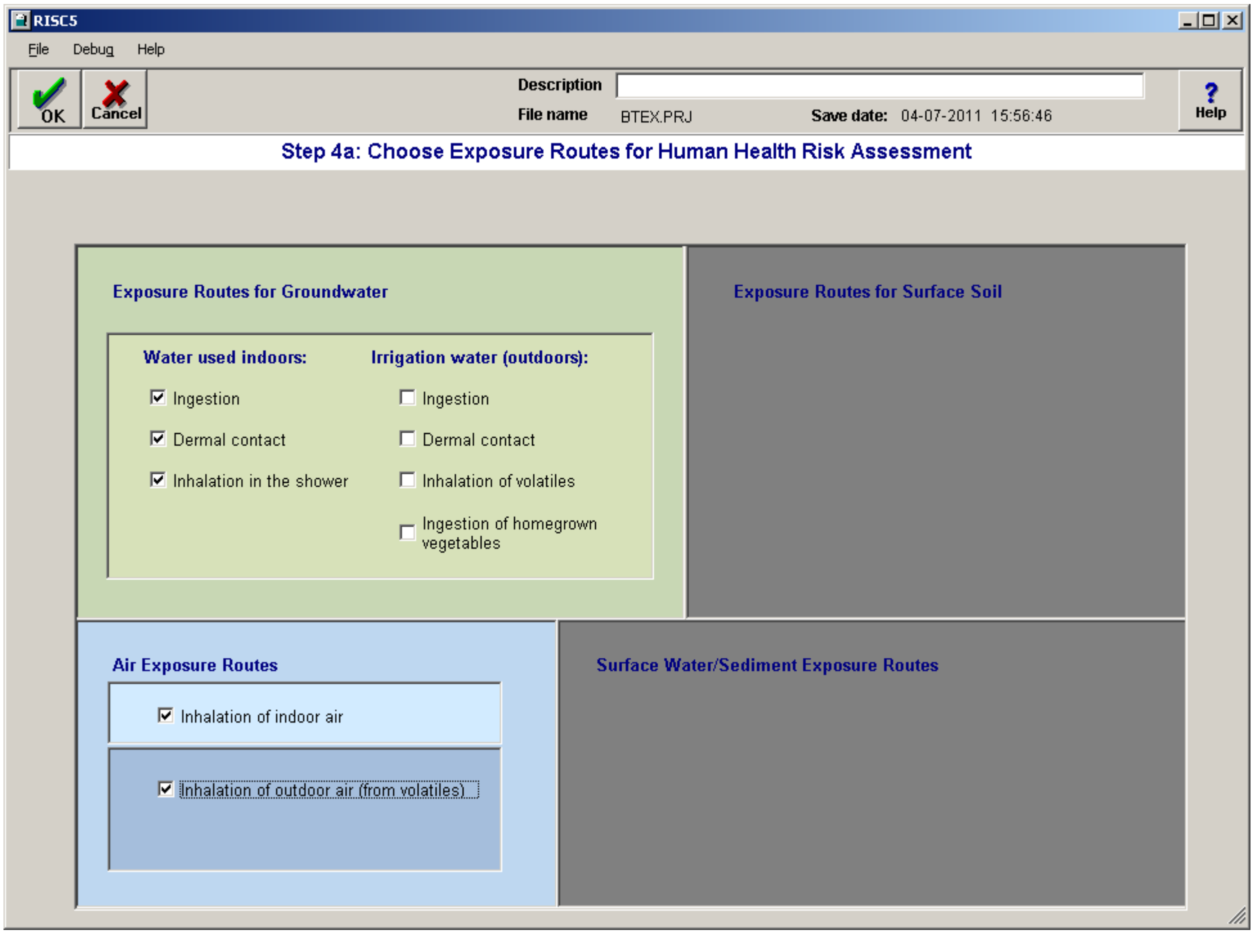
FIGURE 6-1. Step 4 Main Screen for Human Health Risk Assessment.

6.1.1 Choose Exposure Routes

The purpose of this step is to identify the exposure pathways that will be used in the risk assessment. This screen will appear differently based on the choices that were made in Step 2. Figure 6-2 shows the exposure pathways available for a groundwater source that can be used as an indoor water supply and the emissions from groundwater to indoor air and outdoor air are being modeled.



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Step 4a: Choose Exposure Routes for Human Health Risk Assessment

Exposure Routes for Groundwater

Water used indoors:
☑ Ingestion
☑ Dermal contact
☑ Inhalation in the shower

Irrigation water (outdoors):
☐ Ingestion
☐ Dermal contact
☐ Inhalation of volatiles
☐ Ingestion of homegrown vegetables

Exposure Routes for Surface Soil

Air Exposure Routes
☑ Inhalation of indoor air
☑ Inhalation of outdoor air (from volatiles)

Surface Water/Sediment Exposure Routes

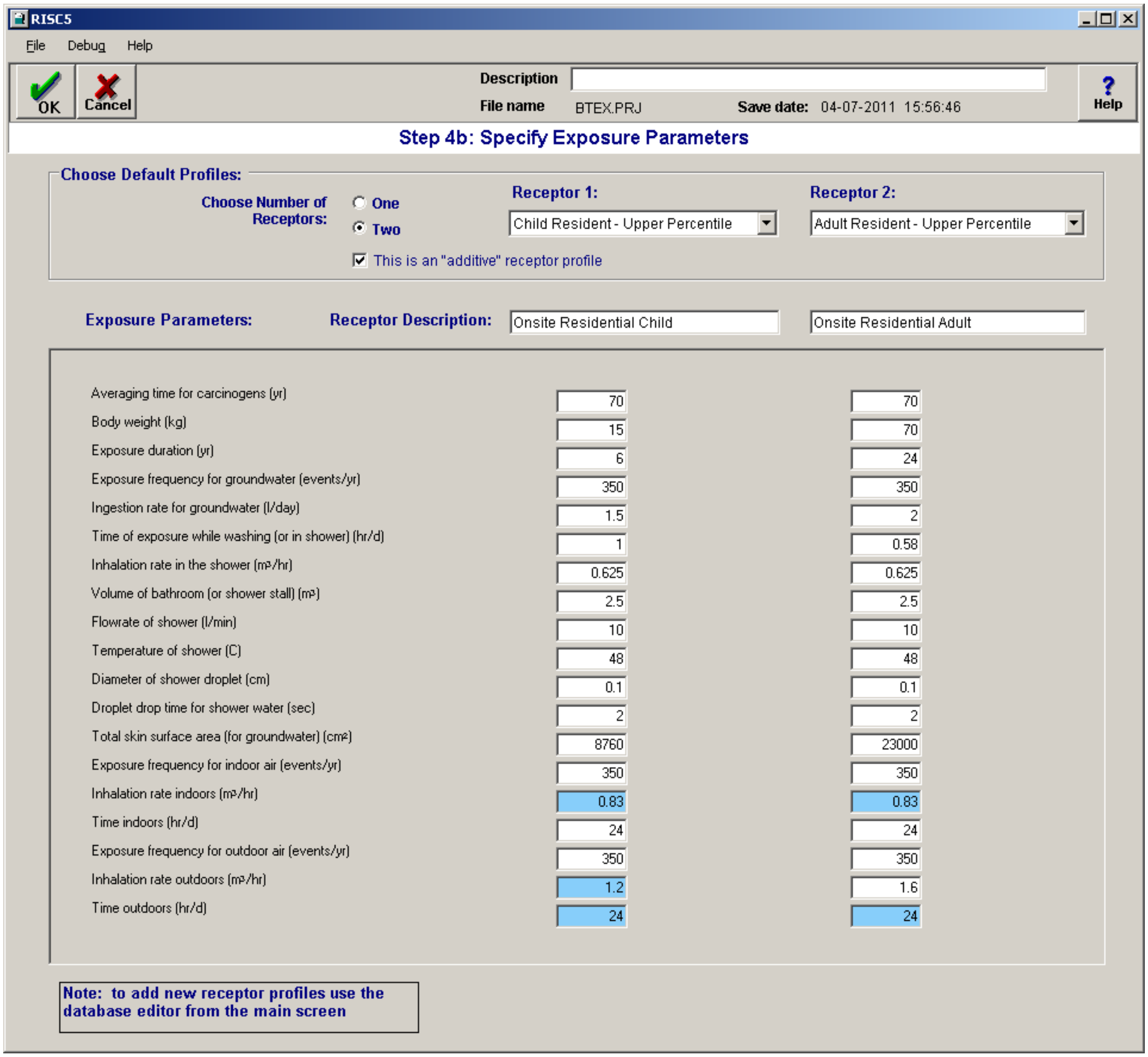
Figure 6-2. Step 4a Showing Options for a Groundwater Source with Volatile Emissions to Indoor and Outdoor Air.

6.1.2 Enter Exposure Parameters

In this step, the type(s) of receptors to be considered in the risk assessment will be identified and the exposure parameter data for each receptor of concern will be reviewed or revised. The decisions that must be made in this step are:

- 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 the default exposure parameters appropriate for this scenario or do they need to be modified to reflect site-specific conditions?

Figure 6-3 shows the input screen with two receptors chosen and the additive receptor profile option chosen.



Description
File name BTEX.PRJ
Save date: 04-07-2011 15:56:46

Step 4b: Specify Exposure Parameters

Choose Default Profiles:

Choose Number of Receptors: ○ One ● Two

Receptor 1: Child Resident - Upper Percentile

Receptor 2: Adult Resident - Upper Percentile

☑ This is an "additive" receptor profile

Exposure Parameters:	Receptor Description: Onsite Residential Child	Onsite Residential Adult
Averaging time for carcinogens (yr)	70	70
Body weight (kg)	15	70
Exposure duration (yr)	6	24
Exposure frequency for groundwater (events/yr)	350	350
Ingestion rate for groundwater (l/day)	1.5	2
Time of exposure while washing (or in shower) (hr/d)	1	0.58
Inhalation rate in the shower (m^3/hr)	0.625	0.625
Volume of bathroom (or shower stall) (m^3)	2.5	2.5
Flowrate of shower (l/min)	10	10
Temperature of shower (C)	48	48
Diameter of shower droplet (cm)	0.1	0.1
Droplet drop time for shower water (sec)	2	2
Total skin surface area (for groundwater) (cm^2)	8760	23000
Exposure frequency for indoor air (events/yr)	350	350
Inhalation rate indoors (m^3/hr)	0.83	0.83
Time indoors (hr/d)	24	24
Exposure frequency for outdoor air (events/yr)	350	350
Inhalation rate outdoors (m^3/hr)	1.2	1.6
Time outdoors (hr/d)	24	24

Note: to add new receptor profiles use the database editor from the main screen

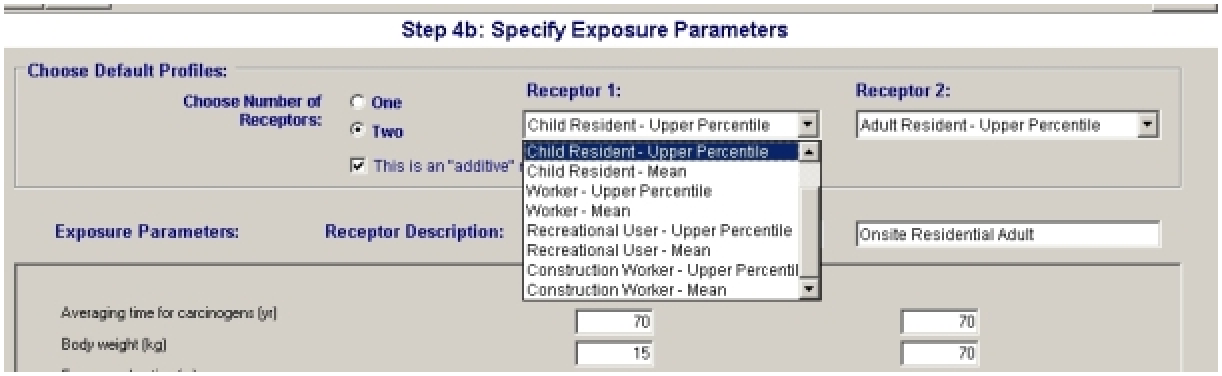
FIGURE 6-3. Step 4b Input Screen for the Pathways Shown in Figure 6-2.

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 side-by-side. For example, one might examine the effect of changing exposure assumptions by comparing very conservative exposure parameter estimates ("upper percentile") 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 "upper percentile" inputs correspond to the conservative parameter estimates. USEPA used to refer to the upper percentile exposure defaults as the "Reasonable Maximum Exposure" (RME) scenario.

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. The additive scenario is only used for carcinogenic risk; for non-carcinogenic risk the two exposures are not assumed to be additive and the results will be presented separately for each receptor.

The "Receptor Descriptions" text boxes may be used to enter a more appropriate name for the receptor being considered. For example, if the scenario being considered is a future residential onsite scenario, the receptor could be called "Onsite Residential Child" and "Onsite Residential Adult". This labels will be used in the tables of model output shown in Step 6.

When the exposure value is changed from the "default profile", the edit box will be highlighted in blue to indicate that the value does not match the default profile shown at the top of the screen. To reload the default profiles, reselect the receptor from the drop-down boxes in the top panel (as shown below):



Step 4b: Specify Exposure Parameters

Choose Default Profiles:

Choose Number of Receptors: ○ One ● Two

☑ This is an "additive"

Receptor 1: Child Resident - Upper Percentile

Receptor 2: Adult Resident - Upper Percentile

Exposure Parameters:

Receptor Description: Onsite Residential Adult

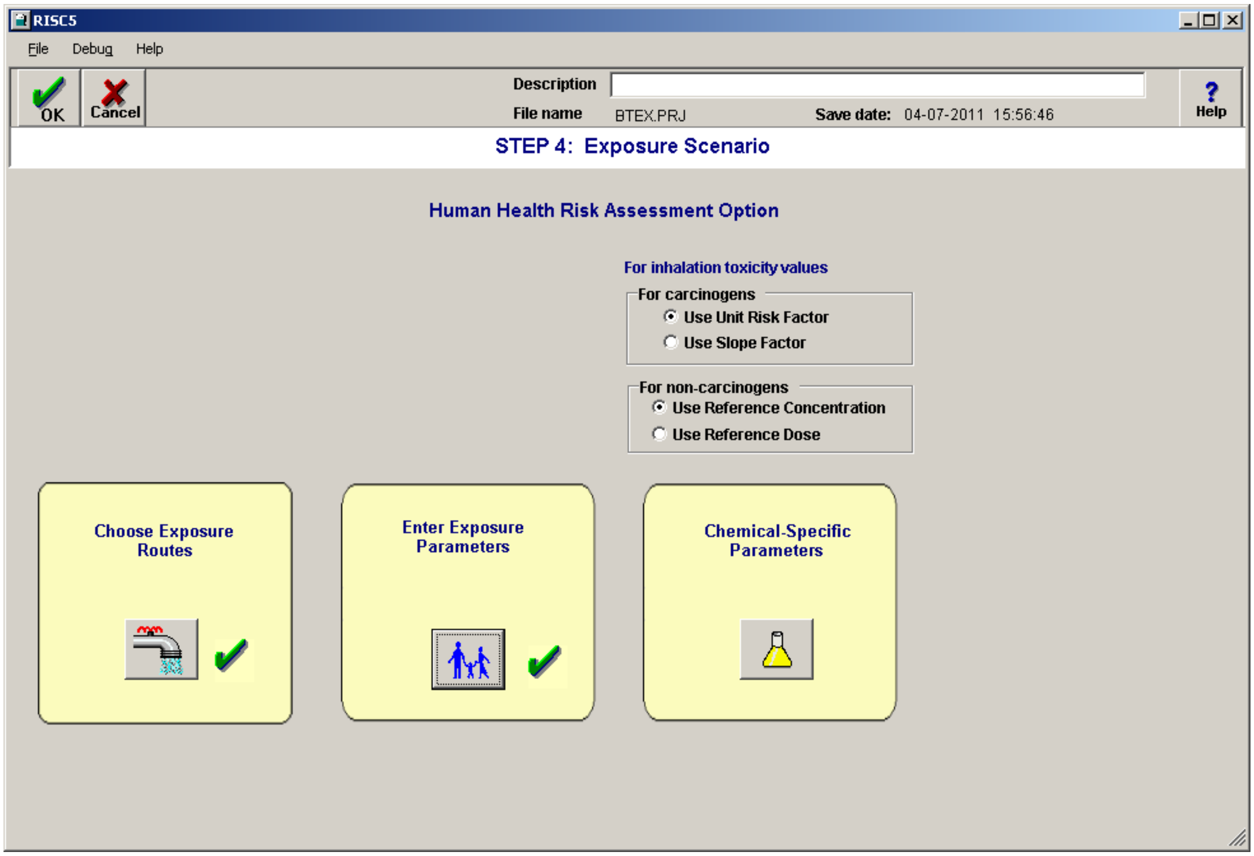
Averaging time for carcinogens (yr) 70 70

Body weight (kg) 15 70

6.1.3 Chemical-Specific Parameters

In this step, the chemical-specific parameters are reviewed and/or revised. Note, the parameters shown are the ones required for the exposure pathways chosen; this is not a complete list of the chemical parameter values that are in the main chemical database. Any changes made in this screen will be saved with the project file only; they will not affect the permanent chemical database.

For the scenarios that have an inhalation pathway, the main Step 4 screen will be modified slightly to allow the used to choose which type of inhalation toxicity to use. Figure 6-4 shows the Step 4 main screen with this choice available.



Description

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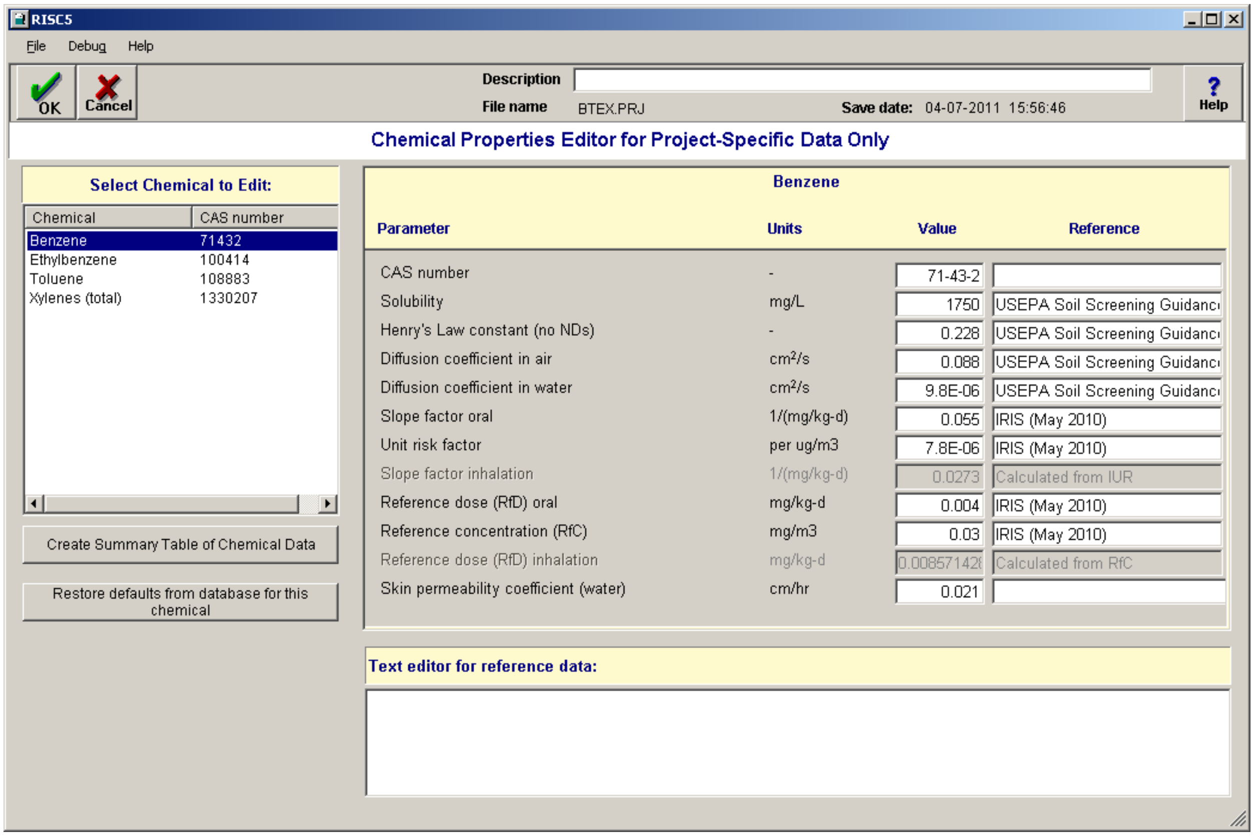
For inhalation toxicity values

For carcinogens
● Use Unit Risk Factor
○ Use Slope Factor

For non-carcinogens
● Use Reference Concentration
○ Use Reference Dose

Figure 6-4. Step 4 Main Screen with Inhalation Toxicity Selections.

Figure 6-5 shows the Chemical-Specific Parameters with the inhalation toxicity choices shown in Figure 6-4. Note, that since the “Unit Risk Factor” and the “Reference Concentration” options were made, the inhalation slope factor and inhalation reference dose are grayed out and are not available for editing.



Description

File name BTEX.PRJ

Save date: 04-07-2011 15:56:46

Chemical Properties Editor for Project-Specific Data Only

Select Chemical to Edit:

Chemical	CAS number
Benzene	71432
Ethylbenzene	100414
Toluene	108883
Xylenes (total)	1330207

Benzene

Parameter	Units	Value	Reference
CAS number	-	71-43-2	
Solubility	mg/L	1750	USEPA Soil Screening Guidanc
Henry's Law constant (no NDs)	-	0.228	USEPA Soil Screening Guidanc
Diffusion coefficient in air	cm²/s	0.088	USEPA Soil Screening Guidanc
Diffusion coefficient in water	cm²/s	9.8E-06	USEPA Soil Screening Guidanc
Slope factor oral	1/(mg/kg-d)	0.055	IRIS (May 2010)
Unit risk factor	per ug/m3	7.8E-06	IRIS (May 2010)
Slope factor inhalation	1/(mg/kg-d)	0.0273	Calculated from IUR
Reference dose (RfD) oral	mg/kg-d	0.004	IRIS (May 2010)
Reference concentration (RfC)	mg/m3	0.03	IRIS (May 2010)
Reference dose (RfD) inhalation	mg/kg-d	0.00857142	Calculated from RfC
Skin permeability coefficient (water)	cm/hr	0.021	

Text editor for reference data:

Figure 6-5. Chemical-Specific Parameters in Step 4.

6.2 ECOLOGICAL RECEPTORS AND RISK ASSESSMENT

The ecological food web model is presented in Appendix T. Setting up the ecological risk assessment in Step 2 will be forthcoming in the next User's Guide revision.

7.0

Calculate Exposure and Risk

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 (note, some of the items listed cover more than one exposure pathway):

1. Ingestion of contaminated soil and/or sediment.
2. Dermal contact with contaminated soil and/or sediment.
3. Ingestion of contaminated drinking water.
4. Dermal contact with contaminated groundwater (while showering), irrigation water or surface water (while swimming).
5. Inhalation while showering or of irrigation water spray (from sprinklers etc.).
6. Inhalation of indoor air or outdoor air.
7. Ingestion of home-grown vegetables (grown in contaminated soil).
8. Ingestion of home-grown vegetables (watered with contaminated groundwater).
9. Ingestion of surface water or irrigation water (e.g. while swimming).

Ingestion of soil, dermal contact with soil, inhalation of outdoor air and indoor air represent some of the more common exposure pathways for many petroleum contaminated sites (e.g. former gas stations). The irrigation water pathways will usually only be of concern if the house water is provided by a municipality but groundwater is used outside to irrigate in the garden.

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 CALCULATION OF INTAKE (DOSE)

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 7.1.9 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.

7.1.1 Ingestion of Soil or Sediment

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 or sediment by ingestion is estimated as follows:

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

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

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 or sediment [mg/kg]
C_{ave} = time-averaged concentration of chemical in soil or sediment over the exposure duration [mg/kg]
IR = soil ingestion rate [mg/day]
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]

7.1.2 Dermal Contact with Soil or Sediment

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:

$$\mathrm{CADD} = \frac{\mathrm{C_{max}} \times \mathrm{SA} \times \mathrm{AAF} \times \mathrm{AF} \times \mathrm{EF}}{\mathrm{BW} \times 365\ \frac{\mathrm{d}}{\mathrm{yr}}} \times 10^{-6}\ \frac{\mathrm{kg}}{\mathrm{mg}} \qquad \textbf{(7-2a)}$$

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

where

C_{max} = maximum 7-year average concentration of chemical in soil or sediment [mg/kg]
C_{ave} = time-averaged concentration of chemical in soil or sediment 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]
AF = soil-to-skin adherence factor [mg/cm^2/event]

The skin surface area available for dermal exposure will vary seasonally and between receptors. For example workers would most likely have less skin exposed than children playing in the summer.

7.1.3 Ingestion of Groundwater

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

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

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

where

C_{max} = maximum 7-year average concentration of chemical in water [mg/l]
C_{ave} = time-averaged concentration of chemical in water over the exposure duration [mg/l]
IR = water ingestion rate [l/day]

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 Exposure to Groundwater, Surface Water or Irrigation Water

During showers and baths receptors may absorb dissolved contaminants across the skin into the bloodstream. Similarly, outdoor exposure to irrigation water or surface water could also be potential exposure pathways 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:

$$\text{CADD} = \frac{C_{max} \times SA \times ET \times PC \times EF}{BW \times 365\ \frac{d}{yr}} \times 10^{-3}\ \frac{l}{cm^3} \tag{7-4a}$$

$$\text{LADD} = \frac{C_{max} \times SA \times ET \times PC \times EF \times ED}{LT \times BW \times 365\ \frac{d}{yr}} \times 10^{-3}\ \frac{l}{cm^3} \tag{7-4b}$$

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]
PC = chemical-specific skin permeability constant [cm/hr]
ET = bath or shower duration [hr/day]

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 or from Irrigation Water (Sprinklers)

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. Similarly, chemicals can volatilize to outdoor air from groundwater spray.

$$\text{CADD} = \frac{C_{max} \times InhR \times ET \times EF}{BW \times 365\ \frac{d}{yr}} \tag{7-5a}$$

$$\text{LADD} = \frac{C_{ave} \times InhR \times ET \times EF \times ED}{LT \times BW \times 365\ \frac{d}{yr}} \tag{7-5b}$$

where

C_{max} = maximum concentration of chemical in bathroom or outdoor air [mg/m^3] (calculated from the *maximum 7-year average groundwater* concentration)
C_{ave} = time-averaged concentration of chemical in either bathroom air or outdoor [mg/m^3] (calculated from the *maximum average groundwater* concentration over the exposure duration)
$InhR$ = inhalation rate [m^3/hr]
ET = shower duration or time spent in the sprinkler [hr/day]

These equations assume that the concentration in the bathroom air is known. RISC5 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 Indoor or Outdoor Air

In this exposure pathway the inhalation of chemicals in breathing space air (either inside or out) is considered. The intake is computed as follows:

$$\mathrm{CADD} = \frac{\mathrm{C_{max}} \times \mathrm{InhR} \times \mathrm{ET} \times \mathrm{EF}}{\mathrm{BW} \times 365\ \frac{\mathrm{d}}{\mathrm{yr}}} \tag{7-6a}$$

$$\mathrm{LADD} = \frac{\mathrm{C_{ave}} \times \mathrm{InhR} \times \mathrm{ET} \times \mathrm{EF} \times \mathrm{ED}}{\mathrm{LT} \times \mathrm{BW} \times 365\ \frac{\mathrm{d}}{\mathrm{yr}}} \tag{7-6b}$$

where

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

7.1.7 Ingestion of Home-Grown Vegetables Grown in Contaminated Soil

This exposure route is identical to 7.1.8 (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).

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

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

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 [-]

Workers and trespassers are not expected to be exposed via this pathway.

7.1.8 Ingestion of Home-Grown Vegetables Irrigated With Groundwater

This exposure route is identical to 7.1.7 (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) .

$$CADD = \left[\frac{\left(RCF \times IR_{vr} + ABCF \times IR_{va}\right) \times FI \times EF}{BW \times 365 \dfrac{d}{yr}} \right] \times C_{\max} \times 10^{-3} \frac{kg}{g} \tag{7-8a}$$

$$LADD = \left[\frac{\left(RCF \times IR_{vr} + ABCF \times IR_{va}\right) \times IR_{r} \times FI \times EF \times ED}{LT \times BW \times 365 \dfrac{d}{yr}} \right] \times C_{ave} \times 10^{-3} \frac{kg}{g} \tag{7-8b}$$

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 RISC5, the concentration in irrigation water may be estimated using the groundwater models. Workers and trespassers are not expected to be exposed via this pathway.

7.1.9 Ingestion of Irrigation Water or Surface Water

Ingestion of irrigation or surface water may occur if children are playing in sprinklers or if the irrigation water is used to fill a swimming pool. The intake equation is similar to 7.1.3, ingestion of groundwater, however in this case the ingestion rate is specified per hour spent in the water body. Intake from ingestion of contaminated irrigation or surface water is estimated using the following equations:

$$\mathrm{CADD} = \frac{\mathrm{C_{max}} \times \mathrm{IR_{iw}} \times \mathrm{ET_{iw}} \times \mathrm{EF}}{\mathrm{BW} \times \mathit{365}\ \frac{\mathrm{d}}{\mathrm{yr}}} \times \mathit{10}^{-3}\ \frac{\mathrm{l}}{\mathrm{ml}} \qquad \textbf{(7-9a)}$$

$$\mathrm{LADD} = \frac{\mathrm{C_{ave}} \times \mathrm{IR_{iw}} \times \mathrm{ET_{iw}} \times \mathrm{EF} \times \mathrm{ED}}{\mathrm{LT} \times \mathrm{BW} \times \mathit{365}\ \frac{\mathrm{d}}{\mathrm{yr}}} \times \mathit{10}^{-3}\ \frac{\mathrm{l}}{\mathrm{ml}} \qquad \textbf{(7-9b)}$$

where

C_{max} = maximum 7-year average concentration of chemical in irrigation or surface water [mg/l]
C_{ave} = time-averaged concentration of chemical in irrigation or surface water over the exposure duration [mg/l]
IR_{iw} = water ingestion rate [ml/hr]
ET_{iw} = exposure time for irrigation water [hr/day]

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*:

$$IELCR_{ij} = SF_{ij}\, LADD_{ij} \qquad \textbf{(7-10)}$$

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:

$$IELCR_t = \sum IELCR_{ij} \qquad \textbf{(7-11)}$$

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:

$$HQ_{ij} = CADD_{ij} / RfD_{ij} \tag{7-12}$$

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:

$$\mathrm{HI} = \sum \sum \mathrm{HQ}_{\mathrm{ij}} \tag{7-13}$$

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.

8.0

Calculate Clean-Up Levels

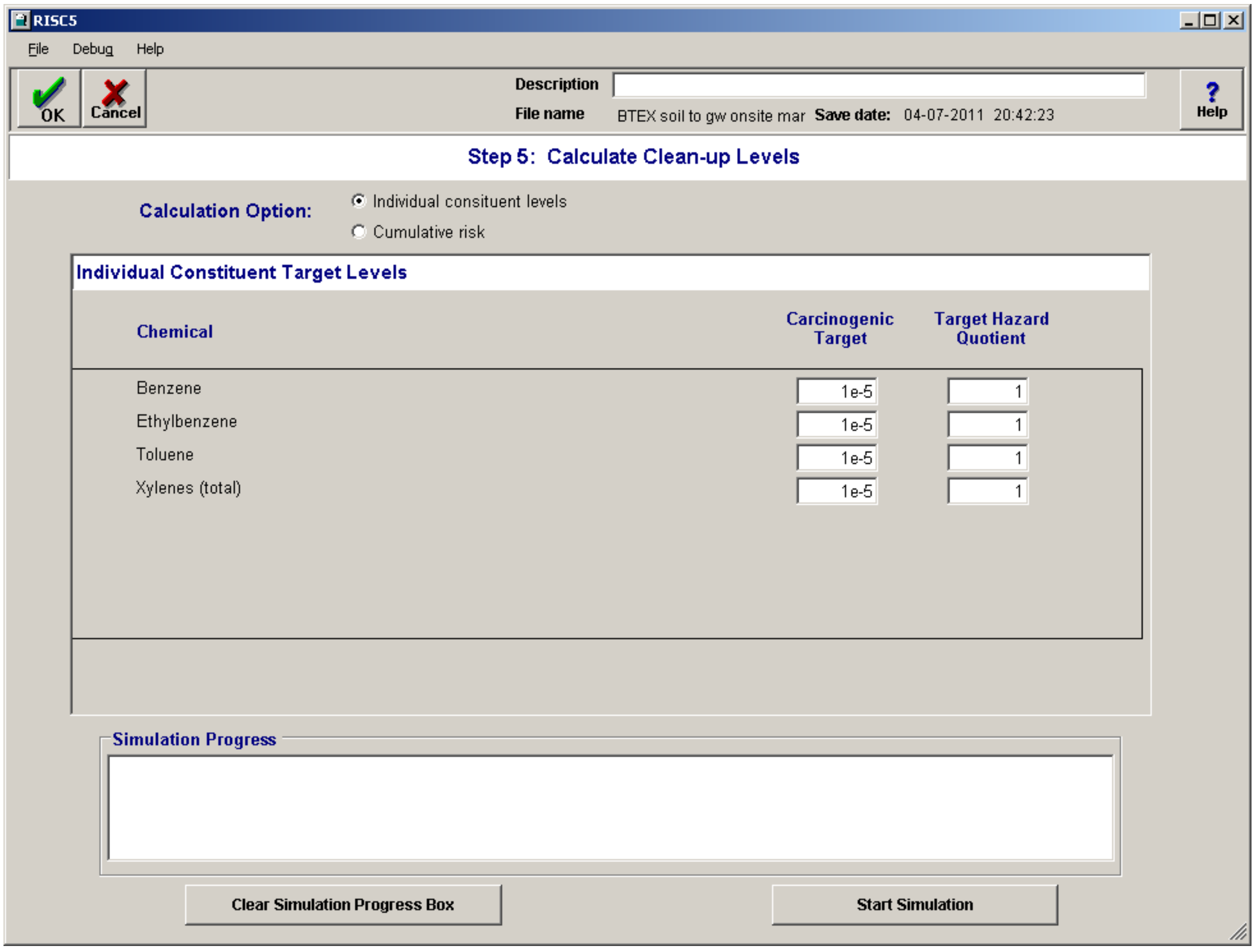
When the "Calculate Clean-up Levels" option is chosen from Step 5, RISC can be used to "back-calculate" clean-up levels using the models and assumptions selected in the current analysis. In the "forward risk" assessment (i.e. "Calculate Risk" option), risk is calculated from input or estimated receptor point concentrations and receptor input parameters. In the back-calculation, the user specifies target risks or target concentrations (e.g. maximum contaminant levels [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.

8.1 BACKGROUND

There are several options for selecting targets in Step 5. The user may choose to calculate clean-up levels for each chemical individually (not considering risk from the other chemicals present) or a "cumulative" scenario may be chosen 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 water) 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 surface and groundwater concentrations are linked in that they are calculated by the same model and therefore only one or the other may be specified for calculating clean-up levels.

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.

Figure 8-1 shows the initial input screen for specifying target risk and hazard indices for cases that do not contain surface water or groundwater as exposure media. Note, the when the screen is opened for the first time in a given scenario, it is defaulted to the "Individual" clean-up level option. This may be changed to "Cumulative" by selecting the option button at the top of the screen.



Description

File name BTEX soil to gw onsite mar **Save date:** 04-07-2011 20:42:23

Step 5: Calculate Clean-up Levels

Calculation Option:
● Individual constituent levels
○ Cumulative risk

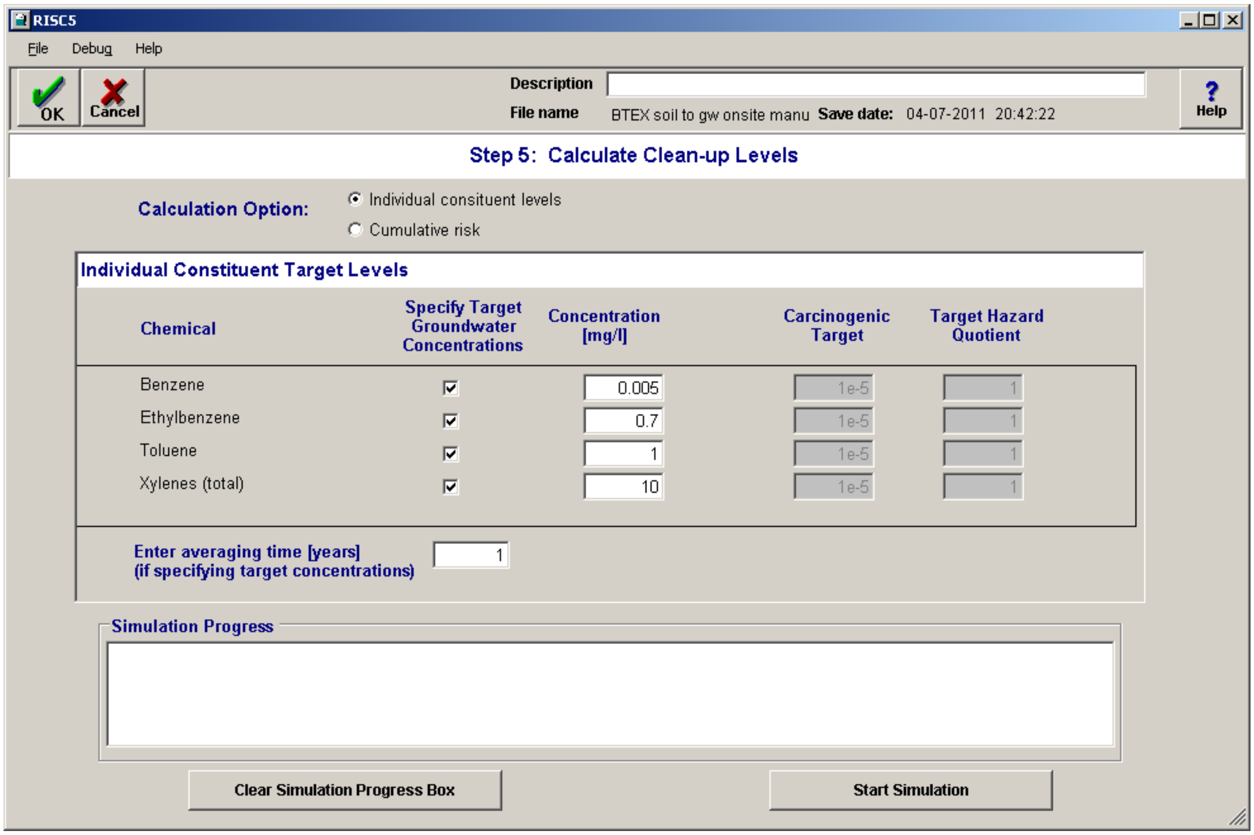
Individual Constituent Target Levels

Chemical	Carcinogenic Target	Target Hazard Quotient
Benzene	1e-5	1
Ethylbenzene	1e-5	1
Toluene	1e-5	1
Xylenes (total)	1e-5	1

Simulation Progress

Figure 8-1. Specifying Individual Constituent Target Levels.

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 maximum contaminant levels (MCLs) in groundwater under the "Individual Constituent Levels" option. This same option is available for surface water pathways as well.



Description

File name BTEX soil to gw onsite manu **Save date:** 04-07-2011 20:42:22

Step 5: Calculate Clean-up Levels

Calculation Option: ● Individual consituent levels ○ Cumulative risk

Individual Constituent Target Levels

Chemical	Specify Target Groundwater Concentrations	Concentration [mg/l]	Carcinogenic Target	Target Hazard Quotient
Benzene	☑	0.005	1e-5	1
Ethylbenzene	☑	0.7	1e-5	1
Toluene	☑	1	1e-5	1
Xylenes (total)	☑	10	1e-5	1

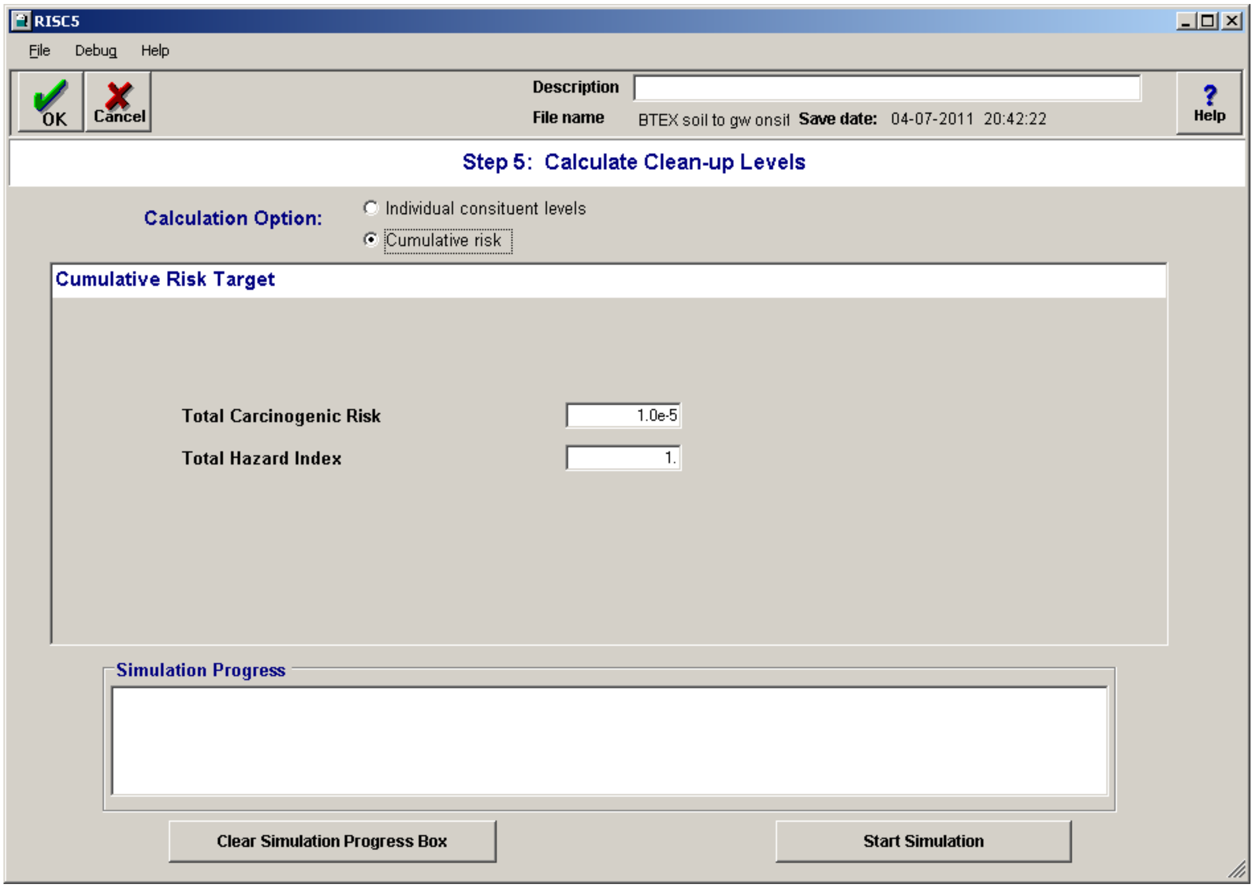
Enter averaging time [years] (if specifying target concentrations): 1

Simulation Progress

Figure 8-2. Specifying Target Groundwater Concentrations.

To use risk or hazard targets, rather than the water concentrations, uncheck the box directly after the chemical name. This will disable the target concentration input box and will enable the target carcinogenic risk and hazard quotient boxes. Note, that there is an input box for the length of time that the concentration in the exposure media should be averaged.

Figure 8-3 shows the input screen for the “Cumulative risk” option. There is only one box for target carcinogenic risk and one box for target hazard quotient.



Description

File name BTEX soil to gw onsit **Save date:** 04-07-2011 20:42:22

Calculation Option:
- ○ Individual consituent levels
- ● Cumulative risk

Total Carcinogenic Risk 1.0e-5

Total Hazard Index 1.

Figure 8-2. Specifying Target Groundwater Concentrations.

The back-calculation code is run by clicking on the "Start Simulation" button. If fate and transport models are used, the code must be run iteratively until the source concentrations converge to meet the target. This may require the models to be run a number of times, so the simulation time may quite a bit 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.

When a back-calculation is performed, 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, the source concentrations of each chemical are increased or reduced proportionately to each other in order until the target is reached. Therefore, after a cumulative risk back-calculation has been performed, each chemical concentration maintains the same ratios as were originally specified in Step 3. For example if a cumulative option is chosen for a case with benzene and xylenes as the chemicals concern, if their original concentrations specified in Step 3 were 1 mg/kg and 0.25 mg/kg, then the calculated clean-up levels will show the benzene concentration being 4 times the xylenes concentration.

8.2.1 Individual Constituent Level Option

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. For scenarios with both surface water and groundwater concentrations being modeled, the user will only have the opportunity to enter surface water concentrations. The reason for this is that the calculated surface water concentrations are dependent on the groundwater concentration, therefore they will be used as the overall target.
- 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 there are multiple exposure pathways, RISC will sum the risk contribution from each pathway to get the total risk for an individual chemical. 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 a soil source is used with the TPH option, 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 the TPH value calculated at the clean-up levels may differ for each chemical modeled.

8.2.1 Cumulative Risk Option

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 will reflect the additive effects from each chemical.
- 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 Exposure 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 of RISC. Target groundwater or surface water exposure point concentrations are not specified for direct pathways since the exposure point concentrations are input by the user. The steps used to calculate clean-up levels for direct scenarios are:

1) 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.
2) 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.
3) 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 Modeled Exposure Pathways (using fate and transport models)

For scenarios that use fate and transport models to estimate the exposure concentration, the clean-up levels are calculated for the source area. The approach used to calculate clean-up levels using models differs slightly from the steps described for the direct exposure pathways. 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) Segregate the chemicals of concern into carcinogens and non-carcinogens. Some chemicals may be in both groups.
2) For the cumulative risk option, the fractional contribution towards the total risk or total hazard is calculated for each chemical in the two groups.
3) 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.

4) 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 the above step 2. This involves:
    a) The clean-up level (solution) for the limiting chemical must be "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 7 iterations.
5) 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.
6) The total risk is compared against the target risk specified. If the target is not met (within a certain tolerance), 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):

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

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

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.

$$\mathbf{LADD_{ij} = CONCcarci\ FACTORcarcj} \qquad \textbf{(8-2a)}$$

$$\mathbf{CADD_{ij} = CONCnoni\ \ FACTORnonj} \qquad \textbf{(8-2b)}$$

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:

$$\mathbf{LADD_{i} = CONCcarci \sum_{j} FACTORcarcj} \qquad \textbf{(8-3a)}$$

$$\mathbf{CADD_{i} = CONCnoni \sum_{j} FACTORnonj} \qquad \textbf{(8-3b)}$$

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:

$$\mathbf{CONCcarc_{i} = TR_{i} / \sum_{j} (SF_{ij} * FACTORj)} \qquad \textbf{(8-3a)}$$

$$\mathbf{CONCnon_{i} = THQ_{i} / \sum_{j} (RfD_{ij} * FACTORj)} \qquad \textbf{(8-3a)}$$

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. If there are more than one type of exposure media, the risk from all of these pathways will be summed to meet the target risk. 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 both carcinogens and non-carcinogenic chemicals are present, both the target risk and the target hazard will be met. The original concentration ratios relative to each other (entered in Step 3) will be maintained.

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

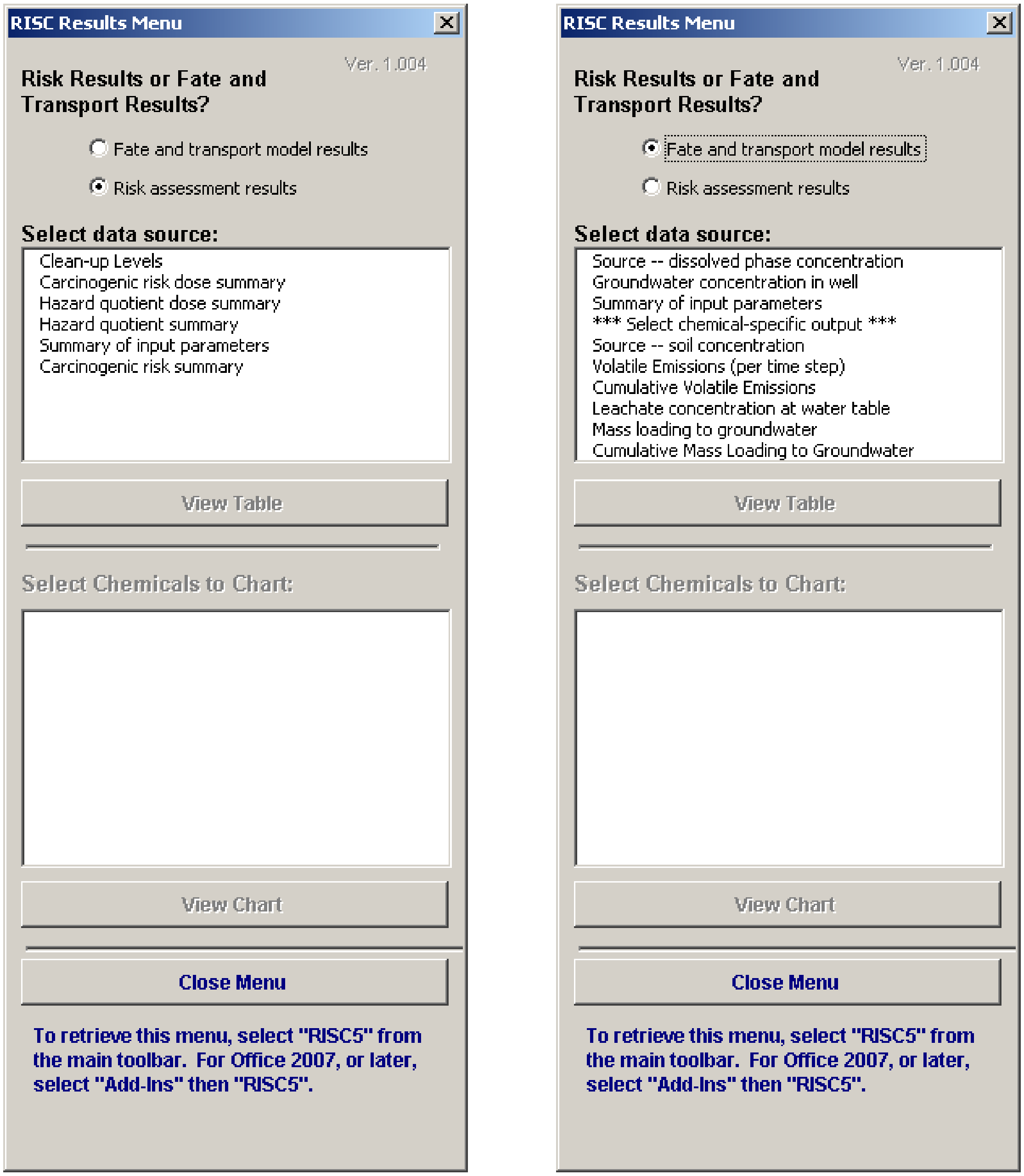
9.0

Step 6: View Results

After a successful risk calculation has been performed, the results can be viewed in Excel.

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. 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.

In Step 6 in Excel, the output tables come up automatically, i.e. they do not need to be created by clicking on the RISC output menu. The fate and transport results (if any) can be viewed by choosing “Fate and Transport Results” from the top of the RISC menu. The following figure shows the two options of the RISC Excel results menu.



Risk Results or Fate and Transport Results?

○ Fate and transport model results

● Risk assessment results

To retrieve this menu, select "RISC5" from the main toolbar. For Office 2007, or later, select "Add-Ins" then "RISC5".

Risk Results or Fate and Transport Results?

● Fate and transport model results

○ Risk assessment results

To retrieve this menu, select "RISC5" from the main toolbar. For Office 2007, or later, select "Add-Ins" then "RISC5".

Figure 9-1. The Excel Results Menu Showing the "Risk Assessment" and "Fate and Transport Model" Results Options.

10.0

Chemical Database

The RISC software contains a large chemical database that can be viewed or modified using the *Master Database Editor*. The chemical database contains physical and chemical parameters used in fate and transport modeling, toxicity values, and absorption adjustment factors for 128 chemicals.

The chemical database can be viewed by using the *Master Database Editor* and selecting the button entitled "Create Summary Table of All Data". 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).

This chapter will be revised in the next update of the RISC5 User's Guide.

10.1 PHYSICAL/CHEMICAL PROPERTIES

10.1.1 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.

10.1.2 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:

$$H' = \frac{H}{RT} \tag{10-1}$$

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] ($R = 8.2 \times 10^{-5}$)
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).

10.1.3 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)

10.1.4 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.

$$\log K_{oc} = 0.779 \log K_{ow} + 0.46 \tag{10-3}$$

$$\log K_{oc} = -0.602 \log S + 0.656 \tag{10-4}$$

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.

10.1.7 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.

10.1.8 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.

10.1.9 Degradation Rates

Degradation rates may be used in all of the fate and transport models in RISC with the exception of the Johnson and Ettinger.

The default degradation rate in the RISC database represents the minimum (slow) 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 default degradation rate 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 are assumed to be media-specific, i.e., they 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).

10.1.10 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 10-1). 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:

$$B_{va} = B_{vBaes} \times (1 - 0.85) \qquad \textbf{(10-5)}$$

$$B_{vr} = B_{vBaes} \times (1 - 0.85) \qquad \textbf{(10-6)}$$

For water:

$$RCF = B_{vBaes} \times (1 - 0.85) \times K_d \qquad \textbf{(10-7)}$$

$$ABCF = B_{vBaes} \times (1 - 0.85) \times K_d \qquad \textbf{(10-8)}$$

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.

10.2 TOXICOLOGICAL PROPERTIES

10.2.1 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 10-2. 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.

10.2.2 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.*

10.2.3 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:

$$\mathrm{RfDi}\left(\frac{\mathrm{mg}}{\mathrm{kg}\cdot\mathrm{d}}\right)=\mathrm{RfC}\left(\frac{\mathrm{mg}}{\mathrm{m}^3}\right)\times\frac{20\mathrm{m}^3}{\mathrm{d}}\times\frac{1}{70\mathrm{kg}} \tag{10-9}$$

Likewise, to calculate an SFi from a URF, the following equation is used:

$$\mathrm{SFi}\left(\frac{\mathrm{kg}\cdot\mathrm{d}}{\mathrm{mg}}\right)=\mathrm{URF}\left(\frac{\mathrm{m}^3}{\mu\mathrm{g}}\right)\times\frac{\mathrm{d}}{20\mathrm{m}^3}\times 70\mathrm{kg}\times\frac{1000\,\mu\mathrm{g}}{\mathrm{mg}} \tag{10-10}$$

10.2.4 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).

10.2.5 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:

$$\log K_p = -2.72 + 0.71 \log K_{ow} - 0.0061MW \qquad \textbf{(10-11)}$$

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.

11.0

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USEFUL WEB PAGES

The Risk Assessment Information System (RAIS) [Highly Recommended Web Site]:
http://rais.ornl.gov

U.S. EPA Risk Based Decision Making and Underground Storage Tanks home page:
http://www.epa.gov/oswer/riskassessment/oust_rbdm.htm

U.S. EPA New Exposure Factors Handbook:
http://cfpub.epa.gov/ncea/cfm/recordisplay.cfm?deid=12464

U.S. EPA Integrated Risk Information System (IRIS):
http://www.epa.gov/iris/

U.S. EPA Regional Screening Levels (Formerly USEPA Region 9 Preliminary Remediation Goals (PRGs), Region 3 Risk-Based Concentrations and Region 6 Human Health Screening Levels:
http://www.epa.gov/region9/superfund/prg/index.html

Association for the Environmental Health of Soils:
http://www.aehs.com

Texas Risk Reduction Program (TRRP):
http://www.tceq.texas.gov/remediation/trrp/trrp.html

Guidance documents for calculating clean-up levels for TPH mixtures search from (document number #366 or RG-366/TRRP-27):
http://www.tceq.texas.gov/publications/rg/rg-366_trrp_27.html

RISC5 User’s Guide

TABLE OF APPENDICES

R Review of Risk Integrated Software for Cleanups (RISC) v4.0

temporary Groundwater Mixing Zone Model (directly beneath source)

APPENDIX A: VADOSE ZONE MODEL

A.1 MODEL DESCRIPTION

The Vadose Zone model in RISC (version 5) 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, vii) first-order degradation in the leachate, viii) the presence of non-aqueous phase liquid (NAPL, i.e., free phase or residual phase concentrations), and ix) chemicals that are parts of larger mixtures (e.g. TPH).

This model is similar to the vadose zone model presented by Unlü et al. (1992), which is called the VADSAT model, with the exception of several significant differences that are discussed. The most significant difference 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 different soil properties from the rest of the vadose zone which can dramatically affect vapor emissions to the surface. Note RISC5 does not use the saturated zone portion of the VADSAT model.

The purpose of the Vadose Zone model is to predict (1) loading to groundwater and (2) volatilization rates to be used in the outdoor air model (if selected). The groundwater loading term may be used as a source input to the saturated zone model (Appendix B) when the leaching model is linked with the saturated zone model. Similarly, 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.

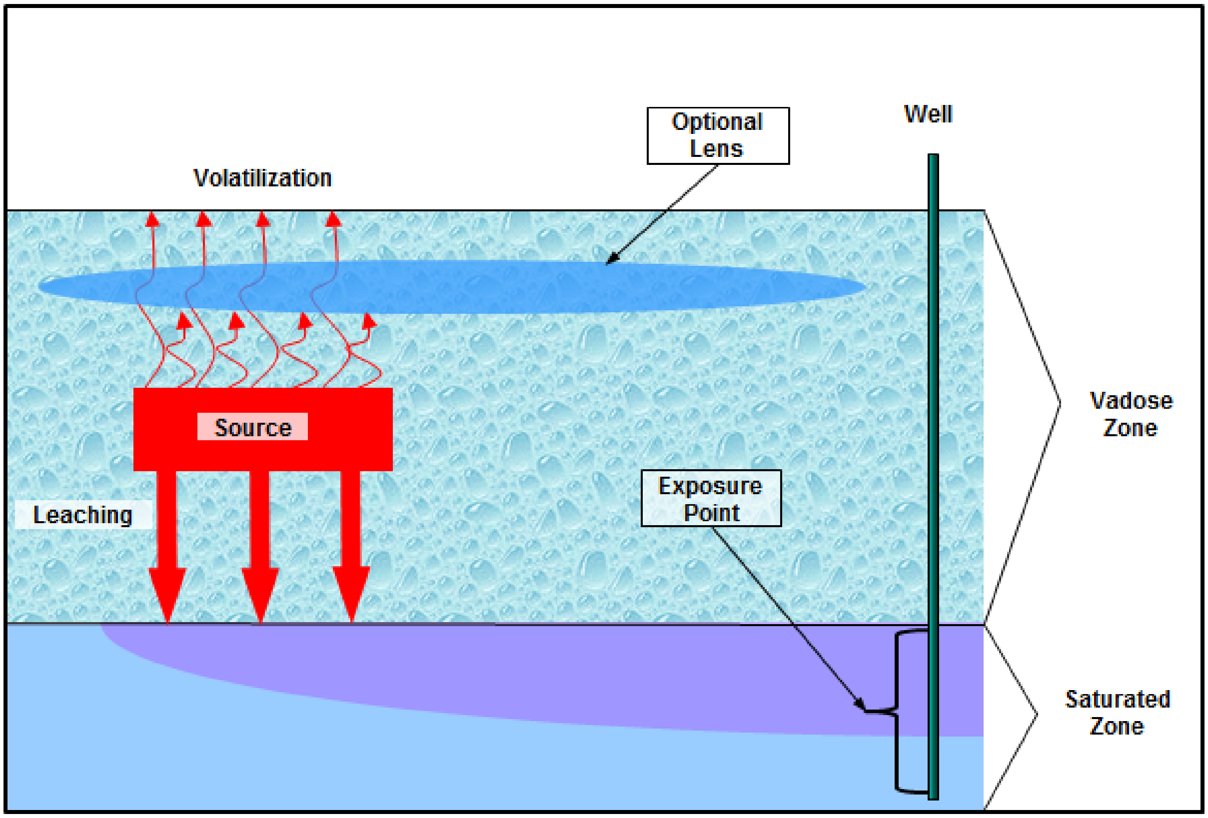

FIGURE A-1. Schematic of the Vadose Zone Model.

This appendix describes the equations used in the vadose zone model. These equations 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 saturated zone model used to predict concentrations in a downgradient well.

A.2 APPLICATIONS OF THIS MODEL

This is a partial list of the main applications and assumptions of the vadose zone model:

- The model estimates the mass loading to groundwater from a vadose zone source and estimates the volatile emissions from the soil surface. Source depletion occurs due to volatilization and leaching. Mass balance is accounted for in that the source depletes over time due to these processes.
- The estimated leaching rate may be coupled with the saturated zone model (Appendix B) or an onsite mixing model (Appendix T) to predict groundwater concentrations.
- The volatilization flux predicted by this model can be used to estimate concentrations in outdoor air (Box Model, Appendix F).

- The source term can account for the presence of a residual phase source (such as non-aqueous phase liquid [NAPL]), however, it does not model the movement of NAPL in the vadose zone. Raoult's Law is used to limit dissolved phase concentrations and vapor concentrations when the source concentrations exceed their saturation levels. It is a dissolved phase and volatile loss model only. 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.
- The model will predict losses due to degradation (first-order) in the leachate as it moves downwards through the unsaturated zone. If "0" is entered for the degradation rate; degradation will not be simulated. Degradation is assumed to occur in the dissolved phase only, in the region below the source and extending to the water table. That is, when the chemical is sorbed to the soil, it is not subject to degradation (this is a conservative, but typical assumption for dissolved phase models). To be conservative, the biological degradation is not simulated for the source zone (i.e., the only losses from the source are leaching and volatilization).
- The model accounts for the presence of non-aqueous phase liquid (NAPL) by limiting the dissolved phase concentration in the source region to the chemicals' effective solubility limit (using Raoult's Law). This is important because if the dissolved phase concentrations are not limited then groundwater concentrations may be greatly over-estimated and source mass (and longevity) will be underestimated. Depending on the scenario being simulated, ignoring Raoult's Law may not be conservative because the source depletes too fast, thereby under-estimating potential long-term carcinogenic and non-carcinogenic risk.
- The source is assumed to be located in the vadose zone. The region in the vadose zone below the source and above the top of the source 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.
- It is important to choose the source concentration and source dimensions 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 length and width of the source in the vadose zone is projected onto the water table and becomes the footprint of the groundwater source size.
- If the groundwater is already contaminated there are several ways to model the situation. Here are two ways to handle that type of situation:

    1. The model can be run so that the start of the model simulation coincides with the estimated date that the spill occurred, rather than the present day. Then the model can be run through to the present day using the current site information to calibrate the model to ensure that the model predicts the current (measured) distribution of contaminants in the soil and groundwater.

    2. If contaminants have already reached the groundwater aquifer, the leaching part of the model could be skipped, using a groundwater model instead. For the groundwater model, the source term could be modeled as either a saturated soil source or a dissolved phase groundwater source. 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 groundwater model with a constant source.

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 (uniform concentration), finite source that depletes with time, while the vadose zone above and below the source is assumed to be "clean" at the start of the simulation.

Beneath the source zone, solute transport of leachate is assumed to be one-dimensional towards the water table. Dissolved phase transport accounts for advection and dispersion processes; mass loss may occur through a first-order degradation reaction. The one-dimensional transport equation (including adsorption) in this zone is given by:

$$R \frac{\partial C_w}{\partial t} = D_x \frac{\partial^2 C_w}{\partial x^2} - \bar{v} \frac{\partial C_w}{\partial x} - \mu C_w \qquad \text{(A-1)}$$

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-xx) [-]

In equation A-1, the x-axis is assumed to be aligned with the direction of fluid flow, that is vertically downward. The model considers dispersion in the direction of fluid flow only (longitudinal dispersion). The advection-dispersion equation is used to solve for aqueous-phase concentration with depth below the source. The concentration of the leachate predicted at the water table will be used with the infiltration rate to estimate mass loading to the groundwater model (if used in the scenario).

A note on nomenclature: In this appendix the variables 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, whereas MW_{TPH} refers to the molecular weight of the TPH mixture.

A.3.1 INITIAL AND BOUNDARY CONDITIONS

In the unsaturated zone, 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-20 and A-21. At a "long distance" below the source (way below the depth to the water table) the concentration gradient is assumed to always equal zero.

$$\frac{\partial C_w}{\partial x}(\infty, t) = 0 \tag{A-4}$$

The solution for the advection-dispersion equation (A-1) with the above boundary conditions is given by van Genuchten and Alves (1982)

$$C_w(x,t) = C_0 e^{-\beta t} B(x,t) \tag{A-5}$$

where

$$B(x,t) = \frac{1}{2}\exp\left[\frac{(\bar{v}-w)x}{2D_x}\right] erfc\left[\frac{xR-wt}{2\sqrt{D_x Rt}}\right] + \frac{1}{2}\exp\left[\frac{(\bar{v}+w)x}{2D_x}\right] erfc\left[\frac{xR+wt}{2\sqrt{D_x Rt}}\right] \tag{A-6}$$

and

$$w = \bar{v}\sqrt{1 + \frac{4D_x R}{\bar{v}^2}\left[\mu - \beta\right]} \tag{A-7}$$

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-20 and A-21 [-]

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 (using Raoult's Law) 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 (i.e. the concentration gradient driving the diffusion rate changes with each time step). 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 [g/cm^2/d]
D_{eff} = effective diffusion coefficient in soil [cm^2/s]
C_{vs} = vapor-phase concentration of chemical in the source area [g chemical/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 (i.e., 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:

$$C_{vs} = K_H C_{ws}\left(\frac{L}{1000cm^3}\right)\left(\frac{g}{1000mg}\right) \tag{A-11}$$

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:

$$D_{eff\,v} = D_{air}\left(\frac{\theta_{a_v}^{\;10/3}}{\theta_{T\,v}^{\;2}}\right) + D_{water}\,\frac{1}{K_H}\left(\frac{\theta_{W\,v}^{\;10/3}}{\theta_{T\,v}^{\;2}}\right) \tag{A-12a}$$

$$D_{eff\,lens} = D_{air}\left(\frac{\theta_{a\,lens}^{\;10/3}}{\theta_{T\,lens}^{\;2}}\right) + D_{water}\,\frac{1}{K_H}\left(\frac{\theta_{W\,lens}^{\;10/3}}{\theta_{T\,lens}^{\;2}}\right) \tag{A-12b}$$

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 [cm3 pores/cm3 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):

$$D_{eff} = \frac{(h_v + h_{lens})}{\dfrac{h_{lens}}{D_{eff\,lens}} + \dfrac{h_v}{D_{eff\,v}}} \qquad \text{(A-13)}$$

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:

$$\frac{dm}{dt} = -\beta m = -\left[\bar{v}\,\theta_w + \frac{K_H D_{eff}}{L_d}\right] C_w \qquad \text{(A-14)}$$

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:

$$1 > \sum_{i=1}^{N} \frac{C_{T_i} \rho_b}{S_i \left(\rho_b K_{oc_i} F_{oc} + \theta_w + \theta_a K_{H_i} \right)} \qquad \text{(A-15)}$$

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 (A-15) 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

$$C_w = \frac{C_T \rho_b}{\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H} \qquad \text{(A-16)}$$

Again, it is assumed that C_T is the total concentration in soil, accounting for 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

$$C_w = xS \qquad \text{(A-17)}$$

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

$$x = \frac{m}{m_{TPH}} \qquad \textbf{(A-18)}$$

$$x = \frac{F_i MW_{TPH}}{MW_i F_{TPH}} \qquad \text{(A-19)}$$

where

m = total moles of component [mol] ($\frac{\rho_b L_w F_i}{MW_i} A$)

m_{TPH} = total moles of hydrocarbon mixture [mol] ($\frac{\rho_b L_w F_{TPH}}{MW_{TPH}}$ A)

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 estimated using 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, it is assumed that if immiscible phase is present initially, then it is present for the entire simulation time, however the individual mole fraction of the chemical decreases with each time step. 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

$$\beta = \frac{qMW_{TPH}S}{\rho_b L_w F_{TPH} MW} + \frac{D_{eff} K_H MW_{TPH} S}{\rho_b L_d L_w F_{TPH} MW} = \beta_w + \beta_v \qquad \text{(A-20)}$$

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

$$m = m_0 \exp(-\beta\, t) \qquad \text{(A-21)}$$

where

m_0 = initial moles of chemical per area [mol/cm^2]

The aqueous concentration decreases similarly

$$C_w = C_{w0} \exp(-\beta\, t) \tag{A-22}$$

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:

$$C_{ws} = \frac{C_T \rho_b}{\left(\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H\right)} \tag{A-23}$$

which when inserted into Equation A-14 yields:

$$\beta = \frac{q}{(\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H) L_w} + \frac{D_{eff} K_H}{(\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H) L_d L_w} = \beta_w + \beta_v \tag{A-24}$$

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:

$$k_r = \frac{q}{K_{su}} \tag{A-26}$$

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, $\bar{v}$:

$$\bar{v} = \frac{q}{\theta_w} \tag{A-29}$$

where

$\bar{v}$ = seepage velocity (actual water flow rate 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:

$$Q(L_u,t) = q\ C(L_u,t) \cdot \left(\frac{L}{1000cm^2} \right) \tag{A-30}$$

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

$$R = 1 + \frac{\rho_b F_{oc} K_{oc}}{\theta_w} \tag{A-31}$$

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.

Degradation rate = 0.693 / (half-life)

Half-life = 0.693 / (degradation rate)

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:

$$\ln \alpha_L = -4.933 + 3.811 \ln x_m \quad x_m \le 2m \tag{A-33a}$$

$$\ln \alpha_L = -2.727 + 0.584 \ln x_m \quad x_m \ge 2m \tag{A-33b}$$

where

$\boldsymbol{x_m}$ = distance from the source to the observation location [m]

A.7 DATA REQUIREMENTS

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-air)/ (mg/L-H_2O)	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 to reduce the volatilization rate). 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.

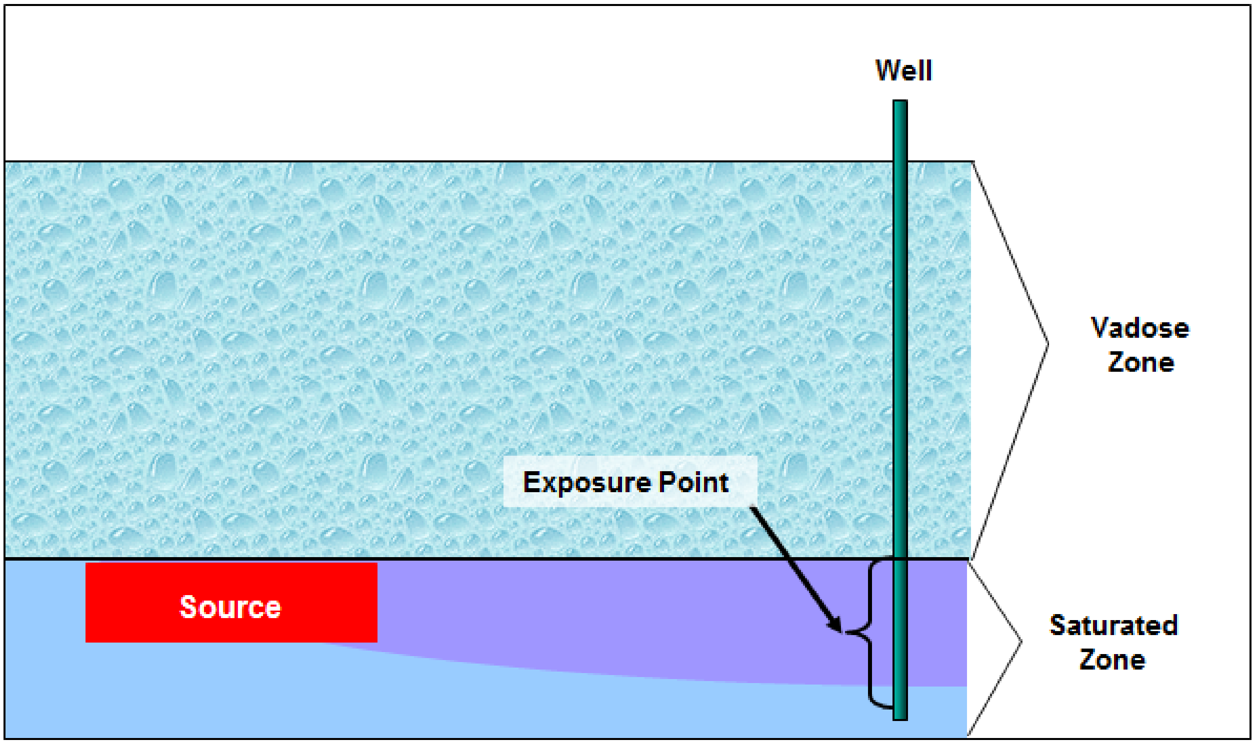

FIGURE B-1. Saturated Zone Model with Source in Groundwater

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 (Yeh, 1981):

$$\frac{\partial\, n_e C_w}{\partial\, t} = \nabla\left(n_e D_x\right)\frac{\partial^2 C_w}{\partial\, x^2} + D_y\,\frac{\partial^2 C_w}{\partial\, y^2} + D_z\,\frac{\partial^2 C_w}{\partial\, z^2} - \bar{v}\,\frac{\partial C_w}{\partial\, x} - \mu C_w + \frac{\dot{M}}{\theta}$$

$$R\,\frac{\partial\, C_w}{\partial\, t} = D_x\,\frac{\partial^2 C_w}{\partial\, x^2} + D_y\,\frac{\partial^2 C_w}{\partial\, y^2} + D_z\,\frac{\partial^2 C_w}{\partial\, z^2} - \bar{v}\,\frac{\partial C_w}{\partial\, x} - \mu C_w + \frac{\dot{M}}{\theta} \tag{B-1}$$

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

$$R = 1 + \frac{\rho_b F_{oc} K_{oc}}{\theta} \qquad \text{for organic chemicals} \tag{B-2a}$$

$$R = 1 + \frac{\rho_b K_d}{\theta} \qquad \text{for inorganic chemicals} \tag{B-2b}$$

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

$$D_x = \frac{\alpha_x V}{\theta},\quad D_y = \frac{\alpha_y V}{\theta},\quad D_z = \frac{\alpha_z V}{\theta} \tag{B-3}$$

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

$$V = K\,i \tag{B-4}$$

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

$$\bar{v} = \frac{V}{\theta} \tag{B-5}$$

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

$$\ln \alpha_x = -3.795 + 1.774 \ln x - 0.093 (\ln x)^2 \tag{B-6}$$

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:

$$\alpha_y = \frac{\alpha_x}{\tau_1},\qquad \alpha_z = \frac{\alpha_y}{\tau_2} \tag{B-7}$$

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.

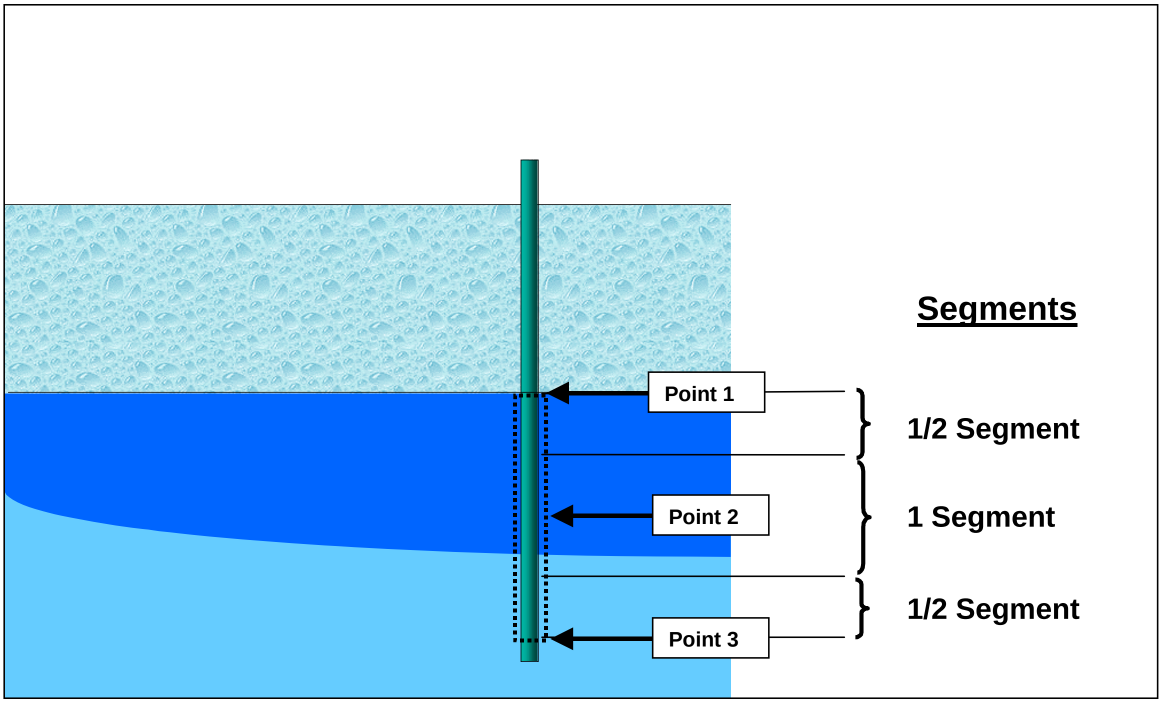

Figure B-2. Vertically Averaging the Concentration Over the Length of the Well Screen (showing 3 averaging points)

For the case shown in Figure B-2 the average concentration would be calculated from the following equation

$$C_{ave} = \frac{\frac{1}{2}C_1 + C_2 + \frac{1}{2}C_3}{2} \tag{B-8}$$

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:

$$\dot{M} = A \cdot V \cdot C_{gw} \cdot \left(\frac{1000 l}{m^3} \right) \tag{B-9}$$

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.

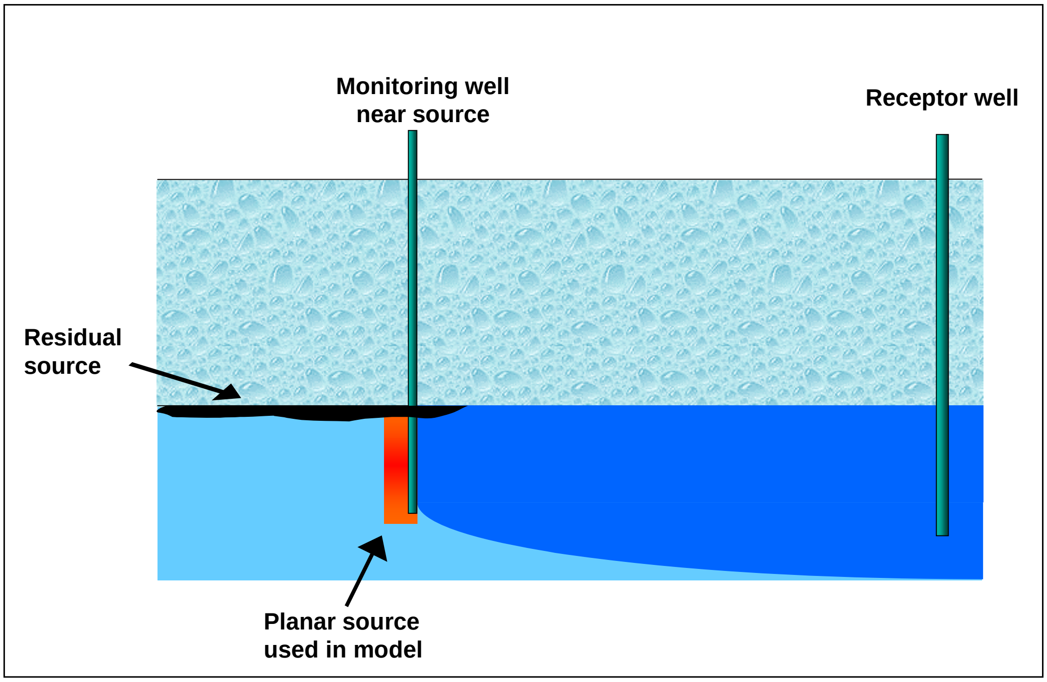

Figure B-3. Schematic of Groundwater Model With a Residual Source

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.

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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. This model was specifically designed for NAPL sources at the water table, however it can be used for any source where the user has measured soil concentrations and an estimate of the sources extent, at the water table.

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). 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.

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.

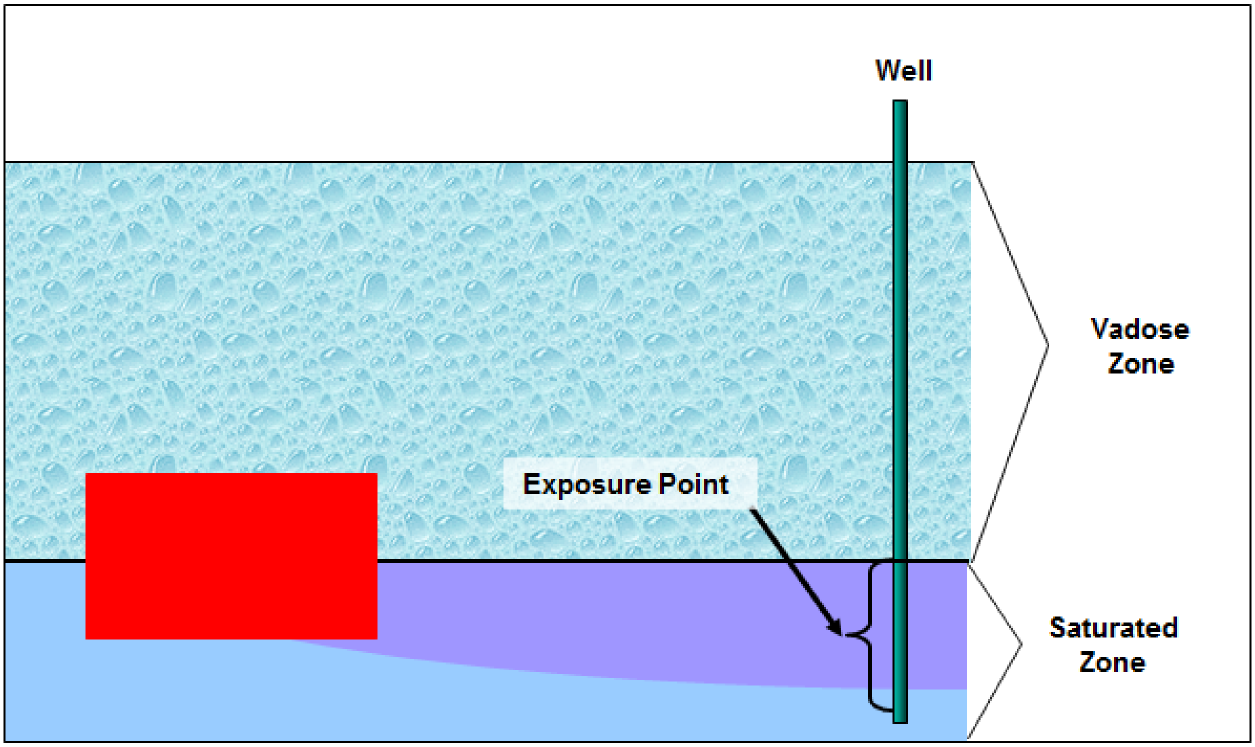

FIGURE C-1. Saturated Soil Model with Source in and above the Water Table

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 (both above and below the water table) is calculated as follows:

$$Mass = \frac{C_T \rho_b \; H \; W \; L \; \left(1E6\, cm^3/m^3\right)}{\left(1000\, g/kg\right)} \tag{C-1}$$

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

$$1 > \sum_{all\ chemicals} \frac{C_T \rho_b}{S_i \left(\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H\right)} \tag{C-2}$$

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:

$$C_w = \frac{C_T \rho_b}{\rho_b K_{oc} F_{oc} + \theta_w + \theta_a K_H} \qquad \text{(C-2a)}$$

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:

$$S_{eff_i} = \left(\frac{C_{T_i}}{C_{TPH}}\right)\left(\frac{MW_{TPH}}{MW_i}\right) S_i \qquad \text{(C-3)}$$

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 CONTRIBUTION FROM ABOVE AND BELOW WATER TABLE

The mass flux contribution from the unsaturated zone portion of the source (Q1) is calculated from:

$$Q1 = q\ A_{horz} C_{w(S1)} \qquad \text{(C-4)}$$

where

$Q1$ = mass flux contributed from the portion of the source (Source Region 1) in the unsaturated zone (due to infiltration) [g/cm^2/d]
$C_{w(S1)}$ = dissolved phase concentration of contaminant at the water table [mg/L] (where S1 indicates source region 1)
q = net infiltration rate in the unsaturated zone [cm/d]
A_{horz} = horizontal area of the source (cm^2) (source length x source width)

The dissolved phase concentration (*C*), is calculated using the equilibrium partitioning equation (checking for residual levels, as all of the soil sources in RISC).

The mass flux contribution from the saturated portion of the source (*Q2*) is calculated from:

$$Q2 = v\ A_{vert} C_{w(S2)} \tag{C-5}$$

where

$Q2$ = mass flux exiting the source contributed by the saturated portion of the source (Source Region 1) (mass flux due to groundwater flow [g/cm^2/d]

$C_{w(S2)}$ = dissolved phase concentration of contaminant in the saturated portion of the source [mg/L] (where S2 indicates source region 2)

v = darcy flux [cm/d] (hydraulic conductivity x hydraulic gradient)

A_{vert} = vertical area of the source (cm^2) (*saturated* source thickness x source width)

If the water table is fluctuating, the mass contributions are adjusted accordingly by adjusting the vertical area of the source for the period of high water table.

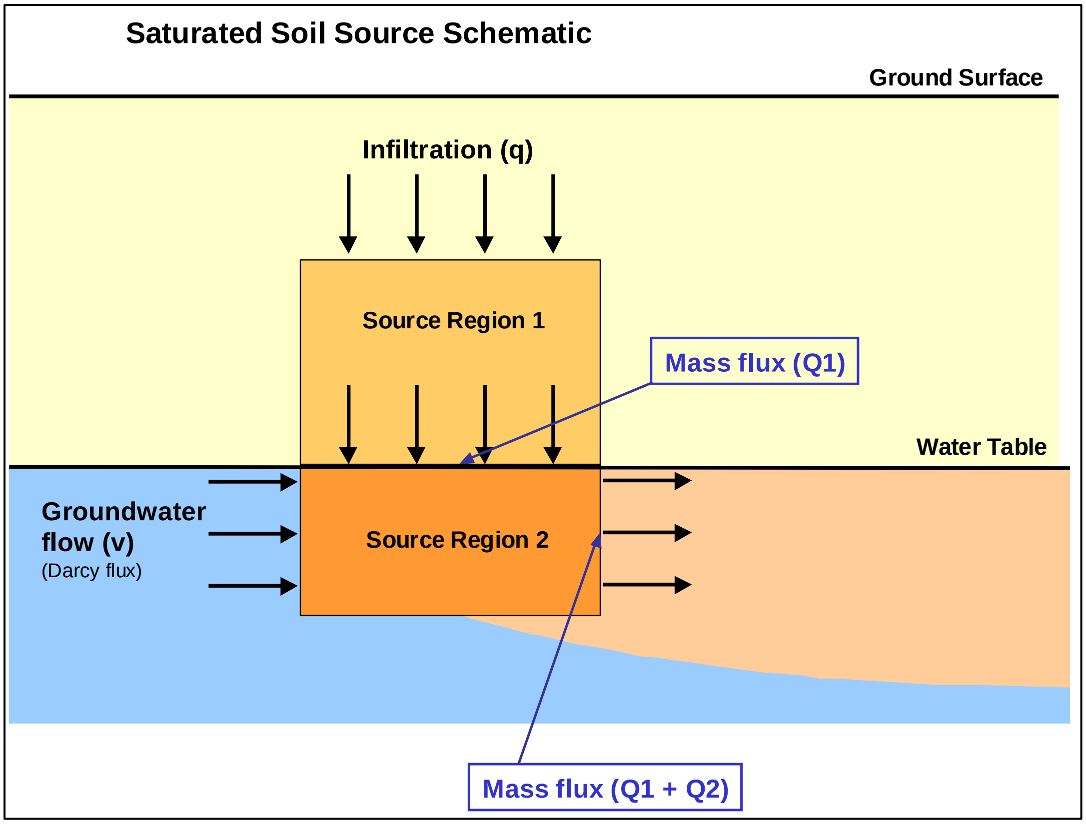

Figure C-1. Saturated Soil Schematic.

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
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

Table C-1. Data Requirements for the Saturated Soil Model
(Page 2 of 2)

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.

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APPENDIX D: JOHNSON AND ETTINGER MODEL

(VAPOR INTRUSION WITHOUT DEGRADATION)

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.

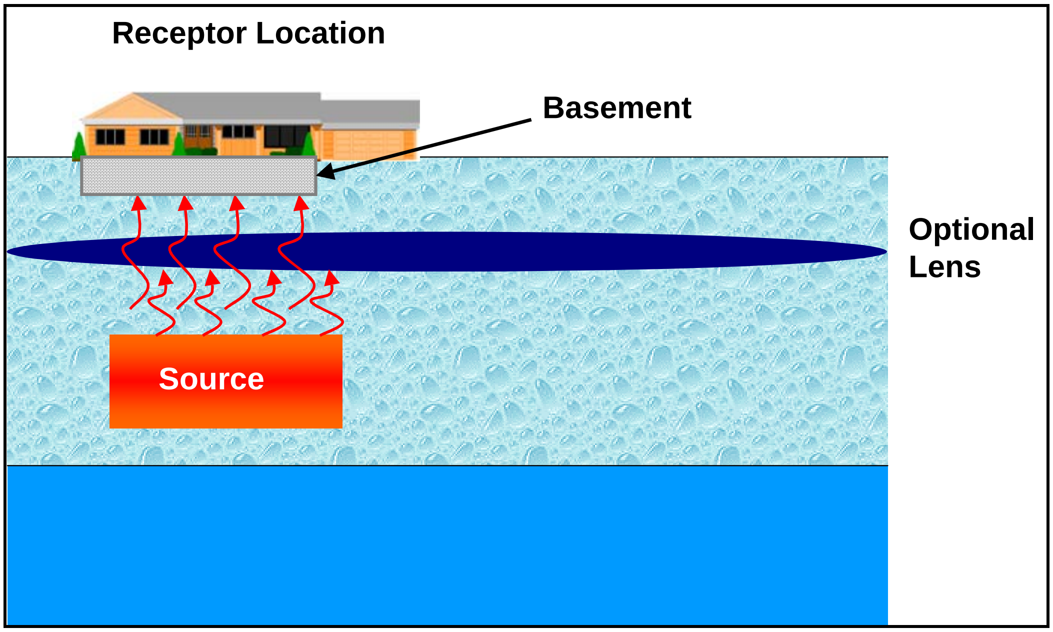

Figure D-1. Schematic of the Vapor Transport Model.

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:

$$E = \frac{A_B \left(C_{vs} - C_{vf} \right) D_{eff}}{L_T} \tag{D-1}$$

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 [g/cm^3]

C_{vf} = vapor concentration in the soil just outside the building foundation [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:

$$E = Q_{soil} C_{vf} - \frac{Q_{soil}\left(C_{vf} - C_{indoor}\right)}{\left[1 - \exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right)\right]} \tag{D-2}$$

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}:

$$C_{vf} = \frac{\left[C_{vs}\left[\frac{D_{eff} A_B}{Q_{soil} L_T}\right]\left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) - 1\right] + C_{indoor}\right]}{\left[\left[\frac{D_{eff} A_B}{Q_{soil} L_T}\right]\left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) - 1\right] + \exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right)\right]} \tag{D-3}$$

Substituting D-3 into equation D-2 yields:

$$E = \frac{\left[\left[\frac{D_t^{eff} A_B C_{vs}}{L_T}\right]\left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) - \left[\frac{C_{indoor}}{C_{vs}}\right]\right]\right]}{\left[\left[\frac{D_T^{eff} A_B}{Q_{soil} L_T}\right]\left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) - 1\right] + \exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right)\right]} \qquad \text{(D-4)}$$

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:

$$Q_B C_{indoor} = E \qquad \text{(D-5)}$$

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

$$C_{indoor} = \frac{C^*_{indoor}\left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right)\right]}{\left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) + \left[\frac{D_{eff} A_B}{Q_B L_T}\right] + \left[\frac{D_{eff} A_B}{Q_{soil} L_T}\right]\left[\exp\left(\frac{Q_{soil} L_{crack}}{D_{crack} A_{crack}}\right) - 1\right]\right]} \qquad \text{(D-6)}$$

where

$$C^*_{indoor} = \frac{D_{eff} A_B C_{vs}}{Q_B L_T} \qquad \text{(D-7)}$$

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):

$$Q_{soil} = \frac{2\pi(\Delta P)k_v X_{crack}}{\mu \ln\left[2Z_{crack} / r_{crack}\right]} \qquad \frac{r_{crack}}{Z_{crack}} << 1 \qquad \text{(D-8)}$$

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:

$$r_{crack} = \frac{\eta A_B}{X_{crack}} \tag{D-9}$$

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):

$$C_{vs} = \frac{C_T \rho_b K_H}{\theta_a K_H + \theta_w + \rho_b F_{oc} K_{oc}} \left(\frac{kg}{1E6mg} \right) \qquad \text{(D-10)}$$

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

$$C_{vs} = \frac{x_i P_v{}^{i} MW_i}{RT} \qquad \text{(D-11)}$$

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

$$x_i = \left(\frac{C_T}{C_{TPH}} \right) \left(\frac{MW_{TPH}}{MW} \right) \qquad \text{(D-12)}$$

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

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

The groundwater vapor transport model is the Johnson and Ettinger model described in Appendix D. In this case (volatilization from groundwater), the soil gas concentration is calculated from the groundwater concentration by multiplying the groundwater concentration and the chemical's Henry's Law coefficient. The capillary fringe is treated as another layer (with different air and water contents – see the depth-weighted average approach shown in Appendix D).

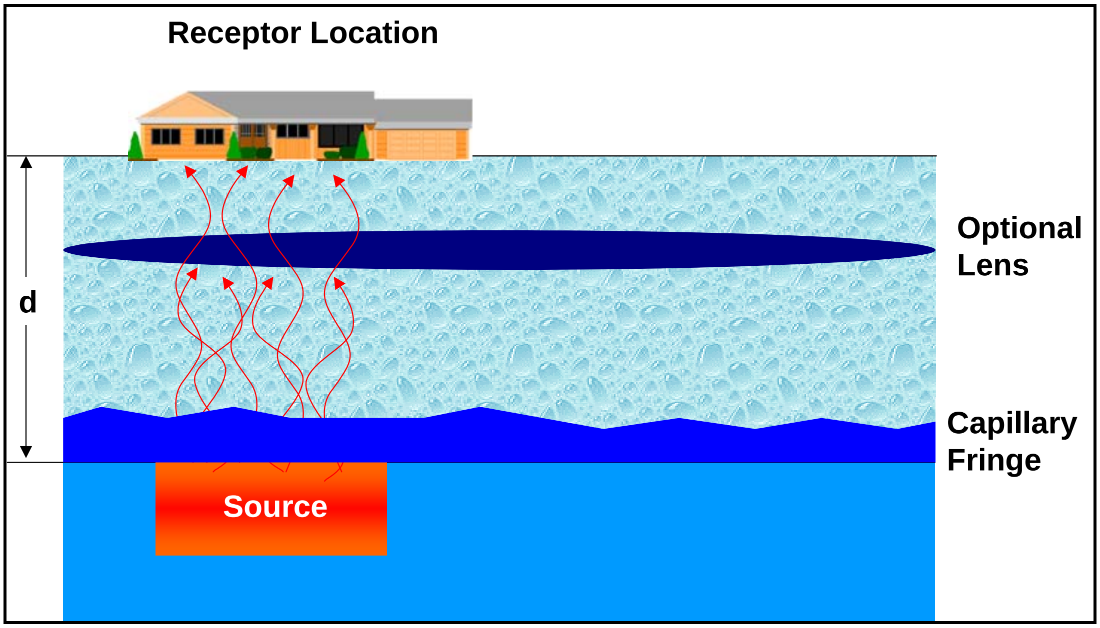

Figure E-1. Schematic of the Vapor Transport Model from Groundwater into Buildings.

E.2 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:

$$C_{vs} = C_{gw} K_H \left(\frac{L}{1000 cm^3} \right) \cdot \left(\frac{g}{1000 mg} \right) \tag{E-2}$$

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 water table surface because the vapor concentrations would be 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.2.1 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. The overall diffusion coefficient is given by:

$$D_{eff} = (d_{cap} + d_v + d_{lens} + d_{bldg})\left[\frac{d_{cap}}{D_{eff\ cap}} + \frac{d_v}{D_{eff\ v}} + \frac{d_{lens}}{D_{eff\ lens}} + \frac{d_{bldg}}{\eta D_{eff\ bldg}}\right]^{-1} \qquad \text{(E-3)}$$

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):

$$D_{eff\,i} = D_{air}\frac{\theta_{ai}^{\;3.33}}{\theta_{Ti}^{\;2}} + \frac{D_{water}}{K_H}\frac{\theta_{wi}^{\;3.33}}{\theta_{Ti}^{\;2}} \tag{E-4}$$

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)]

The following two figures illustrate options for calculating vapor intrusion from groundwater when the receptor is located downgradient of the source region.

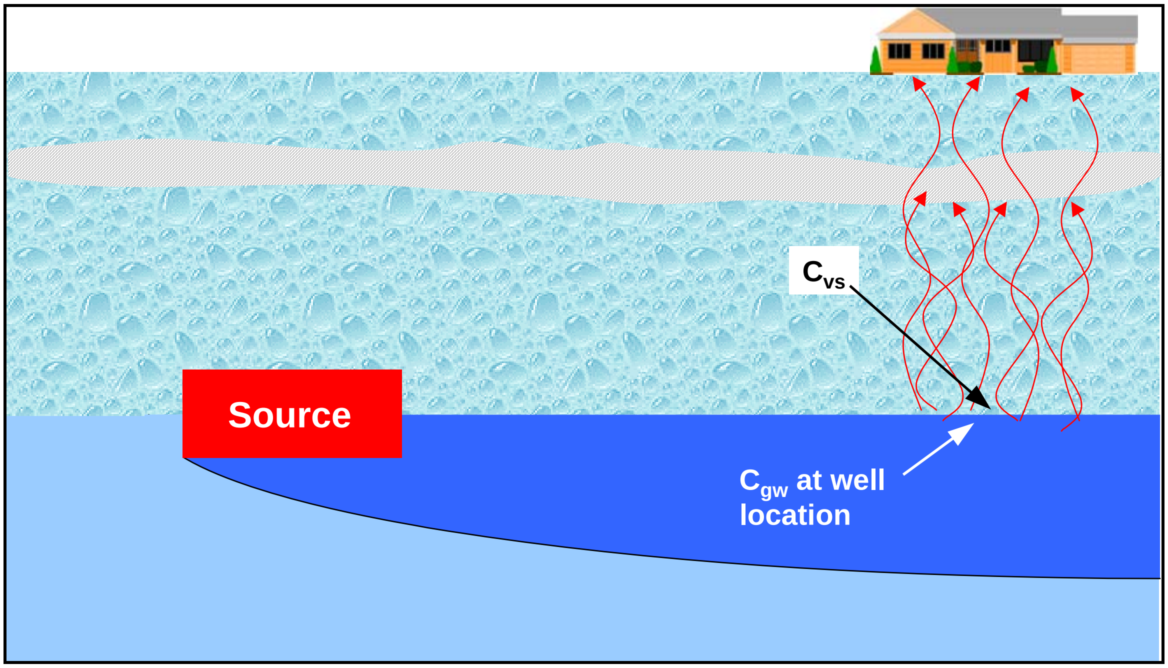

Figure E-2. Vapor Transport from Groundwater Using a Saturated Zone Fate and Transport Model to Estimate Source Concentrations

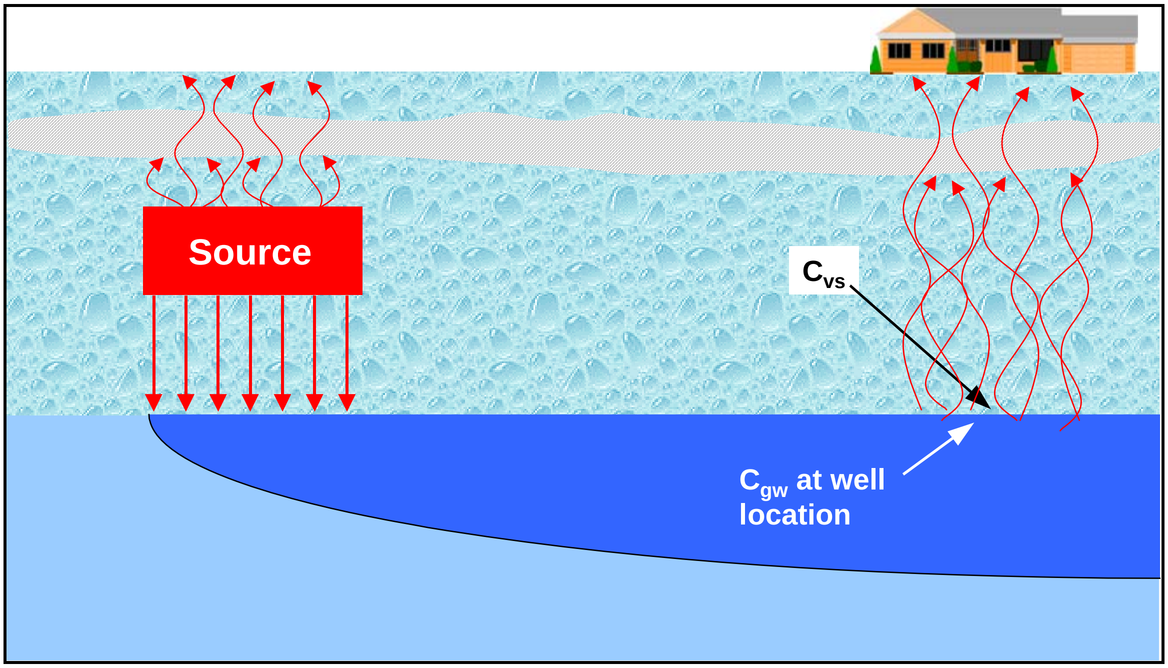

Figure E-3. Vapor Transport from Groundwater Using a Linked Vadose Zone and Dissolved Phase Transport Model

E.3 REFERENCES

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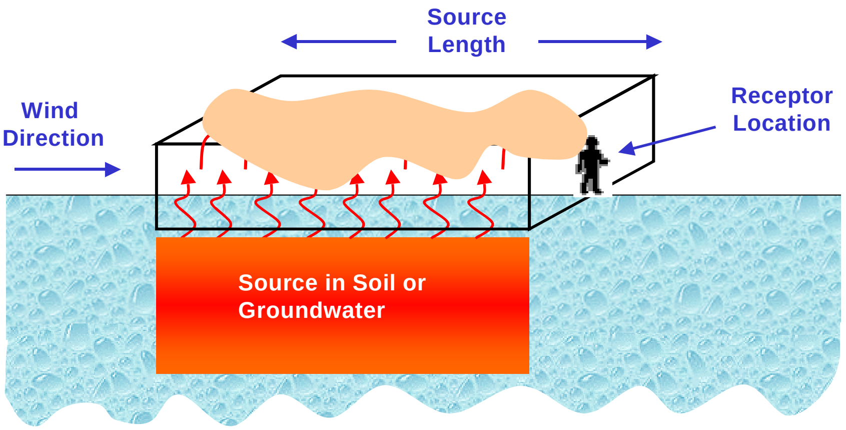
APPENDIX F: OUTDOOR AIR MODEL

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 the unsaturated zone model (discussed in Appendix A).

- 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

$$F = \frac{D_{eff}\left(C_{vs} - C_{vf}\right)}{L_d} \tag{F-2}$$

$C_{outdoor}$ = 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 the unsaturated zone model (Appendix A). 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 emission rate calculated by the unsaturated zone model as a source term. This means that the volatile emission rate changes (decreases) every time step as the soil concentration decreases.

APPENDIX G: VOLATILIZATION IN THE SHOWER AND 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:

$$C_{sh} = \frac{M_{sh}}{V_{sh}} \tag{G-1}$$

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:

$$M_{sh} = f_v > Q > time_{sh} > C_w > 60 \text{ min/hr} \tag{G-2}$$

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):

$$K_{\mathrm{L}} = \left[\frac{1}{k_l} + \frac{1}{K_H k_g} \right]^{-1} \tag{G-3}$$

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 °C: $\mu = 100 \cdot 10^{y}$

and

$$y = \frac{1301}{998.33 + 8.1855(T - 20) + 0.00585(T - 20)^2} - 3.30233 \qquad \text{(G-7)}$$

If T > 20 °C: $\mu = 1.002 \cdot 10^{y}$

and

$$y = \frac{-1.3272(T - 20) - 0.001053(T - 20)^2}{T + 105} \qquad \text{(G-8)}$$

Volatilization is assumed to be a first-order process, described by the differential equation:

$$\frac{dC_{sw}}{dt} = -K'_L \, aC_{sw} \qquad \text{(G-9)}$$

Integrating G-9 yields:

$$C_{sw} = C_w e^{-\frac{K'_L 6t}{d(3600)}} \qquad \text{(G-10)}$$

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:

$$C_{air} = \frac{\dot{M}}{W \cdot H \cdot u} \tag{G-12}$$

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:

$$\dot{M} = Q_{sprinkler} \cdot f_v \cdot C_w \tag{G-13}$$

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.

		Typical Range of Values	
	Units	**Minimum**	**Maximum**
SPRINKLER DATA			
Temperature of water	^oC		
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: PARTICULATE EMISSIONS MODEL

H.1 MODEL DESCRIPTION

The particulate emissions (or dust) model is used to predict the concentration of dust particles in the breathing zone directly overlying contaminated surface soil. The dust particles are also called “fugitive dust” because their presence in the air is caused by wind erosion, not point source emissions. Fugitive dusts results from particle entrainment from the soil surface; thus contaminant concentrations in the surface soil horizon (e.g., the top 2 centimeters) are of primary concern for this pathway. For volatile emissions, the contaminants can originate from the entire soil column. In contrast, the top 2 centimeters of surface soil is the source for dust emissions. Note, these top 2 centimeters are likely to be depleted of volatile contaminants at most sites, therefore this pathway is usually only important for non-volatile organic and inorganic contaminants, such as metals.

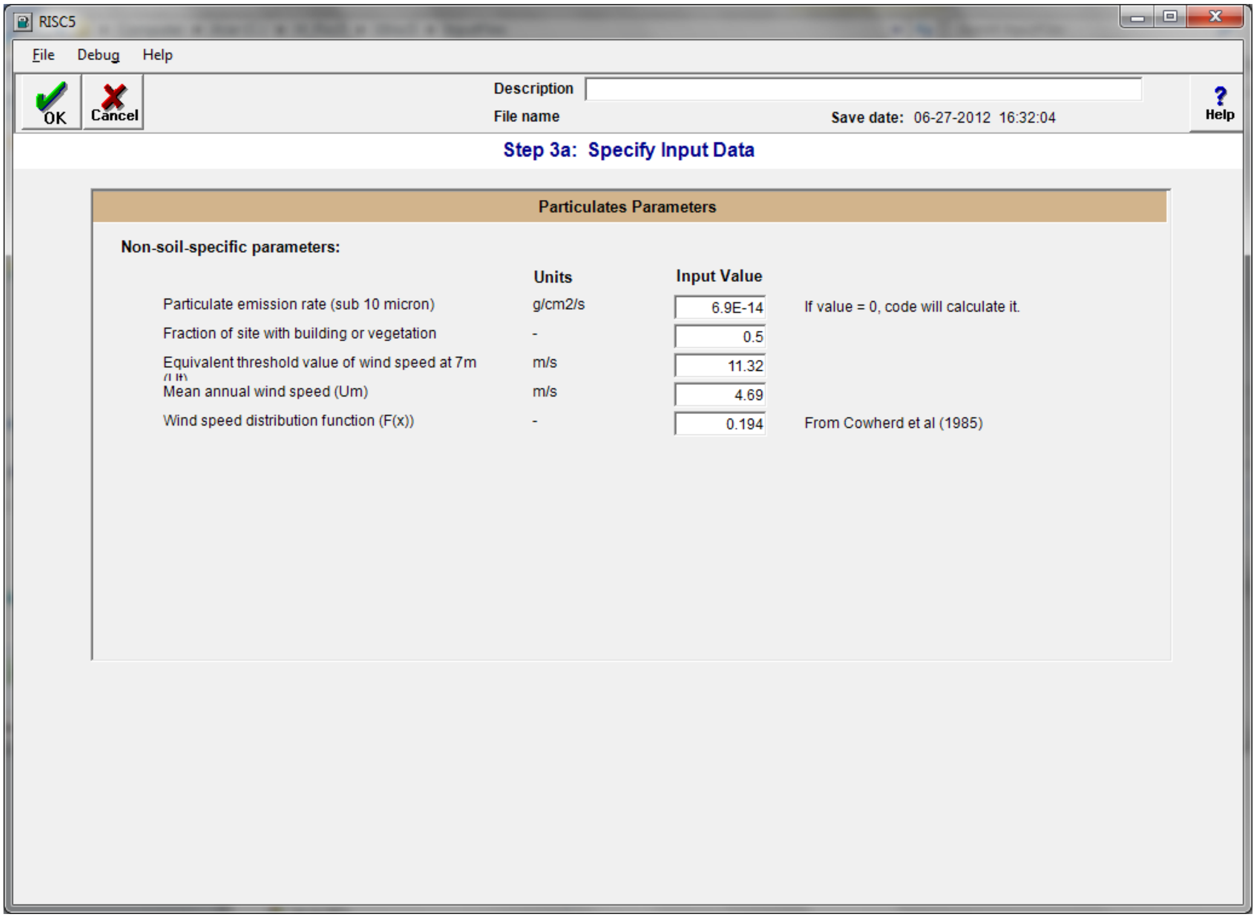
It is generally assumed that, although humans can breathe particles up to 150 µm (microns) in size, most of the large particles are trapped by the nose and mouth. It is assumed that all particles less than 10 microns may be transferred to the lungs, and therefore available for uptake into the body. This sub 10 micron range is usually referred to as PM10 and it represents the respirable, dust-sized particles.

There are two ways that uptake from dust emissions can be modeled in RISC5:

1. The Particulate Emission Factor (PEF) may be specified directly by the user. The particulate emission factor is combined with the outdoor air “box” model (Appendix F) to estimate the concentration of particulates, and hence, contaminants in the air. This is the approach taken in ASTM, 2002.
2. The particulate emission can be calculated using the algorithm presented by Cowherd et al. (1985). Once the particulate emission rate is calculated, the outdoor air concentration is estimated using the outdoor “box” model (Appendix F). This is the approach used in the US EPA Soil Screening Guidance (1996) and the UK CLEA model (2009).

H.2 OPTION 1: SPECIFYING A PEF FACTOR

In this option, the user specifies the particulate emission factor explicitly. Figure S-1 shows the input screen for the particulate data in Step 3a.



Description

File name

Save date: 06-27-2012 16:32:04

Step 3a: Specify Input Data

Particulates Parameters

Non-soil-specific parameters:

	Units	Input Value	
Particulate emission rate (sub 10 micron)	g/cm2/s	6.9E-14	If value = 0, code will calculate it.
Fraction of site with building or vegetation	-	0.5	
Equivalent threshold value of wind speed at 7m (Ut)	m/s	11.32	
Mean annual wind speed (Um)	m/s	4.69	
Wind speed distribution function (F(x))	-	0.194	From Cowherd et al (1985)

FIGURE H-1. Input Screen for Particulate Data

The first parameter is the particulate emission rate (sub 10 micron) in g/cm^2/s. If this value is greater than zero, then the particulate emission rate specified will be used (it will not be calculated using the particulate emission model). The default value shown for particulate emission rate, 6.9E-14 g/cm^2/s, is from the ASTM (1995).

H.3 OPTION 2: CALCULATING A PEF FACTOR

The algorithm used to calculate a Particulate Emission Factor (PEF) is based on the USEPA 1996 Soil Screening Guidance. This approach assumes that dust is generated by wind action alone (as opposed to, for example, trucks driving on a dirt road or playing sports on a dirt field). If there is reason to believe that other factors could be significant contributors to airborne dust levels, another method for estimating exposure should be used.

The air concentration of PM10 is calculated by

$$J_w = 0.036 \times (1 - V) \times (U_m / U_t)^3 \times F_{(x)} \times \frac{1}{3{,}600 \ \ s/hr} \times \frac{m^2}{1E4cm^2} \qquad \text{(H-1)}$$

where

J_w = particulate emissions factor [g/cm^2/s]
V = fraction of the site with building or vegetative cover [dimensionless]
U_m = mean annual wind speed [m/s]
U_t = threshold value of wind speed at height of 10 m, [m/s] (Discussed in the CLEA attachment to this appendix.)
$F(x)$ = wind speed distribution function from Cowherd et al (1985) [dimensionless] (Discussed in the CLEA attachment to this appendix.)

H.3.1 INPUT PARAMETER VALUES

The default values used in RISC5 are from the USEPA Soil Screening Guidance document (USEPA 1996), see Table S-1. At the end of this appendix, however, the section of the UK CLEA technical background document is presented with an alternative set of default input parameters.

Table H-1. Summary of Input Parameters.

Definition (units)	Parameter Symbol	Default Value	Source
Fraction of vegetative cover (-)	V	0.5 (50%)	U.S. EPA, 1991
Mean annual wind speed (m/s)	Um	4.69	EQ, 1994
Equivalent threshold value of wind speed at 7 m (m/s)	Ut	11.32	U.S. EPA, 1991
Function dependent on Um/Ut derived using Cowherd et al. (1985) (unitless)	F(x)	0.194	U.S. EPA, 1991

H.4 REFERENCES

ASTM. 1995. Standard Guide to Risk-Based Corrective Action Applied at Petroleum Release Sites, ASTM E1739-95.

EQ (Environmental Quality Management). 1994. Revisions to VF and PEF Equations. Memorandum #5099-3. Prepared for Office of Emergency and Remedial Response, U.S. Environmental Protection Agency, Washington DC.

U.K. Environment Agency. January 2009. Updated Technical Background to the CLEA Model. SC050021/SR3. http://www.environment-agency.gov.uk/static/documents/Research/CLEA_Report_-_final.pdf

U.S. Environmental Protection Agency. 1991. Risk Assessment Guidance for Superfund, Volume I: Human Health Evaluation Manual (Part B, Development of Risk-Based Preliminary Remediation Goals). Iterim. Publication 9285.7-01B, Office of Emergency and Remedial Response, Washington, DC. NTIS PB91-921359/CCE.

U.S. Environmental Protection Agency. May 1996. Soil Screening Guidance: Technical Background Document, Office of Solid Waste and Emergency Response, EPA/540/R-95/128.

APPENDIX I: IRRIGATION WATER MODEL

I.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.

I.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.

I.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.

I.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.

I.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. (The equation numbers need to be updated.)

I.6 REFERENCES

Walden, J.T and Spence. L.R. 1997. Risk-Based BTEX Screening Criteria for a Groundwater Irrigation Scenario*.* *Journal of Human and Ecological Risk Assessment*, Vol. 3, No. 4, pp. 699-722.

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 indoor. The model can consider both diffusive and advective transport through the soil and into the building foundation. When run with a degradation rate equal to zero, this model is identical to the Johnson and Ettinger model (Johnson and Ettinger, 1991, Appendix D).

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.

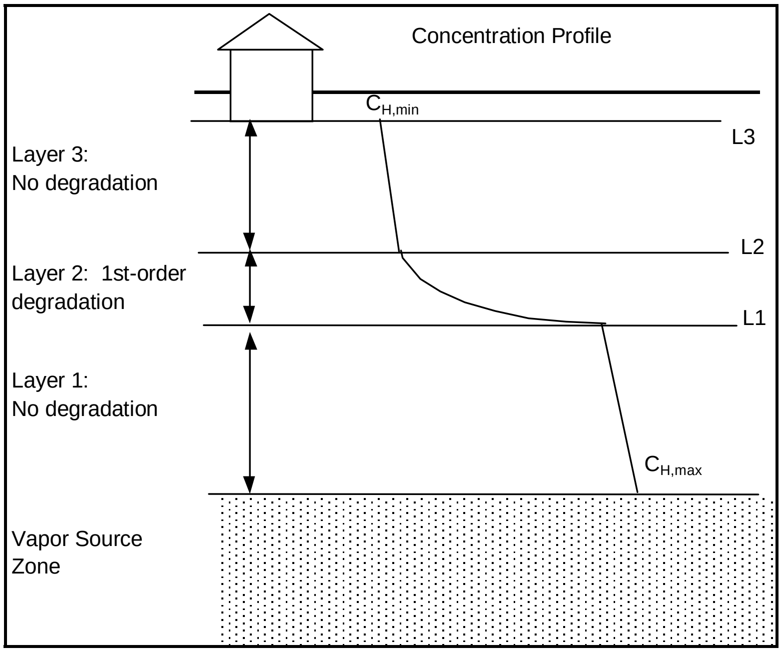


Figure J-1. Schematic of the Dominant Layer Vapor Transport Model.

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 ($0<z<L_1$):

$$C_v(z) = C_{vs} - (C_{vs} - C_{v2})\left(\frac{z}{L_1}\right) \tag{J-1}$$

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.

$$D_i^{eff} = D_{air}\left(\frac{\theta_a^{3.33}}{\theta_T^2}\right) + \frac{D_{water}}{K_H}\left(\frac{\theta_m^{3.33}}{\theta_T^2}\right) \tag{J-5}$$

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 CALCULATING ATTENUATION AND INDOOR AIR CONCENTRATIONS

Similar to Johnson and Ettinger (1991) for enclosed spaces the attenuation factor is calculated from:

$$\alpha = \frac{C_{indoor}}{C_{vs}} = \frac{1-\beta}{(1-\beta)\left(\frac{Q_B}{2\phi\gamma\psi}\right) + \left(\beta\left(\frac{Q_B}{Q_{soil}}\right)-1\right)\left(\frac{1+\gamma\psi-4\psi^2}{2\gamma\psi^2}\right)} \qquad \text{(J-6)}$$

where:

$$\beta = 1-\exp\left(\frac{Q_{soil}L_{crack}}{D_{crack}A_{crack}}\right) \qquad \text{(J-7)}$$

$$\gamma = \left(\frac{D_1^{eff}}{D_2^{eff}}\right)\left(\frac{\exp(-\eta)-\exp(\eta)}{\eta}\right)\left(\frac{L_2-L_1}{L_1}\right) \qquad \text{(J-8)}$$

$$\psi = \frac{1}{\exp(-\eta)+\exp(\eta)-\gamma} \qquad \text{(J-9)}$$

$$\phi = \left(\frac{A_B D_3^{eff}}{L_3-L_2}\right)\frac{1}{\left[\sigma-(1/\psi)-\gamma+4\psi\right]} \qquad \text{(J-10)}$$

$$\sigma = \left(\frac{D_3^{eff}}{D_2^{eff}}\right)\left(\frac{\exp(-\eta)-\exp(\eta)}{\eta}\right)\left(\frac{L_2-L_1}{L_3-L_2}\right) \qquad \text{(J-11)}$$

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:

$$E = C_{indoor} * Q_B \qquad \text{(J-12)}$$

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:

$$C_H^{\max} = C_w K_H \qquad \text{(J-15)}$$

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.

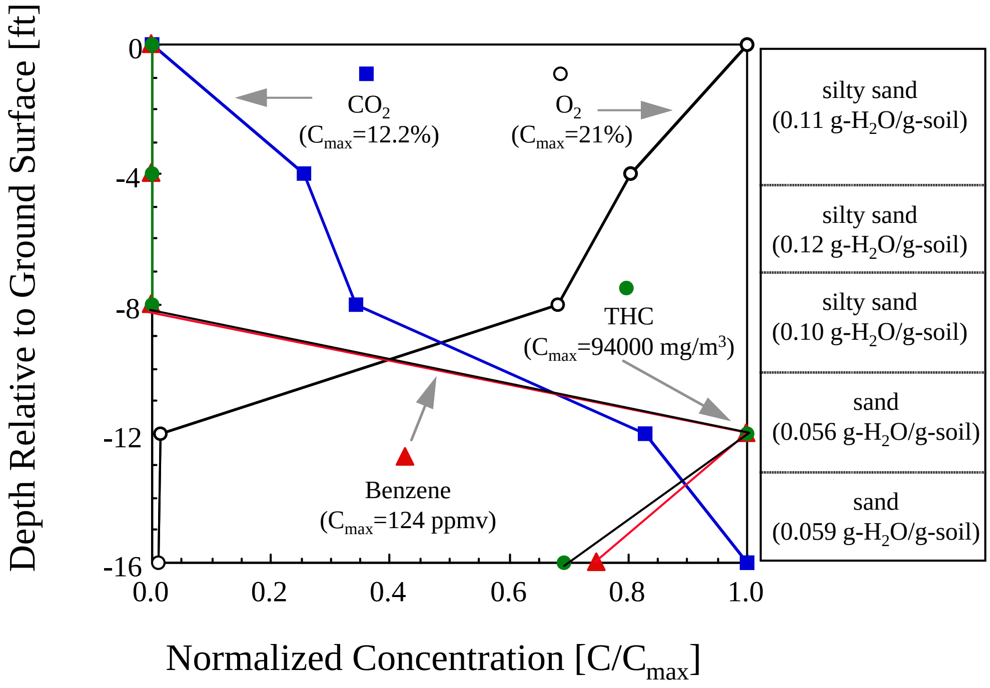


Figure J-2. Data Used for the Example Problem, from BP (1997).

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 MODEL PARAMETERS USED IN EXAMPLE PROBLEM

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.

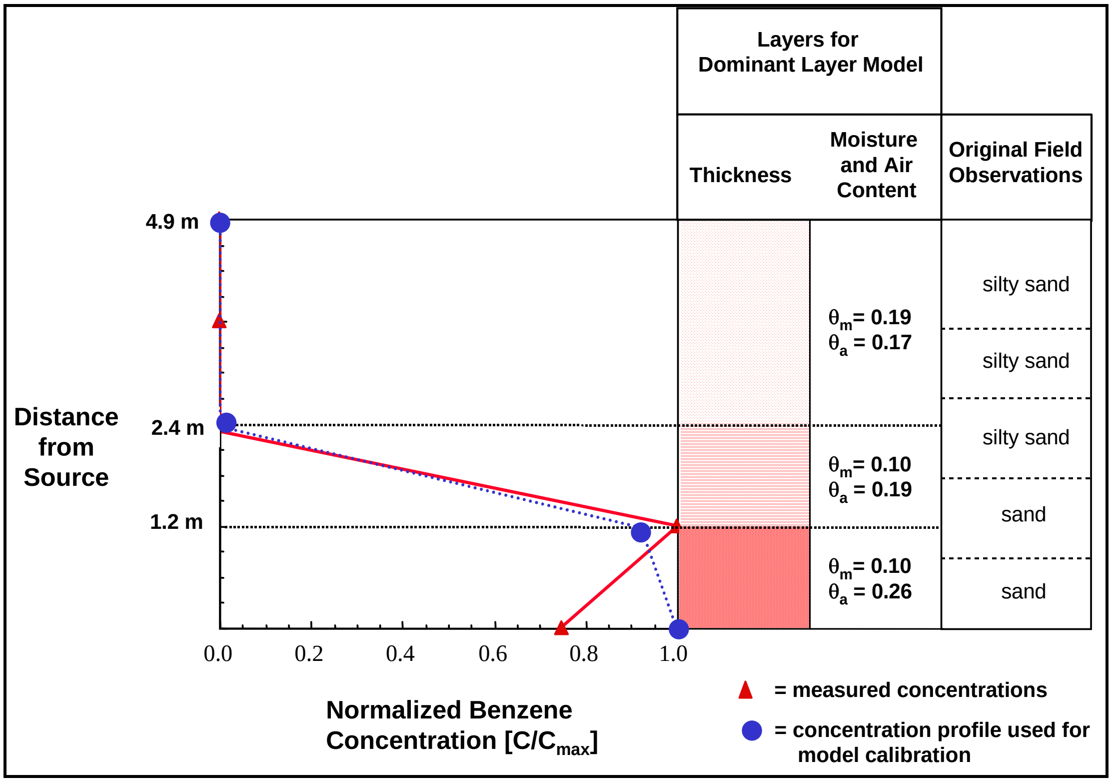


Figure J-3. Layers for the Dominant Layer Model.

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.

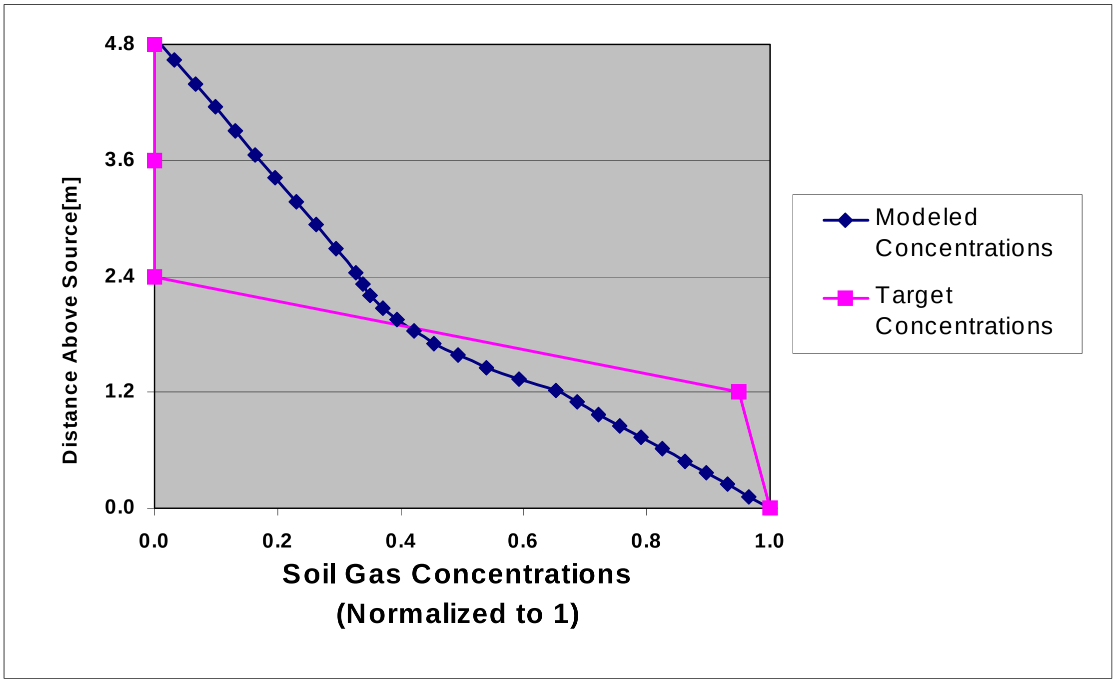


Figure J-4. Model Results Using the Reported Diffusion Coefficients, the "Base Case"

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.

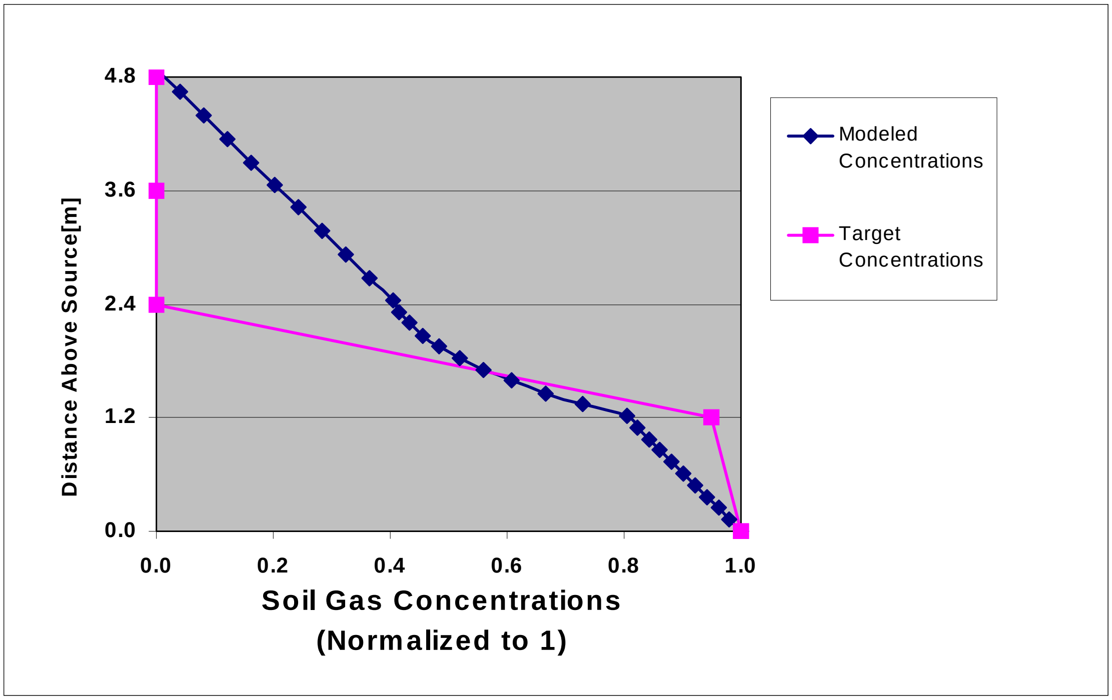


Figure J-5. Model Results for the "Dry Case" in Bottom Layer

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.

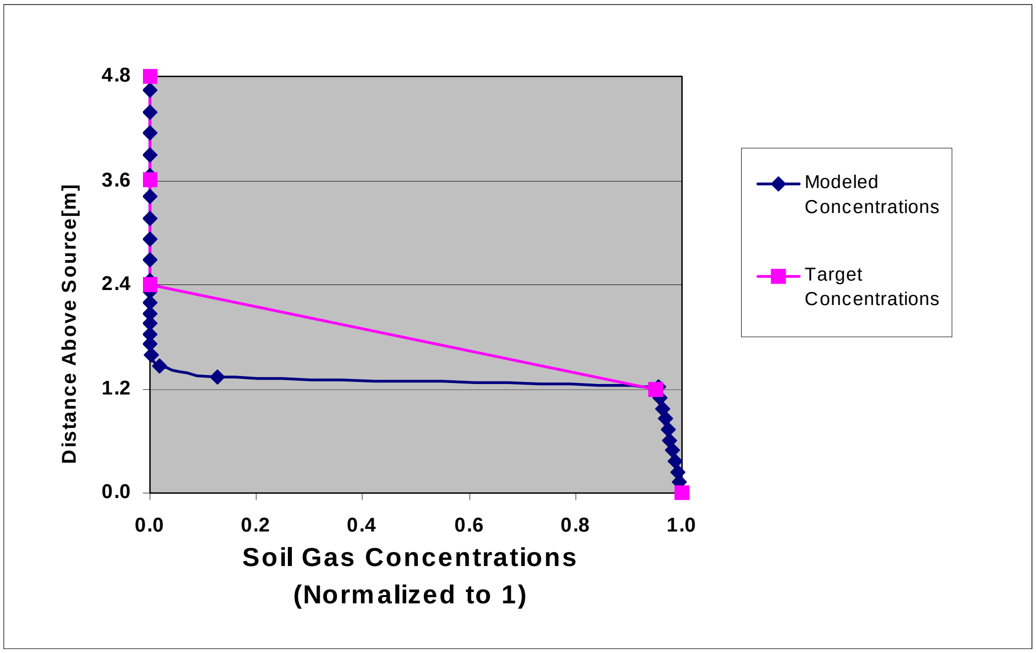


Figure J-6. Model Results Using a Dry Bottom Layer and a Wet Middle Layer

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).

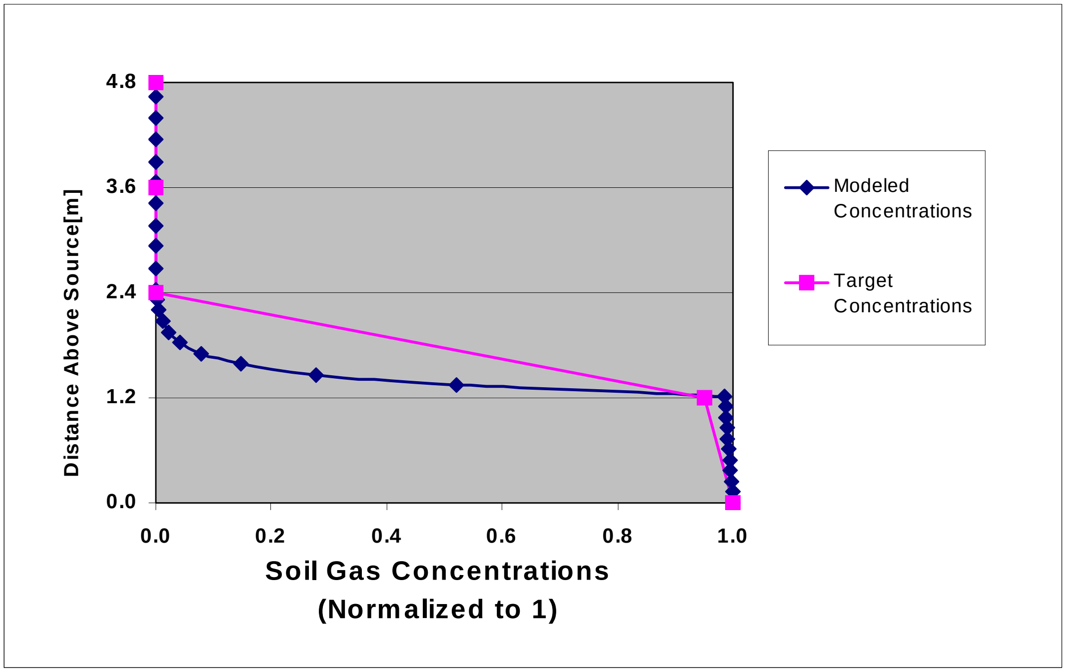


Figure J-7. Model Results With A Degradation Rate of 0.007/d

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-3.

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

British Petroleum. 1997. Summary of Field Activities Hydrocarbon Vapor Migration Research Project BP Oil Test Site Paulsboro, New Jersey. Prepared by Integrated Science and Technology, Inc.. Cleveland, OH. February.

Howard, P.H., et al. 1991. Handbook of Environmental Degradation Rates, Lewis Publishers Inc., Chelsea, MI.

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., December 1998. 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.

Millington, J.J. and Quirk, J.P. 1961. Permeability of Porous Solids. Trans. Faraday Soc., 57. 1200-1207.

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 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.

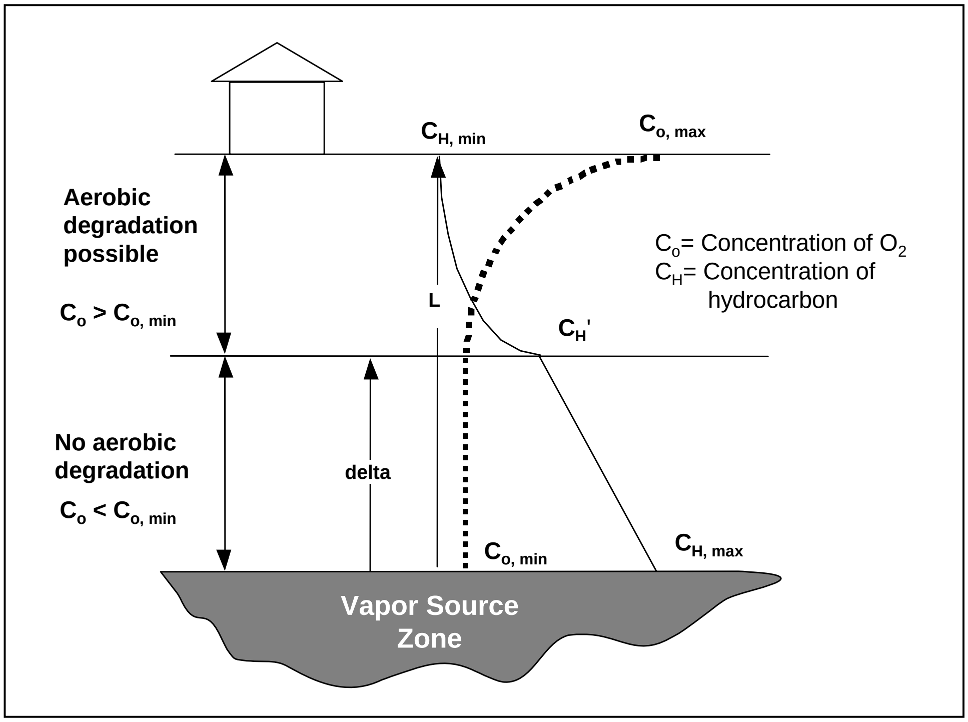


Figure K-1. Schematic of the Oxygen-Limited Vapor Transport Model.

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 building foundation. 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 Concentrations?	No	No	Yes	No
Considers Pressure-Driven Flow by Building?	Yes	Yes	Yes	Yes
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.

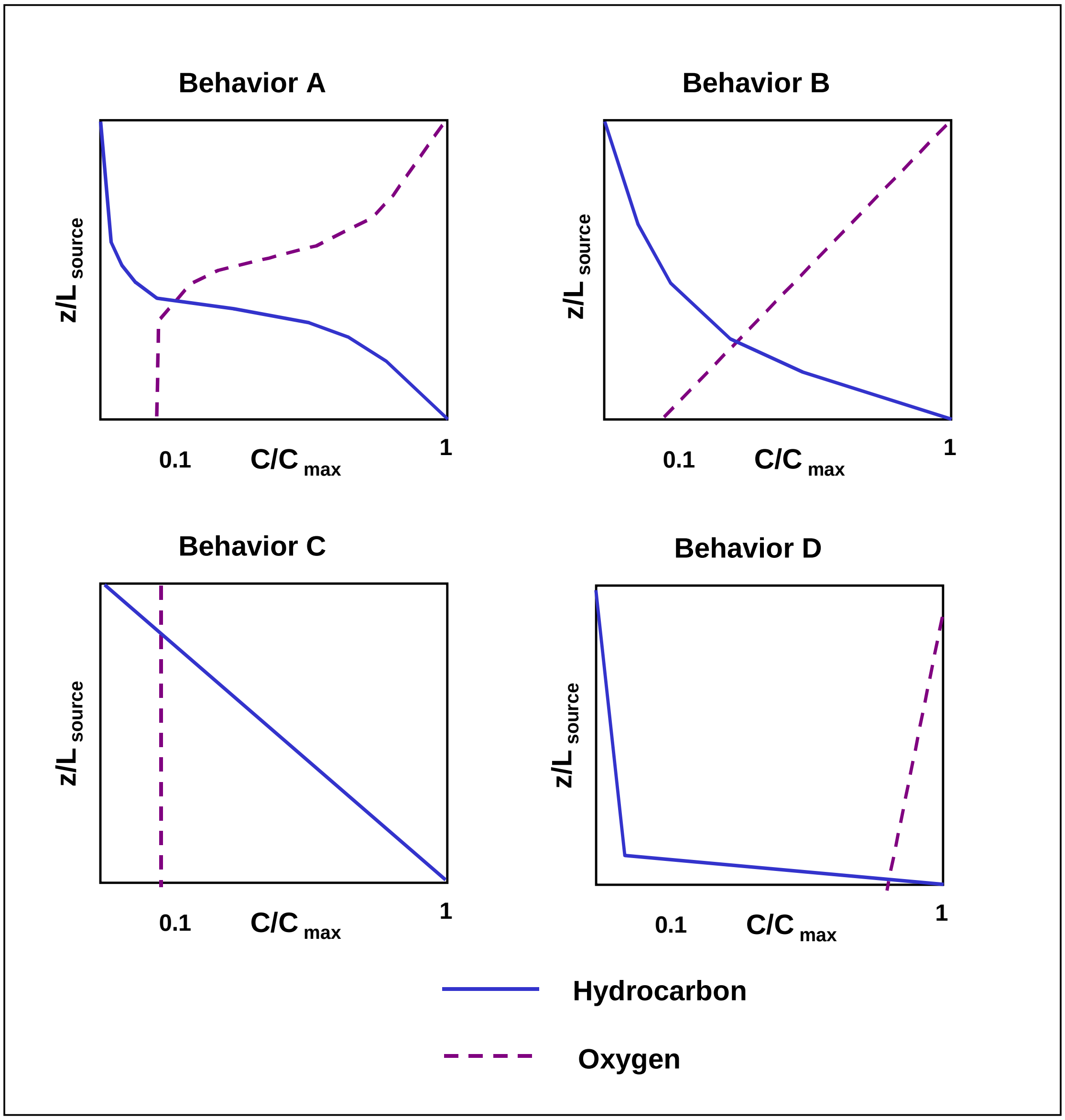


Figure K-2. Four Generalized Soil Gas Profiles

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 air concentrations 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:
$$0 = D_{eff\_H} \frac{\partial^2 C_H}{\partial z^2} \tag{K-1}$$

oxygen:
$$0 = D_{eff\_O2} \frac{\partial^2 C_{O2}}{\partial z^2} \tag{K-2}$$

For the region $\delta < z < L$ where the oxygen concentration is not limited ($C_{02} > C_{02,min}$):

chemical:
$$0 = D_{eff\_H} \frac{\partial^2 C_H}{\partial z^2} - \frac{\lambda \theta_m}{K_H} C_H \tag{K-3}$$

oxygen:

$$0 = D_{eff\_O2}\frac{\partial^2 C_{O2}}{\partial z^2} - \beta\frac{\lambda\theta_m}{K_H}C_H \qquad \text{(K-4)}$$

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.

$$D_{eff\_H} = D_{air\_H}\left(\frac{\theta_a^{3.33}}{\theta_T^2}\right) + \frac{D_{water\_H}}{K_H}\left(\frac{\theta_m^{3.33}}{\theta_T^2}\right) \qquad \text{(K-5)}$$

$$D_{eff\_O2} = D_{air\_O2}\left(\frac{\theta_a^{3.33}}{\theta_T^2}\right) + \frac{D_{water\_O2}}{K_{HO2}}\left(\frac{\theta_m^{3.33}}{\theta_T^2}\right) \qquad \text{(K-6)}$$

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 $z = 0$:

$$C_H = C_H^{\max} \quad \text{and} \quad \frac{\partial C_O}{\partial z} = 0 \qquad \text{(K-7)}$$

at $z = \delta$:

$$\boldsymbol{C_H = C'_H} \quad \text{and} \quad \boldsymbol{C_O = C_{O\,min}} \qquad \text{(K-8)}$$

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 $\delta < z < L$ (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

$$\eta_j = \sqrt{\frac{\lambda_j \theta_m}{D_{eff\_H} K_H}} \tag{K-14}$$

$$A_j = \frac{C_H^{'} e^{-\eta_j \delta}}{e^{-2\eta_j L} \left[\dfrac{\eta_j \dfrac{D_{eff\_H}}{K_j} - 1}{\eta_j \dfrac{D_{eff\_H}}{K_j} + 1} \right] + e^{-2\eta_j \delta}} \tag{K-15}$$

$$B_j = C_H^{'} \left\{ e^{-\eta_j \delta} - \frac{e^{-\eta_j \delta}}{e^{-2\eta_j L} \left[\dfrac{\eta_j \dfrac{D_{eff\_H}}{K_j} - 1}{\eta_j \dfrac{D_{eff\_H}}{K_j} + 1} \right] + e^{-2\eta_j \delta}} \right\} \tag{K-16}$$

$$D_j = \frac{\left(C_O^{amb} - C_O^{\min} \right) - \left(1 + \dfrac{D_{eff\_O}}{K_O} \right) \left[\sum \beta_j \left(\dfrac{D_{eff\_H}}{D_{eff\_O}} \right) \left(B_j \eta_j e^{\eta_j \delta} - A_j \eta_j e^{-\eta_j \delta} \right) \right] + \left[\sum \beta_j \left(\dfrac{D_{eff\_H}}{D_{eff\_O}} \right) \left(A_j \eta_j e^{-\eta_j \delta} + B_j \eta_j e^{\eta_j \delta} \right) \right]}{\left[\dfrac{D_{eff\_O}}{K_O} + L - \delta \right]} \tag{K-17}$$

$$E_j = C_O^{\min} - D_j \delta - \sum \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}} \right) \left(A_j \eta_j e^{-\eta_j \delta} + B_j \eta_j e^{\eta_j \delta} \right) \tag{K-18}$$

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* = δ (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:

$$C_H^{'} = \frac{C_H^{\max}}{1+\left\{\dfrac{\eta_j \delta e^{-2\eta_j \delta}}{e^{-2\eta_j L}\left[\dfrac{\eta_j \dfrac{D_{eff\_H}}{K_j}-1}{\eta_j \dfrac{D_{eff\_H}}{K_j}+1}\right]+e^{-2\eta_j \delta}}+\eta_j \delta+\dfrac{\eta_j \delta}{e^{-2\eta_j L}\left[\dfrac{\eta_j \dfrac{D_{eff\_H}}{K_j}-1}{\eta_j \dfrac{D_{eff\_H}}{K_j}+1}\right]+e^{-2\eta_j \delta}}\right\}} \qquad \text{(K-19)}$$

$$0 = \sum \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(\frac{C_H^{\max}-C_H^{'}}{\delta}\right)-D_j \qquad \text{(K-20)}$$

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:

$$D_j = \sum \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(\eta_j A_j + \eta_j B_j\right) \qquad \text{(K-21)}$$

$$E_j = C_O^{amb} - \left[\sum \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(A_j \eta_j e^{-\eta_j \delta} + B_j \eta_j e^{\eta_j \delta}\right)\right] - D_j L - \frac{D_{eff\_O}}{K_O}\left[\sum \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(-A_j \eta_j e^{-\eta_j \delta} + B_j \eta_j e^{\eta_j \delta}\right) + D_j\right] \qquad \text{(K-22)}$$

To determine which case is applicable, the concentration of oxygen at $z = 0$ must be calculated and then compared with C^{min}_O:

$$C_O(z=0) = \sum \beta_j \left(\frac{D_{eff\_H}}{D_{eff\_O}}\right)\left(A_j + B_j\right) + E_j \qquad \text{(K-23)}$$

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:

$$E(z=0) = D_{eff\_H} \frac{\left(C_H^{\max} - C'_H\right)}{\delta}, \quad if\ \delta > 0 \tag{K-24}$$

$$E_{area}(z=0) = D_{eff\_H}\left(A_j\eta_j - B_j\eta_j\right), \quad if\ \delta = 0 \text{ (i.e. CO>C}^{\text{min}}_{\text{O}}) \tag{K-25}$$

$$E_{area}(z=0) = D_{eff\_H}\left(A_j\eta_j e^{-\eta jL} - B_j\eta_j e^{\eta jL}\right) \tag{K-26}$$

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.

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):

$$K_j = \frac{Q_{soil}}{A_B} \frac{\exp\left(\frac{Q_{soil}L_{crack}}{D_{crack}A_B\eta}\right)}{\left[\exp\left(\frac{Q_{soil}L_{crack}}{D_{crack}A_B\eta}\right) - 1\right]} \tag{K-28}$$

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.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:

$$C_H^{\max} = C_w K_H \tag{K-34}$$

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-2.

Table K-2. 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-2. 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.

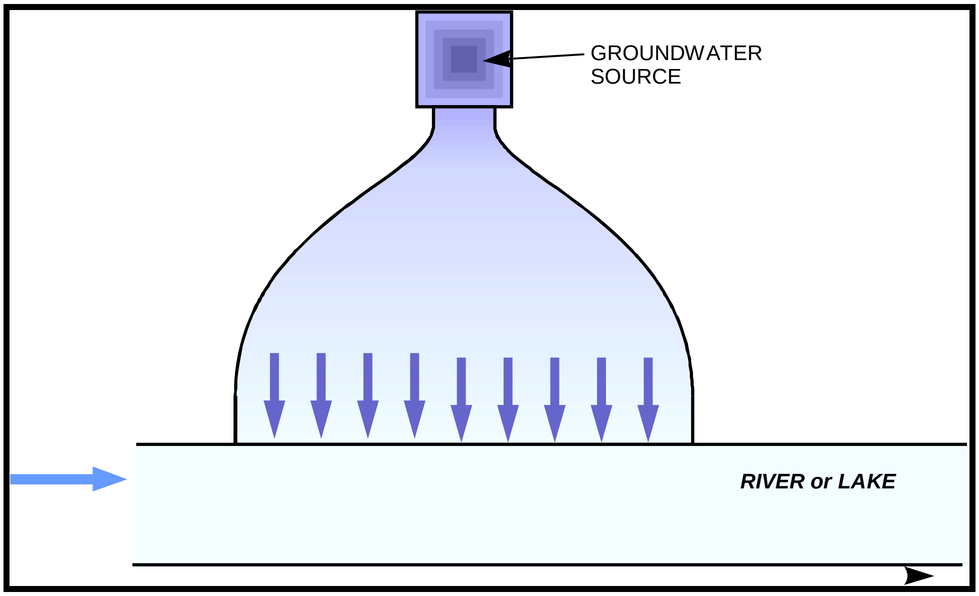

Figure L-1. Surface Water Mixing Model Geometry.

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:

$$V\frac{dC_{sw}}{dx} = W(t) - QC_{sw} - \mu_{sw}VC_{sw} \qquad \text{(L-1)}$$

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:

$$c = \frac{W}{Q + \mu_{sw}V} \qquad \text{(L-2)}$$

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:

$$C_{sed} = C_{gw} K_d \tag{L-5}$$

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:

$$K_d = F_{oc} * K_{oc} \tag{L-6}$$

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 of 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:

$$C_{sw} = \frac{W}{Q + kV} = \frac{3.16E7\,\dfrac{mg}{d}}{\left[200\,\dfrac{m^3}{d} + \left(\dfrac{0.05}{d}\right)50{,}000m^3\right]}\,\frac{1m^3}{1000l} = 11.7mg\,/\,l$$

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:

$$C_{sw} = \frac{W}{Q_{gw} + Frac_{mix}\left(Q_{sw} + kV\right)} = \frac{3.16E7\,\dfrac{mg}{d}}{100\,\dfrac{m^3}{d} + 0.01 \times \left[100\,\dfrac{m^3}{d} + \left(\dfrac{0.05}{d}\right)\left(50{,}000m^3\right)\right]}\,\frac{1m^3}{1000l} = 14mg\,/\,l$$

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}:

$$Q_{gw} = K_{sw} d_{sw} L_{reach} \left(\frac{h_{gw} - h_{sw}}{L_f} \right) \tag{L-7}$$

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-7 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.

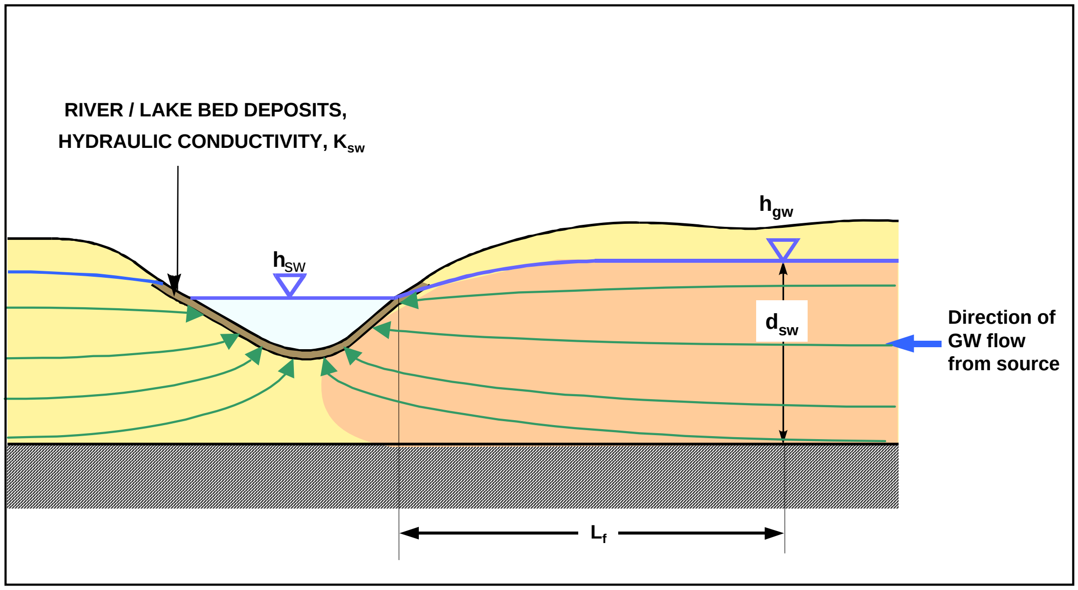

Figure L-2. Cross-Sectional Model Geometry.

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. Figure 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.

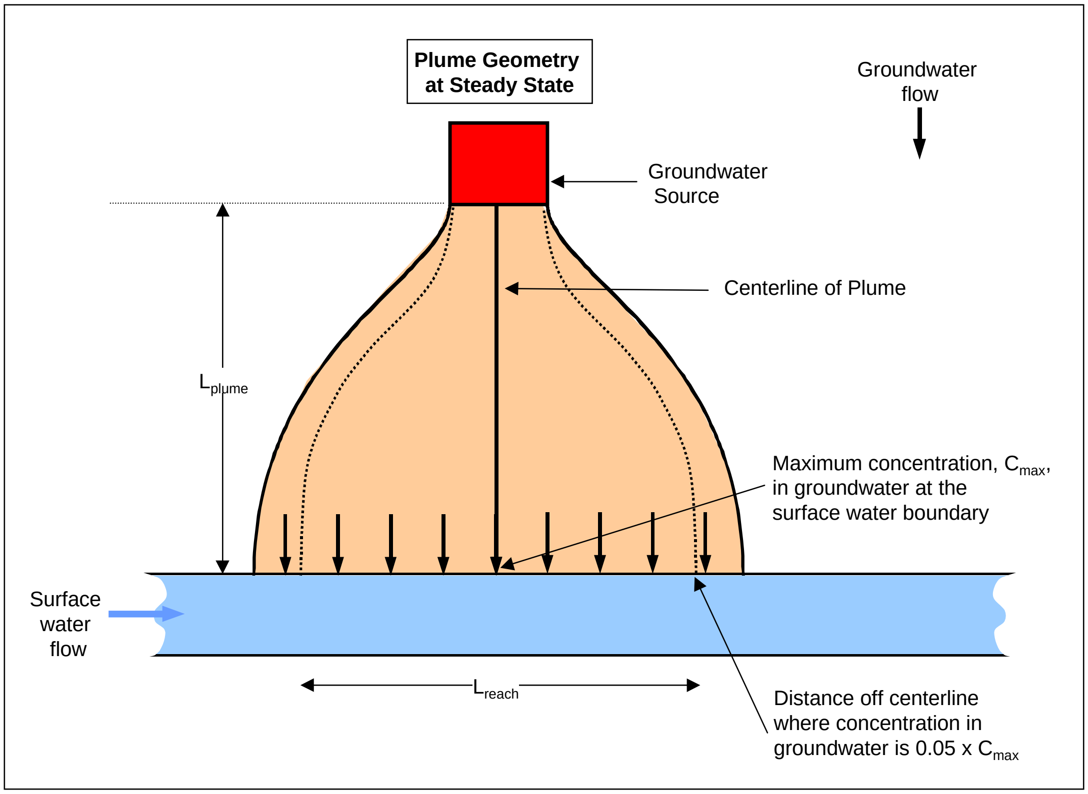

Figure L-3. Calculating the Length of the Reach

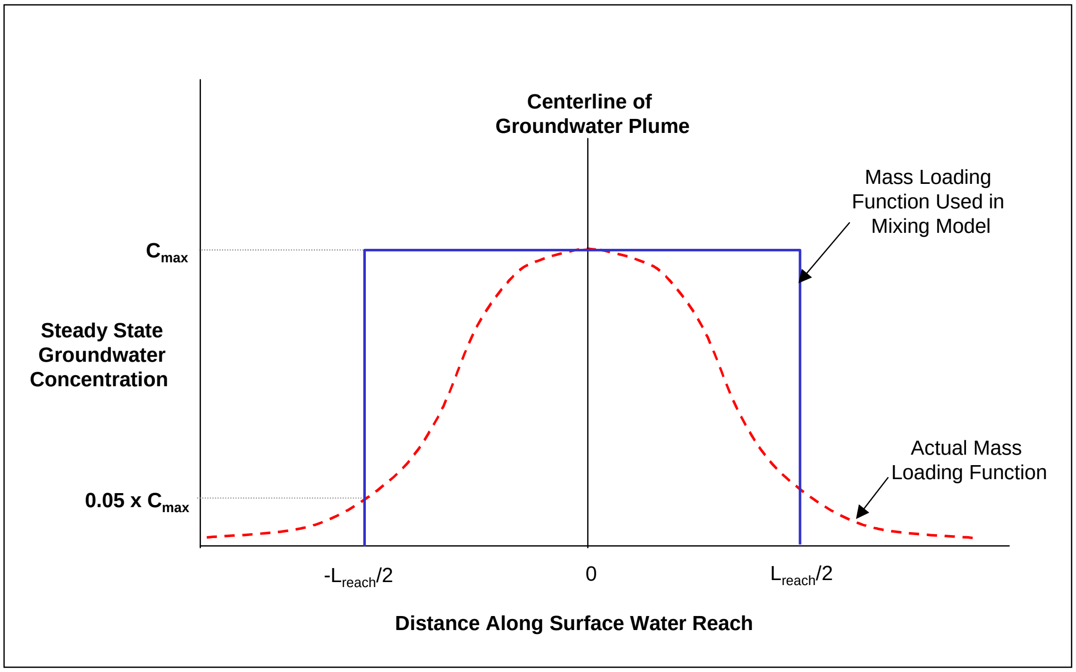

Figure L-4. Calculating the Mass Loading Function

The following equation (Domenico, 1987) is used to estimate the distance off the centerline at which the concentration becomes 5% of the centerline concentration:

$$\begin{aligned} C(x,y,z) = \frac{C_o}{4}\exp&\left\{\frac{x}{2\alpha_x}\left[1-\sqrt{1+\frac{4\lambda\alpha_x}{\upsilon}}\right]\right\} \\ &\left\{erf\left[\left(y+\frac{W_y}{2}\right)\frac{1}{2\sqrt{\alpha_y x}}\right]-erf\left[\left(y-\frac{W_y}{2}\right)\frac{1}{2\sqrt{\alpha_y x}}\right]\right\} \\ &\left\{erf\left[\left(z+\frac{W_z}{2}\right)\frac{1}{2\sqrt{\alpha_z x}}\right]-erf\left[\left(z-\frac{W_z}{2}\right)\frac{1}{2\sqrt{\alpha_z x}}\right]\right\} \end{aligned} \qquad \text{(L-8)}$$

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 α_x/3)

α_z = vertical dispersivity [m] (assumed to be equal to α_x/87)

The length of the surface water reach is calculated by first using Equation L-8 to calculate the centerline concentration at the surface water body edge. Then L-8 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-8 is the relative concentrations. The Domenico equation presented in L-8 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.

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

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.

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.

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.

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 has 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 FLORIDA DEP (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 exceedance 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.

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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.

RISC5 VERSION UPDATE

This appendix was originally prepared for version 4 of the RISC model. As such, it reviewed plant uptake research and plant models that were available at the time. In RISC5, the above-ground portion of the plant uptake (vegetable uptake) is now estimated with the Trapp and Matthies (1995) model. This model considers losses due to volatilization from the plant leaves which is important for volatile or semi-volatile organic chemicals. The updates to this appendix are highlighted in blue text.

Note, this software update only changes the model used for above-ground plant uptake of organic chemicals.

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:

$$C_v = C_{soil} B_v \qquad \text{(O-1)}$$

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:

$$C_v = C_{water} CF \qquad \text{(O-2)}$$

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]

The soil uptake factor, B_v has been divided into two component factors for purposes of modeling exposure in RISC: one uptate factor is used for root vegetables (using the notation B_{vr}) and the other uptake factor is used for above-ground leafy portion of plants (B_{va}). Similarly, the water uptake factor (CF) has been divided into a water uptake factor for the root portions of plants, the root concentration factor (RCF), and an above-ground concentration factor (ABCF) from water.

The next section reviews the most commonly used models for estimating the produce uptake factors.

O.2 VEGETABLE UPTAKE MODELS FOR ORGANIC CHEMICALS

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.

RISC5: Since the time this appendix was originally developed, the Trapp model has been simplified and published by Trapp and Matthies (1995). This will now be used for estimates of uptake for the above-ground portions of the vegetables. A quick review of USEPA risk assessment guidance and models indicates that the USEPA has not published revised approaches to modeling plant update for the human ingestion pathway.

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:

$$\log B_v = 1.588 - 0.578 \log K_{ow} \qquad \text{(O-3)}$$

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:

$$RCF = 10^{0.778\ \log K_{ow} - 1.52} + 0.82 \tag{O-4}$$

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:

$$B_{vr} = \frac{RCF * \rho_b}{\theta_w + (1 - \theta_t) * K_d \rho_s} \approx \frac{RCF}{K_d} \tag{O-5}$$

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 between soil and water [ml/g or L/kg]

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:

$$B_{vr} = \frac{0.01RCF}{K_d} \qquad \text{(O-6)}$$

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):

$$TSCF = 0.748e^{-\frac{(\log K_{ow} - 1.78)^2}{2.44}} \qquad \text{(O-7)}$$

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:

$$SCF = 10^{0.951\log K_{ow} - 2.05} + 0.82 \quad \text{(O-8)}$$

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:

$$B_{vst} = \frac{SCF \times TSCF}{K_d} \quad \text{(O-9)}$$

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 partitioning coefficient between soil and water [ml/g or L/kg]

This ratio may be used to determine wet weight 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 THE TRAPP AND MATTHIES MODEL

The Trapp and Matthies (1995) model is used in RISC5 to estimate concentrations of organic chemicals (any chemical with a non-zero K_{oc} value) in roots and above-ground plants. Is considers:

- translocation to shoots,
- gaseous deposition on leaves,
- volatilization from leaves,
- metabolism and degradation processes, and
- dilution by exponential growth.

Gaseous deposition on leaves is not modeled in RISC; this type of deposition usually occurs due to emissions from combustion facilities and is beyond the scope of the RISC software. For more information on deposition uptake, and the USEPA models used for this pathway, see USEPA (2005). The following two sections (root uptake and above-ground uptake using T&M) are taken directly from the original paper (Trapp and Matthies, 1995).

O.2.3.1TRAPP AND MATTHIES UPTAKE INTO ROOTS

The partition coefficient describes the concentration ratio between two neighboring phases in thermodynamic equilibrium and is a key property for the fate of compounds in the soil-plant-air system. The partition coefficient between soil (pore) water and root plant tissue is calculated from

$$K_{RW} = \left(W_P + L_P K_{OW}{}^{b}\right) \cdot \left(\frac{\rho_P}{\rho_W}\right) \tag{O-10}$$

Where

K_{RW} = partition coefficient between root plant tissue and water [(kg chemical/m^3 of plant)/(kg chemical/m^3 water)]

W_p = water content of the plant tissue (g/g)

L_p = lipid *(fat, i.e. hydrophobic)* content of the plant tissue (g/g)

K_{ow} = chemical-specific octanol/water partitioning coefficient (L/kg) [note this is not logKow; Kow = 10^{logKow})

b = correction exponent for differences between plant lipids and octanol (-)

ρ_P = density of plant tissue (kg/m^3)

ρ_W = density of water (kg/m^3)

Note, the “b” coefficient in Equation O-10 is likely to be plant-specific. For cut bean roots and stems, “b” was found to be 0.75; for macerated barley roots it was 0.77; for barley shoots, 0.95; and for isolated cuticles, 0.97.

This partition coefficient between bulk soil concentrations and roots, K_{RB}, is given as

$$K_{RB} = \frac{K_{RW}}{\rho_B K_d + \theta} \tag{O-11}$$

Where

K_{RB} = partition coefficient between roots and bulk soil [(kg chemical/m^3 of plant)/(kg chemical/m^3 soil)] (Calculated using equation O-10)

K_{RW} = partition coefficient between roots and water [(mass /volume of plant)/(mass/volume of water)]

K_d = distribution coefficient between soil matrix and water (L/kg)

ρ_b = soil bulk density (kg/L) (note the units)

θ = volumetric water content of the soil (cm^3 water/cm^3 soil)

The values calculated using equation O-11 are close to those calculated using equation O-10 and only slightly depend on lipophilicity when K_d is calculated from K_{oc}. A plausible reason for the similar sorption properties of roots and soil is that the humic substances in soil originate from plant material. Note: for fine roots, diffusive exchange with the soil is high, and near-equilibrium conditions are assumed to be achieved. However, for thicker roots (such as below-ground vegetables), equilibrium (predicted by O-10 and O-11) should be considered an upper limit; i.e., the kinetics of uptake control the concentration.

Measurements by E. M. Topp for barley and cress roots indeed support this finding (Trapp, 1994). Schroll and Scheunert (1992) found K_{RW} values of hexachlorobenzene for maize, oat, rape, and barley of between 0.8 and 3.2 but found higher values for lettuce (13.7) and carrot (31.6). Wang and Jones (1994) found that the concentration ratio between carrot and soil of 10 chlorobenzenes varied also with the type of application. However, none of the K_{RW} values (B_{CF} fresh weight) were above 5; most of them were much lower. Their experiments also showed that concentrations in peels were always higher than those in cores, indicating the slow uptake kinetics into the tap root. From all this, it might be concluded that it is sufficient to assume that the concentration in fine roots is usually in or below the order of magnitude of the concentration in soil.

O.2.3.2TRAPP AND MATTHIES UPTAKE INTO ABOVE-GROUND PRODUCE

The Trapp and Matthies approach for calculating concentration of chemicals in above-ground plant parts first calculates the transpiration stream concentration factor that controls the rate of flux of chemical up into the leaves. Once in the leafy portion of the plant, the processes considered are gaseous deposition, volatilization from leaves, transformation and degradation and growth. Note, the RISC5 version of the Trapp and Matthies model does not allow for the deposition of chemicals in the gaseous phase onto leaves; this pathway is usually considered for industrial plant emissions and is assumed not to apply in RISC5.

Transpiration Stream

The “transpiration stream concentration factor” (TSCF, discussed above as well) is defined as the concentration ratio between xylem sap and external solution (soil pore water). The mass transport within the xylem, N_{xy}, is calculated by

$$N_{xy} = Q \cdot C_w \cdot TSCF \qquad \text{(O-12)}$$

Where

N_{XY} = mass transport within the xylem (kg/s)
Q = transpiration stream (m^3/s)
C_W = concentration in soil pore water
TSCF = transpiration stream concentration factor (mg/L)/(mg/L)

Note, if the source term is a soil concentration, then the concentration in the soil pore water is calculated using equilibrium partitioning. The TSCF is related to the K_{ow} and is calculated two different ways (equations O-13 and O-14). The higher calculated value is then used for the mass transport within the xylem (equation O-12).

$$TSCF = 0.784 \ \exp\left[\frac{-\left(\log K_{ow} - 1.78)^2\right)}{2.44}\right] \qquad \text{(O-13)}$$

$$TSCF = 0.7 \ \exp\left[\frac{-\left(\log K_{ow} - 3.07)^2\right)}{2.78}\right] \qquad \text{(O-14)}$$

For substances with intermediate K_{OW}, the equations work satisfactorily. But from the comparison of both empirical equations, it can be seen that TSCF is an uncertain parameter, in particular for very lipophilic substances. In the following, the higher result from following equations (O-13 and O-14) will be used. From theoretical considerations, it follows that TSCF values of nondissociating compounds should maximally be 1.

Gaseous Exchange Between Leaves and Atmosphere (Volatilization from the Leaves)

The partition coefficient between leaves and air, K_{LA} is

$$K_{LA} = \frac{K_{LW}}{K_{AW}} = \frac{K_{LW}}{H'} \qquad \text{(O-15)}$$

Where

K_{LA} = partition coefficient between leaves and air (-)
K_{LW} = partition coefficient between leaves and water [(mass /volume of plant)/(mass/volume of water)] (Calculated from O-10)
K_{AW} (H’) = partition coefficient between air and water (Henry’s Law coefficient), dimensionless form [(mg/l vapor)/(mg/L water)]

can account for losses from volatilization of the chemical from plant leaves, a growth rate constant (λ_g), a metabolism rate constant (λ_m) and a photodegradation constant (λ_m).

O.2.4 CALCULATING UPTAKE 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 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.4 SUMMARY OF RECOMMENDATIONS

In summary, the Trapp and Matthies equations are used to calculate the concentration of contaminants in vegetables. Separate uptake factors are calculated for above-ground and root 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 the vegetable ingestion pathway as it is incorporated into RISC5:

- 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 or groundwater concentration is assumed to be constant. The soil concentration can be specified directly or it may be calculated using the unsaturated zone soil model (Appendix A). Similaryly, for groundwater, the soil pore water (groundwater) concentration may be specified directly by the user or it may be calculated using one of the groundwater models. If a model is used to estimate the soil or groundwater concentrations, a time-weighted average concentration (based on the exposure duration) is calculated for use in the plant uptake equation. (This is the same approach as used in all of the exposure calculations in RISC.)
- Risk modeling is being performed at the USEPA that 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.
- 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.5 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 (B_v)explicitly entered in the chemical database, then this value is used for both above-ground and root portions of the 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.5.1 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:

$$B_{va} = B_{vBaes} \times (1 - W_p) \tag{O-16}$$

$$B_{vr} = B_{vBaes} \times (1 - W_p) \tag{O-17}$$

For water:

$$RCF = B_{vBaes} \times (1 - W_p) \times K_d \tag{O-18}$$

$$ABCF = B_{vBaes} \times (1 - W_p) \times K_d \tag{O-19}$$

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]

W_p = water content of the vegetable [g water/g 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 = soil 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.5.2 ORGANIC CHEMICALS

If the chemical has a non-zero value entered for K_{ow}, then the partioning coefficient from either soil or water into the plant root is calculated using the Trapp and Matthies partitioning equations, O-10 and O-11, for water and soil, respectively.

O.6 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.

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Wild and Jones reported on PAH uptake at three different PAH concentrations, which are reported which were used to calculate B_{vr} for "high", "medium" and "low" concentrations of PAH.

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ADDITIONAL SECTION FROM RISC v. 4:

COMPARISON OF THE BRIGGS EMPIRICAL MODEL, THE TRAVIS AND ARMS MODEL AND OBSERVED PLANT CONCENTRATIONS

This section from the RISC v. 4 model was included because it discusses a comparison of the two previous plant models that were used in RISC and these models may be commonly used by various regulatory agencies.

The relationship of the various soil-to-plant uptake factors to K_{ow} are plotted in Figures O-1 and O-2.

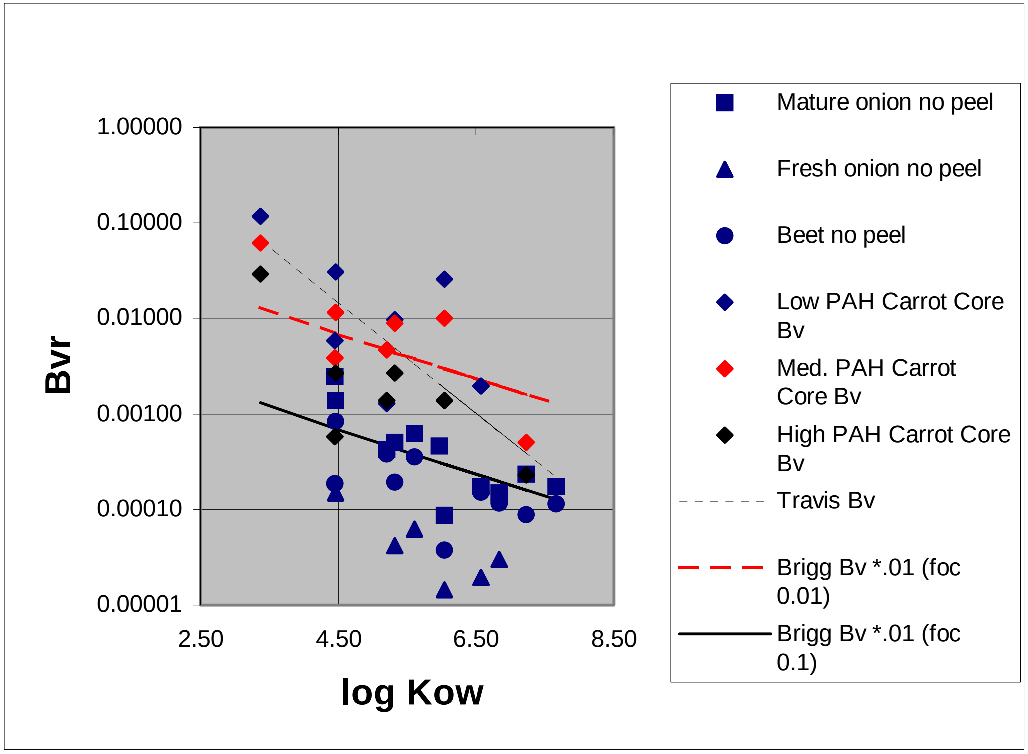

Figure O-1. Wild and Jones (1983) Carrot Core Data For Three Different PAH Concentrations, and Wang and Meresz Peeled Root Vegetable Data as a Function of K_{ow}

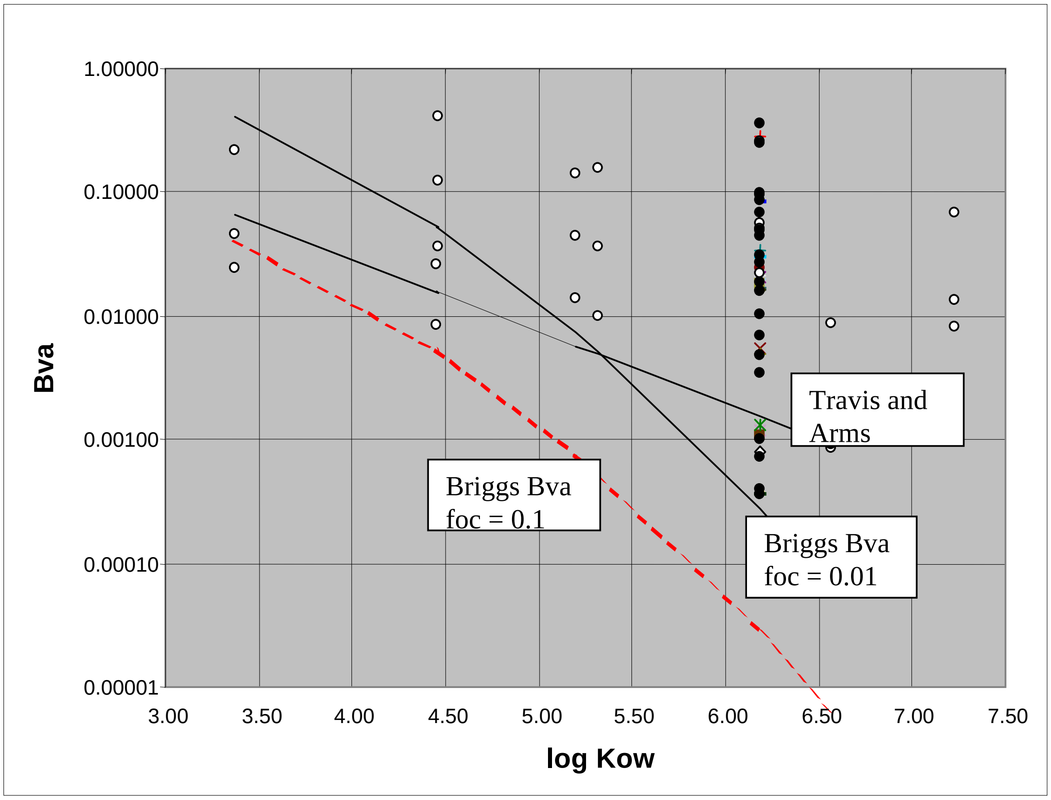

Figure O-2. Comparison of Above Ground Uptake Factors, B_{va}

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."

APPENDIX P

Ecological Risk Assessment for Contaminated Soils

RISC Software Project

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Contents

List of Figures

Acronyms and Abbreviations

BAF	bioaccumulation factor
BCF	bioconcentration factor
BP	BP International
BSAF	biota-sediment accumulation factor
CSM	conceptual site model
Eco-SSL	ecological soil screening level
EPA	U.S. Environmental Protection Agency
ERA	ecological risk assessment
HHRA	human health risk assessment
HQ	hazard quotient
LOAEL	lowest-observed-adverse-effect level
NOAEL	no-observed-adverse-effect level
TRV	toxicity reference value
UCLM	upper confidence limits of the mean

1 Introduction

This report describes a process for food-web modeling to quantify ecological risks from contaminated soils. The document serves two purposes, including 1) use as a stand-alone report to enable the reader to generate “back of the envelope” ecological risks using the algorithms and exposure parameters presented in this document, and 2) the user’s manual text to explain the ecological risk assessment (ERA) component and associated numbers generated by BP International’s (BP’s) Risk-Integrated Software for Clean-ups (RISC) software, version 5 (to be released in 2003).

Generally speaking, regulatory agencies have promulgated few specific practices or formulaic approaches to food-web modeling for ecological receptors. Many aspects of ERA must be tailored to a given site or scenario of interest. However, the approach described here is consistent with state-of-the-practice methods, as well as conceptual guidance issued by the U.S. Environmental Protection Agency (EPA), and similar guidance and policy developed by other regulatory agencies around the world. The following sections describe the conceptual design, derivation of parameters used in the model, and guidelines on the selection of chemicals and receptors of concern, estimation of dietary exposure, and calculation of risk. Examples of representative receptor species and input parameters are provided. This is not intended to be a checklist for regulatory compliance, though the approaches described here can be adapted to meet the requirements of most ERA guidance from regulatory authorities throughout the world.

For those with a high level of theoretical interest, a number of reference books on ERA methods and practice are commercially available, and may be consulted for more depth on many of the topics discussed here. Notable among these for their breadth and practical value are Suter (1993) and Calabrese and Baldwin (1993). Exposure modeling is a specialized technical field in its own right, drawing upon fundamentals of disciplines as diverse as animal behavior, biochemistry, physiology, pharmacology, and statistics. Many general and specific texts are available for those interested in the technical underpinnings of exposure modeling. The RISC software, which is intended to produce Tier 2 screening level target values, permits rapid estimation of chemical exposure and characterization of risk for ecological receptors using standard approaches. In this document, Tier 2 refers to screening criteria to protect higher-level trophic species derived from a modeled food web analysis (not a published set of numbers), with or without the use of site-specific data. It intentionally requires little theoretical knowledge by the user to generate a result. However some knowledge of ERA principles is helpful in interpreting results and critically evaluating the reliability of risk predictions. In practice, the utility of any ecological food-web model is primarily limited by the availability of relevant data on receptors of interest rather than on the selection of a specific analytical technique.

1.1 Unique Aspects of Ecological Risk Assessment

ERA is a process used to characterize the likelihood of adverse effects as a result of chemical exposure to plants and wildlife. Conceptually, the ERA paradigm is similar to that employed in human health risk assessment (HHRA). HHRA practices are generally well codified and may be familiar to the reader. In both ERA and HHRA, potential chemicals of concern are identified, environmental exposure pathways and receptors are described, then exposure levels are estimated and compared to a relevant reference dose or toxicity threshold. There are, however, significant differences between HHRA and ERA, both in terms of regulatory objectives and standard practice. Obviously, these differences result in part from the higher societal value placed upon protection of the human individual. HHRA typically focuses on probabilities of effects, such as cancer risk, to the individual, with fairly rigid regulatory guidelines on the threshold above which risk becomes unacceptable and risk management measures are required. ERA usually focuses solely on effects that have the potential to influence receptor populations, such as survival, growth, and reproduction, and does not place a high priority on protection of the individual.[1] In addition, there typically are no promulgated standards for determining what constitutes unacceptable risk for ecological receptors. Far more decision-making is required during the assessment process and more discretion left to the ecological risk manager to determine appropriate measures, making it impossible to define a universal ERA template. ERA is a rapidly evolving field, with very limited regulatory guidance. Standard practices vary and change rapidly as the underlying science advances. Current local regulatory guidance should be consulted as a part of any ERA.

Other significant differences between HHRA and ERA are driven by the relative complexity of ecological food webs. The ecological risk assessor must evaluate the likelihood of effects on an entire ecosystem composed of numerous, interdependent receptor species, each with specific diet, chemical sensitivity, and life history characteristics. The theoretically potential combinations of ecological receptors, chemicals, and exposure scenarios are virtually infinite, necessitating substantial simplification for evaluation purposes. Knowledge uncertainty about most receptor species and their relevant characteristics is high, necessitating many assumptions on the part of the risk assessor.

The procedure for assessing ecological risk at a particular site, to say nothing of the interpretation of ERA results, is highly subjective, and is typically negotiated between risk assessors, regulators, and stakeholders on a case-by-case basis. Many factors beyond the quantitative risk characterization go into the development of a cleanup goal, including an evaluation of ecological significance of predicted effects, analysis of uncertainty with regard to risk-driving assumptions, regulatory priorities (which vary with time and jurisdiction), and cost-benefit analysis of action. Nevertheless, identifying the framework and parameters for quantifying ecological risk is a necessary first step in the process. Tier 2 screening values can indicate the presence or absence of potential risk, and can be helpful in educating the stakeholders on the assumptions, sensitivities, and limitations of the process. They can also provide insight into where resources should be targeted to reduce the uncertainty.

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[1] There are exceptions to this rule. Risk to ecological receptors of special societal importance, such as those species protected by the federal Endangered Species Act in the United States, is typically assessed at the level of the individual.

1.2 Use of Generic Ecological Screening Benchmarks

Various regulatory agencies around the United States and the world have published soil screening criteria for ERA. Other criteria have been compiled and published for use by risk assessors (see Appendix A of this chapter). Generally speaking, these toxicity benchmarks are not based on food-web exposure routes, and may not even be rigorously risk-based. Those that are derived from toxicological data are likely to be based on direct toxicity data only—in most cases from laboratory exposures of lower trophic order species, such as earthworms or plants. They are low-biased to preclude the possibility of a false negative finding, and will tend to over-predict risk at most sites. For the purposes of this document, they are referred to as Tier 1a criteria, meaning they are non site-specific and reflect direct toxicity only.

Food web modeling, on the other hand, tends to focus on higher trophic order consumer species. The threshold for risk from food-web exposure to soil contaminants may be higher or lower than that of a direct-effect benchmark.

It is also important to bear in mind that these Tier 1a screening-level benchmark concentrations are reported as nominal concentrations of the test chemical associated with toxicity in laboratory tests. They are not bulk soil concentrations associated with adverse effects in the field. For example, most toxicity tests of metals use soluble salts, which are likely to be more bioavailable and more toxic than the stable metal forms that are commonly found in the environment. Equating the lab value to a bulk soil concentration in the field may be an apples-to-oranges extrapolation.

The EPA is currently developing generic Tier 1b ecological soil screening levels (Eco-SSLs), which will at least partially incorporate food-web pathways for assessment of risk to higher trophic order receptors (U.S. EPA 2000). In this document, Tier 1b refers to generic food web criteria (i.e., they protect higher trophic level species and are derived from a food web analysis but with non site-specific data). Eco-SSLs are being developed using food-web models to back-calculate soil concentrations necessary to result in an exposure level that would exceed a published toxicity benchmark (see discussion of food-web modeling approach below). To date, draft Eco-SSLs have been developed for a handful of metals, the pesticide dieldrin, and the explosive compound RDX. Eco-SSLs will provide a valuable and much-needed Tier 1b screening tool to the risk assessor, but even they should not be used as *de facto* cleanup targets. Because Eco-SSLs are designed for use at any site in the United States with contaminated soils, they cannot reflect individual site conditions and their use may result in large over-estimates or even an under-estimate of risk (although the latter is more unlikely due to the deliberate conservative bias built into all screening criteria). The Tier 2 food-web model approach requires more effort than simple comparison with a list of Tier 1a or 1b numbers, but the benefit is that the risk estimate is likely to be more accurate because assumptions are tailored to fit actual site conditions to a greater degree than with generic screening benchmarks.

Potential risks from surface water contamination to aquatic species may be screened using EPA ambient water quality criteria or similar promulgated water quality standards that are designed to protect aquatic life. Careful attention should be paid to the basis of such criteria. Most do not reflect food-web exposure but instead are derived solely from tests on low trophic level aquatic organisms. A variety of published sediment quality standards also exist, though few have been promulgated as regulatory standards.[2]

1.3 Limitations of Food-Web Modeling

The decision to make use of any given approach for chemical risk assessment makes implicit decisions about the nature of the risk. The use of any modeling approach involves many assumptions on the part of the modeler, resulting in many sources of uncertainty. Because it is not possible to completely eliminate uncertainty, an analysis of major sources of uncertainty should be part of any risk assessment.

It must first be recognized that food-web modeling is generally only used to assess dietary ingestion exposure pathways. Other exposure pathways, such as dermal contact and inhalation, may be important for some chemicals and receptors, though it may not be possible to evaluate them quantitatively. Exposure to soil contaminants due to inhalation of volatile vapors and/or airborne particles may be an important source of exposure for terrestrial receptors, especially those that burrow or nest underground. In practice, the inhalation exposure pathway is usually not incorporated into ERA because of the paucity of wildlife toxicity data for inhaled chemicals. Likewise, the dermal exposure route is rarely included in ERA. Inhalation and dermal exposure routes are not inherently complicated to quantitatively assess. Procedures for doing so are described in some regulatory guidance documents (Environment Australia 1997). However, knowledge uncertainty about uptake factors and effect thresholds for non-dietary exposure pathways generally precludes quantitative assessment of risk.

Risk from direct chemical exposure to contaminated soil may sometimes be assessed through toxicity testing under controlled conditions. This approach is frequently used to characterize risk to lower trophic level receptor species that are in intimate contact with contaminated soil, such as plants and soil macroinvertebrates, but is rarely employed with higher trophic level receptors. Food-web modeling is the most commonly used approach to ERA for higher-order consumer species, and dietary exposure to soil contaminants is usually considered the most important exposure route for these species. Nevertheless, non-dietary exposure routes may also result in significant exposure, and should be qualitatively considered when characterizing risk.

Food-web exposure is most likely to be a risk driver for bioaccumulative chemicals. Most chemicals can be taken up into ecological food webs from contaminated soil to some degree, but many do not significantly bioaccumulate under typical field conditions. Plants, for example, do not appreciably take up many petroleum hydrocarbons from contaminated soils due to low water solubility, and such hydrocarbons are readily metabolized (broken down within the body to other forms) by higher vertebrates. As a result, concentrations of these chemicals in biota can be expected to decrease at higher trophic levels. Direct toxicity of soil to lower trophic level receptors may represent a more significant risk than food-web exposure of higher trophic level receptors in such cases. Nevertheless, food-web modeling has value for chemicals with low

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[2] For a compilation of generic sediment screening criteria, see http://response.restoration.noaa.gov/cpr/sediment/squirt/squirt.pdf.

bioaccumulation potential, in that it may be useful to demonstrate that risk to higher trophic levels is low.

Food-web analysis requires detailed information about exposure characteristics and chemical sensitivity of selected receptors. If either of these parts of the risk equation are missing for a given chemical and receptor, accurate evaluation of the food-web risk may not be possible. A common problem with application of the food-web model approach is a lack of suitable toxicity information from dietary exposure studies. If the oral dose-response relationship for a given chemical and receptor is poorly understood, the risk characterization will be highly uncertain and may not accurately reflect true risk or support a good risk management decision process. It is also important to use only studies of ecologically relevant exposure routes and effects, not esoteric pathways or endpoints with unknown relevance to ecological receptors. Identifying the adverse effect threshold for wildlife receptors exposed to soil contaminants is one of the leading and least-acknowledged sources of uncertainty associated with food-web ERAs.

A final practical caution is in order: Because technical opinions vary and regulatory policies are not uniform or well codified, no single modeling approach will satisfy all regulatory reviewers, even within a given agency. Interpretations of findings are somewhat subjective, and may differ widely. Development of a defensible risk-based cleanup target in soils can be accomplished only with direct input and approval of the relevant regulatory authority, and requires evaluation of factors other than risk, such as practicability and cost/benefit of action. Practitioners of ERA should not assume that an approach that has been successfully used at one site will necessarily be approved at another. Regulatory consultation is always prudent.

2 Overview of the Food-Web Modeling Approach

Essential components and example parameters for typical ERA food-web models are described below. These are designed to fulfill the requirements of a Tier 2 screening level risk assessment to remain consistent with the other RISC model components. The objectives of the Tier 2 ERA are to determine the relative contributions of various exposure pathways to total exposure and to assess the potential ecological effects of soil chemical concentrations under highly protective assumptions. Therefore, the model forms suggested are deliberately conservative so that the final exposure estimate will be protective of all or most individuals of a receptor population.

The effects of other environmental media, such as contaminated sediment or surface water, may be incorporated into the same dietary exposure model to assess risk to higher trophic level species (e.g., river otters that feed on fish exposed to contaminated surface water). On the other hand, a direct comparison can be made of media concentrations to appropriate surface water quality criteria for the relevant species. The general approach of this food-web model is consistent with regulatory guidance offered by environmental agencies in many different countries (e.g., United States, Australia, European countries). Basic food-web modeling is not a complex mathematical process. Most calculations involve only simple algebra (see Appendix B). The complexity in food-web modeling lies primarily in the parameterization of models, which requires judgment and numerous assumptions about receptor behavior relating to exposure. Custom food web models are easily coded using standard spreadsheet or data management software, though commercial programs designed for ERA are not widely available. RISC version 5 will be one of the first programs in this regard.

2.1 Elements of Approach

In ERA, food-web modeling is most commonly used to develop a point estimate of risk to a given receptor under one or more fixed sets of exposure assumptions. The most common quantitative expression of risk is the hazard quotient (HQ). The HQ is calculated as the ratio of estimated exposure to a theoretical threshold of adverse effects or toxicity reference value (TRV).

$$\mathrm{HQ} = \frac{\mathrm{Exposure}}{\mathrm{TRV}}$$

When estimated exposure and TRV are expressed in like units, the HQ is a unitless ratio. A fractional HQ (i.e., $\mathrm{HQ} < 1$) indicates that the estimated exposure does not exceed the theoretical threshold, and adverse effects are unlikely to occur. HQs greater than 1 indicate that the potential for adverse effects exists, with the higher the HQ, the higher the potential in an exposed population. As a point estimate of risk, the HQ does not express the probability of adverse effects on a population in a statistically meaningful manner. Rather, it is a tool to eliminate chemicals of concern from further evaluation (those for which $\mathrm{HQ} < 1$), and to identify which chemicals may pose the greatest risk, and which receptors are most at risk.

The exercise of food-web modeling can thus be thought of as two separate processes: exposure assessment (resulting in the numerator of the HQ) and effects assessment (resulting in the denominator of the HQ). Exposure is typically expressed in terms of a daily ingested dose, from all sources, and is usually normalized for body weight of the receptor. A daily dose of chemical X for a given receptor is simply an estimate of the daily ingestion rate of X from all sources, divided by the receptor's body weight. The resulting exposure estimate would have units such as *mg X/kg body wt./day*. One or more TRVs, which are similarly expressed in terms of a daily ingested dose, are then derived from published toxicology studies for comparison.

The exposure estimation approach used here is consistent with EPA wildlife exposure guidance (U.S. EPA 1997). The general structure of the food-web exposure model is described by the following equation:

$$D_{\text{chemical}} = \frac{\sum_i \left(C_i \times M_i \times A_i \times F_i\right)}{W}$$

where:

D_{chemical} = daily ingested dose of chemical from all dietary components (mg/kg-body weight/day)

C_i = concentration of the chemical in dietary component i (mg/kg)

M_i = rate of ingestion of dietary component i (kg/day)

A_i = relative gastrointestinal absorption efficiency for the chemical in dietary component i (fraction)

F_i = area use factor; portion of the daily intake of dietary component i derived from the investigation area (fraction)

W = body weight of receptor species (kg).

Any number of dietary components may be summed to estimate the daily ingestion dose.

Probabilistic exposure modeling methods commonly used in HHRA (e.g., Monte Carlo simulation) may be used in food-web models to incorporate greater realism by treating parameters that are naturally variable or stochastic (e.g., receptor body weight) as distributions. A stochastic HQ may be calculated after application of probabilistic exposure assessment methods by selecting summary statistics of the parameter distributions (e.g., mean, 50th percentile, 90th percentile) to calculate a stochastic point estimate of exposure. However, it is also possible to develop a probability distribution of total exposure for a receptor. This exposure probability distribution allows fuller characterization of risk than the single point estimate of the HQ. Probabilistic modeling methods have historically not been widespread in standard ERA practice, but their use is increasing. The use of probabilistic ERA is supported by U.S. EPA guidance (U.S. EPA 1997), especially as a Tier 3 assessment when traditional, deterministic methods indicate that significant risk exists, and the risk assessor desires to better characterize that risk. For purposes of this document, Tier 3 refers to a more sophisticated analysis than Tiers 1 and 2, and may involve things like stochastic modeling or collection of field data. The use of probabilistic modeling requires an understanding of the stochastic parameter distributions, which may be poorly understood. In cases where the natural variability of a given parameter is not well understood or characterized, application of a stochastic model will add nothing to the understanding of risk and is inadvisable.

As noted previously, a high level of knowledge uncertainty is typically associated with exposure factors and chemical sensitivity for most wildlife species. Critical inputs to the exposure model, such as local dietary composition for a given receptor and variations in feeding behavior, may never have been measured, requiring estimation or extrapolation from data collected for other species or locations. TRVs for wildlife species are very sparse in the literature, and extrapolation from toxicity data on other tested species is usually required. Standard risk assessment practice is to deliberately bias assumptions about uncertain parameters in a conservative or protective direction. While this approach is necessary to prevent a false negative finding in the ERA, and may be mandated by regulatory guidance, conservative assumptions must be noted and re-evaluated by the risk manager when interpreting ERA findings. One method of assessing the significance of uncertainty in the deterministic risk characterization (although it cannot reduce uncertainty) is to evaluate multiple scenarios in parallel, each with its own set of exposure assumptions. It is common practice in ERA to evaluate multiple exposure scenarios and TRVs to assess which assumptions are driving risk calculations. A rapid modeling tool such as RISC permits this type of sensitivity analysis to be readily conducted.

The time course of chemical exposure, which is of interest in ERA, is usually chronic, though there are no standard definitions of what exactly constitutes chronic versus acute exposure for wildlife receptors. Generally speaking, exposure of a duration approaching the lifecycle or breeding cycle of a receptor is regarded as chronic exposure. Food-web models are therefore typically designed to predict chronic exposure, and should only be compared to chronic TRVs. While it is possible to model acute exposure by using short-term exposure assumptions and compare the resulting exposure estimates to acute TRVs, bioaccumulation of contaminants into the food web is typically not the major concern under acute exposure conditions.

2.2 Exposure Assessment

Most of the assumptions and parameters of the model form described above are associated with exposure assessment. Input parameters may be derived from site-specific studies, and such information greatly increases the realism of risk assessments, but site-specific data is usually limited during the screening phase of the assessment. Published sources of information are typically employed. Example parameters and formulas from commonly used published sources of exposure and effects data are presented in Appendix C.

2.2.1 Selection of Representative Receptors

It is not possible or necessary to assess exposure or risk for all receptor species that may occur at a given site. In order to make the complexity of ecological food webs manageable, exposure is typically modeled only for a limited number of species that are representative of the vast majority of species at a site. Exposure and risk predicted for these representative receptors are then extrapolated to predict exposure and risk to other species. The most common approach to selection of representative receptors for dietary exposure assessment is the "feeding guild" approach. A feeding guild is a subset of wildlife species that has similar dietary requirements and foraging habits.

For example, a white-tailed deer (*Odocoileus virginianus*) may be selected as a representative receptor for herbivorous mammals in a woodland habitat. The assessment of risk to white-tailed deer would then be interpreted as applicable to all other mammalian herbivores which are potentially exposed. Apart from being typical of a guild of ecologically similar species that are likely to experience similar exposure conditions, representative receptors may be selected based on knowledge of their feeding behavior and chemical sensitivity. Species that are known or believed to be especially sensitive to a given chemical are often selected as receptors because risk to such species is theoretically protective of the entire guild. This approach is consistent with regulatory guidance mandating that assessments be biased in a protective manner.

Some entire guilds and even taxonomic orders of wildlife receptors, notably amphibians and reptiles, are rarely assessed in food-web models due to a virtual complete lack of dietary toxicity data for suitable representative species. If appropriate information is available, these species can be evaluated using standard model approaches; however, this is rarely possible.

Once chemicals of concern and representative receptors of concern are defined, complete exposure pathways are identified to describe a conceptual site model (CSM) for ecological exposure. Figure 1 illustrates the CSM for a typical terrestrial food-web exposure pathway.

2.2.2 Selection of Dietary Components

Even for selected representative receptors of concern, simplifying assumptions must be made with regard to the number of dietary inputs that are incorporated as model terms. For example, the diet of a raccoon (*Procyon lotor*) in a lakeshore habitat may include dozens of different food items, but for modeling purposes, these can be lumped into generic categories, each representing specific food-web pathways of interest (e.g., fish, insects, or plant material). Standard food-web modeling practice only incorporates the categories of dietary components most likely to represent significant inputs to the total dietary exposure for the chemicals of interest. Often, the entire diet is modeled as being derived from a single food source in order to evaluate a single exposure pathway. Therefore, an omnivorous receptor may be modeled separately as an herbivore, an insectivore, or a carnivore. Insignificant dietary components may be ignored, though it is important to document the basis for such a decision.

It is also standard practice to include direct ingestion of soil that may be entrained in food items or ingested during grooming/preening behavior as a dietary input. In areas of high soil contamination, direct ingestion of soil may be the single largest source of dietary exposure to some chemicals, and should not be discounted. Published studies of incidental soil ingestion are few, and this exposure pathway always has a high degree of uncertainty associated with it. Drinking water, which may contribute to overall exposure, is also typically incorporated as a dietary term, if any surface water exists in the investigation area.

2.2.3 Typical Receptors and Pathways of Concern

Guilds of mammalian and avian receptors that are typically assessed in ERA are discussed below. Typically, species are chosen as representative receptors for a guild when extensive information is available on their life history and toxicology. Many alternative species could be selected, and it is not possible to comprehensively list all potential receptors for all sites. When selecting representative receptors, it is important to remember that risk to selected receptors is intended to represent risk to an entire receptor guild, not just the species that is modeled.

2.2.3.1 Mammalian Terrestrial Exposures

All terrestrial mammals are potentially exposed to soil contaminants through food, direct soil ingestion, and drinking water pathways. Mammals can be broadly divided according to their diet (e.g., into insectivores, carnivores, and herbivores). Chemical concentrations in different food items for these feeding guilds will usually vary widely. Examples of mammalian receptors commonly selected for food-web models in North America are the insectivorous short-tailed shrew (*Blarina brevicauda*), the carnivorous red fox (*Vulpes vulpes*), and the herbivorous muskrat (*Ondatra zibethicus*).

It should be recognized that most wildlife receptors are at least partially omnivorous. Many species are opportunistic feeders, using whatever food resources are readily available, and the composition of their diet will vary by location and season. The raccoon is an example of a common omnivorous mammal with a highly varied diet. This species will eat plant material, as well as terrestrial and aquatic prey, and will adapt its diet to the resources available.

For modeling purposes, it is easier and may be sufficient to assume a simple diet. In Tier 1b or a first pass at Tier 2 screening assessments, it is standard practice to assume that the entire diet is composed of the most-contaminated dietary component. This protective assumption is replaced with more realistic and complicated assumptions in subsequent evaluations. Whenever site-specific information is available as to the composition of any receptor’s diet, it is recommended that this information be incorporated into the food-web model. When relying on published studies about dietary preferences and feeding behavior, care should be taken to choose studies conducted in habitats similar to the site of interest.

2.2.3.2 Avian Terrestrial Exposures

Birds that consume terrestrial food items are exposed to chemical contaminants through the same basic pathways as mammals. There are insectivorous/vermivorous (worm-eating), carnivorous, and herbivorous birds. The vermivorous American woodcock (*Scolopax minor*), the carnivorous red-tailed hawk (*Buteo jamaicensis*), and the herbivorous northern bobwhite (*Colinus virginianus*) are examples of commonly selected representative receptors in North America.

2.2.3.3 Mammalian Aquatic Exposures

If surface water features are present at a site, soil contamination may lead to sediment and water contamination through runoff and groundwater transport pathways. Mammals that consume aquatic food items (e.g., fish, shellfish, aquatic vegetation) are potentially exposed to sediment and waterborne contaminants through this component of their diets. Assessment of this exposure is exactly analogous to soil and is performed in the same manner. It is common practice to model species that consume both terrestrial and aquatic prey by including terms representing both types of dietary components in the same food-web model. Piscivorous (fish-eating) mammals are commonly modeled in ERA. The river otter (*Lutra canadensis*) is a North American receptor species commonly selected to represent piscivorous mammals in ERA. Very few mammalian species subsist primarily on aquatic invertebrates or plants, though many derive some of their diet from these sources. Some species in certain habitats may be an exception to this rule. Raccoons in tidal estuaries, for example, may subsist largely on crustaceans during some periods of the year.

2.2.3.4 Avian Aquatic Exposures

Birds that consume aquatic food items are potentially exposed to chemical contamination through the same generic pathways as mammals. However, the feeding habits of birds that consume aquatic food items are much more diverse. Many birds are highly specialized in their physiology and feeding behavior to exploit a specific aquatic food resource. Waterfowl may be predominately piscivorous, herbivorous, or benthivorous (feeding on bottom-dwelling invertebrates), but many specializations within these general guilds exist. For example, diving piscivorous birds feed primarily on top-water fish, and thus may be expected to have a different prey species composition in their diet and a lower incidental sediment ingestion than wading shorebirds, which feed primarily on benthic (bottom-dwelling) prey. The belted kingfisher (*Ceryle alcyon*), a diving bird, and the great blue heron (*Ardea herodias*), a wading bird, are examples of commonly selected piscivorous avian receptors in North America. Many birds feed primarily on benthic invertebrates, and some have highly specialized body types (i.e., beak and leg length) that make them specialists in specific habitats and prey. The spotted sandpiper (*Actitus macularia*) and lesser scaup (*Aythya affinis*) are examples of commonly modeled benthivorous avian receptors. Few waterfowl are completely herbivorous, but dabbling ducks, such as the mallard (*Anas platyrhynchus*), are commonly modeled as an herbivorous waterfowl.

2.3 Effects Assessment

Toxicity assessment may involve derivation of only a single model parameter, the TRV. However, this parameter has tremendous influence over the risk characterization, comprising the entire denominator of the HQ. Toxicity assessment, including an understanding of the uncertainties involved for wildlife receptors, is one of the most difficult and involved parts of the ERA process. No single parameter in the food-web model is more important to the risk characterization than the TRV. TRVs may be derived directly from the published toxicology literature, but this requires considerable knowledge and professional judgment (see discussion below). A few compendia of wildlife TRVs have been published. The most comprehensive is that of Sample et al. (1996), developed for the U.S. Department of Energy at Oak Ridge National Laboratory (see Tables C-1 and C-2 in Appendix C).

2.3.1 Toxicity Reference Value Derivation

Dietary TRVs are defined by recent EPA guidance as “doses above which ecologically relevant effects might occur to wildlife species following chronic dietary exposure and below which it is reasonably expected that such effects will not occur” (U.S. EPA 2000). In other words, TRVs are estimates of toxicity thresholds. In ERA, TRVs are usually based on no-observed-adverse-effect-levels (NOAELs) or lowest-observed-adverse-effect-levels (LOAELs). A NOAEL is the highest dose that does not produce an adverse effect and a LOAEL is the lowest dose that results in a statistically significant adverse effect. The threshold of the onset of adverse effects for an exposed receptor population lies somewhere between the NOAEL and LOAEL. In a screening-level risk assessment, the NOAEL is typically selected for the TRV.

The objective of ERA is to protect species at the population level. However, most toxicity data are obtained from laboratory exposures of relatively small numbers of individuals. It is important to derive a TRV from studies where the toxic effects measured would be expected to have significant population-level impacts. Examples of appropriate endpoints would be growth, mortality, and reproduction. Other effects commonly reported in toxicity studies include biochemical or physiological changes, which have less defined effects at the individual level, let alone the population level. Such endpoints should not be used as TRVs, even though they may occur at lower exposure levels. Selection of improper TRVs, or values for which the ecological significance to the population is unknown, will result in an uninterpretable risk characterization.

TRVs are specific to both chemicals and the representative receptor species. Ideally, data obtained directly from controlled exposure of the species being modeled would be used. This information is usually not available for wildlife species and a surrogate test species must be chosen. Most mammalian and avian toxicology literature is based on laboratory studies of domestic animal species. TRVs should be selected from studies of taxonomically related species. For example, a dog would theoretically be a better surrogate for a red fox than a mouse, although sensitivity differences between closely related species may occur. Any time a toxicity endpoint is extrapolated to another species, it should be recognized that this introduces a high level of uncertainty into the effects assessment, and therefore to the risk characterization. Regardless of the scientific quality of a toxicity study, the objectives of the original investigator may not be compatible with the objectives of the ERA, thereby rendering the study undesirable for use to derive appropriate threshold doses like NOAELs and LOAELs. The following are examples of ecological relevance criteria that should be assessed during the review of the candidate TRV studies:

- **Taxonomic relationship—**The closer the test species is to the receptor species, the better.
- **Level of biological organization—**Only studies of effects on whole organisms (*in vivo* endpoints) should be used. Effects measured in cell cultures or non-living, biochemical experimental systems (*in vitro* endpoints) are inappropriate for use in ERA.
- **Ecological relevance of the study endpoints—**Endpoints that are meaningful to the population, such as growth, survival, and reproduction, are required.

- **Route of exposure—**Dietary exposure is required.
- **Duration of exposure—**Longer exposure periods are better.

Safety factors are sometimes applied to reference TRVs that are judged to be highly uncertain for a given application. In practice, this usually takes the form of division by a factor of 2 to 100. While the use of TRV safety factors increases the protective bias of a risk characterization, it also results in a risk assessment that is policy-driven rather than science-driven. In effect, it reduces the quantitative meaning of the risk characterization, and introduces risk management steps into the risk assessment. When higher levels of protection are required, safety factors are more appropriately applied outside of the risk assessment process.

Another controversial TRV adjustment practice is allometric scaling of TRVs, as advocated by Sample et al. (1996). The assumption behind this practice is that chemical sensitivity is an inverse function of body size, and that small size results in high metabolism, leading to rapid detoxification. This assumption is certainly false for chemicals that are bio-activated by metabolism (e.g., PAHs) or that are not appreciably metabolized (e.g., chlorinated organics). In the absence of specific knowledge about the relative sensitivities of the test species and the receptor species of interest, the application of TRV scaling factors has little justification. Extrapolation of TRVs should always be acknowledged and considered as a significant source of uncertainty in ERA.

TRVs are typically derived from the literature by reviewing all available dietary toxicity studies and determining the most appropriate study or studies to use as the basis for calculating a TRV. TRVs are typically not directly available from published studies in the form of a chronic daily dose, and often must be calculated by the risk assessor for a given receptor. The derivation process requires careful consideration of information such as the experimental study conditions, the species studied, the exposure route and duration, the toxic effects measured, the chemical form, and the methods used.

Sometimes a study may not provide all relevant information, such as food ingestion rates or body weights of test organisms. In such cases, the risk assessor may need to consult other published sources to estimate these values and calculate a TRV. This process adds further to uncertainty. Often a risk assessor must choose between two or more imperfect studies as a TRV source study. The assessor must weigh the weaknesses and strengths of each candidate study. Familiarity and experience with the toxicology literature is therefore crucial to the process of effects assessment. For screening level ERAs, TRVs are conservatively selected to err on the side of overestimating sensitivity.

3 Application of Food-Web Modeling

The structure of the food-web analysis in the context of using the RISC software is presented in Figure 2. The major steps that require site-relevant input are the identification of the exposure pathways and the selection and description of receptors. The complete description of receptors includes parameterization of the dietary exposure model, which is an important and often time-consuming task to complete. However, this customization of the model parameters to the site provides the principal benefit of the modeling approach. Appendix D presents some sample calculations to illustrate application of the principles described above and highlight some of the factors and uncertainties that may drive even simple risk calculations.

3.1 Steps in Applying the Food-Web Model

Application of food-web models to assessment of risk from soil, surface water, or sediment contamination can be thought of as a five step process.

3.1.1 Step 1—Identify Chemicals of Concern

As in any environmental investigation, selection of chemicals of concern is largely driven by the history of site releases and the magnitude of chemicals present in the area of investigation. Consideration of chemicals of concern for food-web analysis must look beyond bulk soil concentration, however. The physical and biological properties of the chemical can profoundly influence the potential for significant exposure and therefore the risk that the chemical poses to wildlife. For example, volatile chemicals will release from surface soils as a gas in a relatively short period of time in contrast to chemicals that remain in solid or liquid form. Persistent chemicals are likely to pose risk to wildlife over a longer time period than those that rapidly degrade in the environment. Other factors that affect the potential magnitude of risk to wildlife from chemical contamination are the overall tendency for uptake into the food web, how readily the chemical is metabolized and eliminated by biological organisms, and the toxicological sensitivity of the exposed wildlife species. The food-web model approach to risk assessment is especially valuable for persistent, bioaccumulative chemicals, which may be present at higher concentrations in biota than in soil.

As noted previously, many petroleum hydrocarbons are not highly bioaccumulative, due to poor uptake and/or rapid metabolism. The user should always consider the possibility that food-web exposure is not necessarily the highest concern of ERA. Acute toxicity from dermal contact may pose a greater risk than chronic food-web exposure although, as noted previously, the data to quantify this risk may be lacking.

3.1.2 Step 2—Select Representative Receptors

Receptors should be selected on a site-specific basis using available information on the species that makes use of the site as habitat. In order to choose receptors, some information about the habitats present must be known. While it is not necessary to conduct an extensive ecological study, it is highly advisable to conduct an ecological reconnaissance of the site, and estimate the area and extent of various habitats. Species that use onsite habitat for breeding and/or foraging are of particular concern because their level of exposure is high compared to transient species that only migrate through the onsite habitat. Any species occurring onsite with special legal protection (e.g., threatened or endangered species) should be included as a receptor in the food-web analysis, or an appropriate surrogate receptor chosen. In addition, species selected as receptors should be representative of feeding guilds believed to be present at the site, as previously described. Receptors should be chosen to ensure that all the significant, complete exposure pathways to the major feeding guilds in an ecosystem, as identified in the ecological CSM, are included in the ERA.

3.1.3 Step 3—Parameterize Exposure Model

Model parameterization can be a relatively simple process using values from published resources on life history parameters of wildlife receptors, or it can be customized for a site to as great a degree as available data allow. One of the best sources of information is the EPA *Wildlife Exposure Factors Handbook* (U.S. EPA 1993) (refer to Appendix C for exposure parameters for example receptors, as described above). In higher tiers of ERA, field studies are sometimes conducted to develop site-specific receptor life histories. The decision to take such a step is driven by a cost-benefit analysis of the effort required to obtain such data and the cost of a potential remedy. Running a screening model such as RISC should provide insight into the required next steps.

3.1.3.1 Physiological Parameters

Representative body weights for receptors may be difficult to obtain from published sources. Many animals exhibit pronounced sexual dimorphism; that is, large size differences between the genders are the norm. In addition, large variability may exist in size distributions between populations in different locations due to differences in climate or diet. It is important to use a reference value for body weight that is appropriate to the habitat being evaluated. The conservative approach is to use the minimum adult body weight, which will maximize the body weight-normalized exposure (see below).

3.1.3.2 Ingestion Rates

The diet of the receptor species should be reviewed in the published literature to establish the major components. For receptors with diverse diets, the diet may initially be assumed to be composed entirely of the most contaminated food item. If unacceptable levels of risk are predicted, additional effort may be applied to more accurately model actual exposure. Where possible, ingestion rates for food, sediment/soil, and drinking water should be obtained from published literature sources. When ingestion rates for the specific receptor species of interest are not available, they may be estimated using allometric formulas, which are empirical relationships between bioenergetics and body size. For example, Nagy (1987) and Nagy et al. (1999) have developed allometric scaling formulas to estimate daily food ingestion rates of mammals and birds. These formulas require only the body weight of the receptor to estimate total daily ingestion.

$$\text{Mammals:} \quad FIR = 0.235 \times BW^{0.822}$$

$$\text{Birds:} \quad FIR = 0.648 \times BW^{0.651}$$

where:

FIR = food ingestion rate (grams per day on dry-weight basis)

BW = body weight (grams)

Other variants of this basic formula have been developed for subsets of receptors, such as mammalian herbivores and rodents (see Appendix B). Note that it is common to express all food ingestion rates on a dry weight basis in food-web models. Most bioenergetic formulas for estimation of ingestion rates are on a dry weight basis, and analytical results for soil and other environmental media should be expressed on a similar basis. It is important not to mix ingestion terms that are both wet weight- and dry weight-based in the same calculation or large errors in exposure estimates may result.

When surface water is present at a site to be assessed, drinking water ingestion rates can be estimated using the similar allometric approach of Calder and Braun (1983):

$$DIR = 0.059 \times BW^{0.67}$$

where:

DIR = drinking water ingestion rate (liters per day)

BW = body weight (kg)

3.1.3.3 Absorption Efficiency Factor

The absorption efficiency factor, sometimes referred to as a bioavailability factor, is a measure of the fraction of ingested chemicals, relative to the total concentration, that are taken up through the digestive tract of a receptor. Fractional bioavailability factors can be included in exposure modeling when good information is available, but, in the absence of specific data for the receptor of interest, it is typically assumed that the chemical is 100% available ($A_i = 1.0$). In other words, all of the chemical that is ingested is assumed to be absorbed. In screening-level ERAs, 100% bioavailability is an assumption typically required in regulatory guidance.

3.1.3.4 Area Use Factor

A parameter that may be considered in ERA is the area use factor, which is the proportion of total diet that is derived from the site, expressed as a fraction. Species that have very small foraging ranges, such as shrews, may derive their entire diet from a relatively small site, and would have an area use factor of 100% ($F_i = 1.0$). Species with foraging ranges larger than the site are likely to derive only a portion of total diet from the site, and would have an area use factor less than 1.0 (fractional F_i). Area use factor is thus a linear scaler of total exposure. For small sites or receptors that range widely in their foraging behavior, area use factor may profoundly influence the exposure estimate. In a screening risk assessment, the area use factor is typically set at 1.0, which is the worst-case scenario. However, for higher tier assessments, the risk assessor may consider refining the area use factor, based on patterns of suitable habitat within and around the site being evaluated.

3.1.3.5 Dietary Uptake Factors

Estimation of food item concentrations may be necessary when measured biota tissue data are unavailable. Bioaccumulation factors (BAFs), bioconcentration factors (BCFs), and biota-sediment accumulation factors (BSAFs) may all be used to estimate food item concentrations from measured concentrations in soil, sediment, or water. BAFs are a simple ratio of a chemical concentration measured in tissue of a prey organism (e.g., worm) to the medium with which it is in contact (e.g., soil). Both direct accumulation from dermal contact and food-web uptake are reflected in the BAF. The term BCF is sometimes used interchangeably with BAF, but is usually applied only to water. BSAFs are similarly developed to estimate a tissue concentration of aquatic species when only a sediment concentration is known. All of these factors should be used cautiously because they are derived either from laboratory exposures where artificial exposure conditions exist, or from field observations where exposure conditions may be different from the site of interest. Table C-3 in Appendix C lists a number of published uptake factors from soil to common dietary items of wildlife.

3.1.4 Step 4—Determine Exposure Point Concentrations

As described above, estimated exposures from one or more dietary components are summed together with incidental soil/sediment and water ingestion to calculate a total daily exposure. The usual convention is to express all exposure estimates and TRVs on a body weight-normalized basis. Body weight normalization makes inter-species exposures more comparable, and permits direct extrapolation of TRVs between receptors of different size.

The point concentrations used to evaluate each term of the exposure model (i.e., contaminant concentrations in food, soil, and water) can be determined in a number of ways. Common screening-level ERA practice is to first model the maximum detected concentration in the medium as a conservative measure. However, various statistical representations of a data distribution, including means and upper confidence limits of the mean (UCL), may be applied when adequate data are available. Use of the 95% UCL is common, and should result in a protective assessment. Use of statistically derived point estimates of concentration should be performed with caution in the case of small data sets, however. The 95% UCL may be higher than the maximum detected concentration if data scatter is high and data points are few. It may be desirable to perform parallel calculations with different expressions of the environmental concentrations (i.e., mean and max, or mean and UCL).

3.1.5 Step 5—Perform Risk Calculation

The final step to determine risk is calculation of the HQ, which is simply the ratio of estimated exposure to the selected TRV. When examining the results of risk assessments, it should be noted that an HQ greater than 1 is not a *de facto* indicator of unacceptable risk. Many decision points occur in calculation and interpretation of any risk characterization. Typically these are negotiated as much as they are prescribed by regulatory guidance or standard practice. There is no standard or predefined acceptable level of risk, and the HQ is dependent on many input assumptions. Therefore, HQs are open to interpretation.

Risk managers may use a multitude of additional information to decide what actions need to occur, if any. In practice, significant remedial steps are rarely taken for HQs less than 10, though no broad generalizations can be made about HQ interpretation. Comparison of the NOAEL HQ to the LOAEL HQ may be useful to help place a risk calculation into context. It should be remembered that there is *no* adverse effect at an exposure equivalent to the NOAEL. There *may be* an effect at an exposure equivalent to the LOAEL.

It is important to bear in mind that risk predictions are just that—predictions. They are not a guarantee of observed adverse effects. In order to support the development of an appropriate risk management strategy, the risk assessor should critically evaluate all assumptions applied in a food-web model for realism and applicability to the site. Often, in a screening-level ERA, conservative and unrealistic assumptions are applied that result in severe overestimation of risk. When a highly uncertain assumption is determined to be driving a prediction of high risk, it is important to attempt to refine that assumption prior to finalizing the risk characterization or proposing risk management action. Options available to the risk assessor to refine assumptions may include additional literature review, consultation with experts for the species of interest, or conducting site-specific field studies on the feeding habits and exposure of selected receptors. If any site-specific information is available that allows refinement of preliminary assumptions, this adjustment can be made to increase the realism of the risk characterization.

It is often desirable to determine the media concentrations above which the HQ is greater than 1. These can be back-calculated by starting with a total exposure equal to the TRV and determining the soil, water, and/or food concentration that would result in a threshold daily exposure. If a BAF is known for each food item modeled, then the entire food-web equation can be solved for a hypothetical soil concentration that would correspond to a HQ of 1.0.

A sensitivity analysis is recommended to gauge the exposure parameters that have the most influence on the risk estimate. By varying the values of exposure parameters, one can determine which sources and which life history variables are contributing the most and the least to the final total exposure estimate. The use of a software tool such as RISC permits rapid iteration of risk calculations while varying individual input assumptions, thus facilitating such an analysis.

3.2 Ecological Risk Assessment Exit Conditions

A number of circumstances may lead to termination of the risk assessment process. Obviously, one of these is completion of the ERA with a finding of “no significant risk.” Other exit conditions exist that are not strictly risk-based. These include the following:

- Absence of elevated levels of chemicals of potential concern. It is appropriate to compare site chemistry data to local or regional background levels when reliable data exist to permit this comparison. This practice is standard for substances that occur naturally (e.g., metals), however it may also be appropriate for anthropogenic pollutants that are not site-related.
- A finding that no significant exposure pathways exist for ecological receptors. If there is no significant exposure, there can be no significant risk. This condition is not unusual at fully developed industrial sites with no functional ecological habitat or when site soils are completely sealed by pavement. The risk assessor should still consider the possibility of offsite transport of contaminants, or assess the risk under non-industrial future use scenarios.
- A decision to take pre-emptive remedial action. Under some circumstances, such as limited extent of contamination, it may be judged more cost-efficient to implement simple remedial measures (e.g., removal of “hot spots” of contaminated soil) rather than conduct a full ERA. Such action would effectively remove any exposure pathway.

Any early exit from the ERA process requires regulatory “buy-in.” Under certain circumstances or regulatory frameworks, some risk conclusions may be required, even when the exit conditions described above are met. In such cases, the process may be abbreviated without significant expenditure of resources, such as collecting site-specific data.

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Table A-1. Screening benchmark concentrations for the phytotoxicity of chemials in soil

Chemical	Screening Benchmark (mg/kg)	Plant Species	Chemical Form
Aluminum	50	White clover	$Al_2(SO_4)_3$
Antimony	5	--	--
Arsenic	10	[a]	NaH_2AsO_4, $AL(H_2AsO_4)_3$, $Ca(H2AsO4)_2$
Barium	500	Barley	$Ba(NO_3)_2$
Beryllium	10	--	--
Boron	0.5	Corn	H_3BO_3
Bromine	10	--	--
Cadmium	4	[b]	$CdSO_4$, $CdCl_2$, $C_4H_6CdO_6$
Chromium (total)	1	Lettuce	$K_2Cr_2O_7$
Chromium (VI)	--	--	--
Cobalt	20	--	--
Copper	100	Bush beans and little bluestem	$CuSO_4$
Fluorine	200	--	--
Iodine	4	Tomato	KI
Lead	50	[c]	$PbCl_2$,$Pb(NO_3)_2$, PbO
Lithium	2	Orange	$LiSO_4$
Manganese	500	Bush beans	$MnSO_4$
Mercury[d]	0.3	--	--
Molybdenum	2	--	--
Nickel	30	[e]	$NiSO_4$, $NiCL_2$,
Selenium	1	[f]	Na_2SeO_4, $NaSeO_3$
Silver	2	--	--
Technetium	0.2	Wheat and soybean	TcO_4^-
Thallium	1	--	--
Tin	50	--	--
Uranium	5	swiss chard	$UO_2(NO_3)_2$
Vanadium	2	--	--
Zinc	50	[g]	$ZnSO_4$, ZnO
3-Chloroaniline	20	Lettuce	--
2-Chlorophenol	--	--	--
3-Chlorophenol	7	Lettuce	--
4-Chlorophenol	--	--	--
2-Cresol	--	--	--
2,4-Dichlorophenol	--	--	--
3,4-Dichlorophenol	20	Lettuce	--
2,4-Dinitrophenol	20	[h]	--
Di-*n*-butyl phthalate	200	[i]	--
4-Nitrophenol	--	--	--
Pentachlorophenol	3	Lettuce	--
Polychlorinated biphenyls	40	[j]	Aroclor® 1254
Styrene	300	Lettuce	--
2,3,5,6-Tetrachloroaniline	20	Lettuce	--

Table A-1. (cont.)

Chemical	Screening Benchmark (mg/kg)	Plant Species	Chemical Form
Toluene	200	[k]	--
2,4,5-Trichloroaniline	20	Lettuce	--
2,4,5-Trichlorophenol	4	Lettuce	--
2,4,6-Trichlorophenol	--	--	--

[a] Benchmark is based on multiple studies of plants that include corn, spruce, cotton, soybeans, barley and ryegrass.

[b] Benchmark based on multiple studies of plants that include a large range of wild and cultivated plants such as legumes, trees, leafy vegetables and other dicotyledonous plants.

[c] Benchmark based on multiple studies of plants that include autumn olive, red oak, sycamore, Sitka spruce, bluestem, ryegrass, fescue, wheat, oats, corn, radish, and lettuce.

[d] Inorganic mercury.

[e] Benchmark based on multiple studies of plants that include barley, red oak, oats, bush beans, cotton, ryegrass, and corn.

[f] Benchmark based on multiple studies of plants that include sorgrass, alfalfa, and wheat.

[g] Benchmark based on multiple studies of plants that include soybean, wheat, rice, coriander, spinach, beech, cowpea, and corn.

[h] Benchmark based on multiple studies of plants that include soybean, corn, and fescue.

[i] Benchmark based on multiple studies of plants that include corn, soybeans, and fescue.

[j] Benchmark based on multiple studies of plants that include soybean, pigweed, and beet.

[k] Benchmark based on multiple studies of plants that include corn, and fescue.

Table A-2. Screening benchmark concentrations for the toxicity to earthworms and soil microbes of chemicals in soil

Chemical	Earthworm Benchmark (mg/kg)	Earthworm Species	Chemical Form
Aluminum	--	--	--
Arsenic	60	*Eisenia fetida*	KH_2AsO_4
Barium	--	--	--
Boron	--	--	--
Cadmium	20	[a]	$CdCl_2$, $C_4H_6CdO_4$, $Cd(NO_3)_2$, soluble forms
Chromium	0.4	*Octochaetus pattoni*	$K_2Cr_2O_7$
Cobalt	--	--	--
Copper	60	[b]	$CuCl_2$, $Cu(NO_3)_2$, $CuSO_4$, $C_4H_6CuO_4$, $CuNO_3$, soluble forms
Fluorine	--	--	--
Iron	--	--	--
Lanthanum	--	--	--
Lead	500	*Dendrobaena rubida*	--
Lithium	--	--	--
Manganese	--	--	--
Mercury[c]	0.1	*Octochaetus pattoni*	$HgCl_2$
Molybdenum	--	--	--
Nickel	200	*Eisenia fetida*	$C_4H_6NiO_4$
Selenium	70	*Eisenia fetida*	Na_2SeO_3
Silver	--	--	--
Tin	--	--	--
Titanium	--	--	--
Vanadium	--	--	--
Zinc	100	[d]	$Zn(NO_3)_2$, $ZnSO_4$, $ZnCl_2$, $C_4H_6O_4Zn$, soluble forms
Phenol	30	*Eudrilus eugeniae*	--
4-nitrophenol	7	*Eisenia fetida*	--
3-Chlorophenol	10	*Eisenia andrei* and *Lumbricus rubellus*	--
3,4-Dichlorophenol	20	*Eisenia andrei* and *Lumbricus rubellus*	--
2,4,5-Trichlorophenol	9	*Eisenia andrei* and *Lumbricus rubellus*	--
2,4,6-Trichlorophenol	10	*Eisenia fetida*	--
2,3,4,5-tetrachlorophenol	20	*Eisenia andrei*	--
Pentachlorophenol	6	[e]	--

Table A-2. (cont.)

Chemical	Earthworm Benchmark (mg/kg)	Earthworm Species	Chemical Form
Chlorobenzene	40	*Eisenia fetida*	--
1,4-dichlorobenzene	20	*Eisenia fetida* and *Lumbricus rubellus*	--
1,2,3-trichlorobenzene	20	*Eisenia fetida* and *Lumbricus rubellus*	--
1,2,4-trichlorobenzene	20	*Eudrilus eugeniae*	--
1,2,3,4-tetrachlorobenzene	10	*Eisenia andrei* and *Lumbricus rubellus*	--
Pentachlorobenzene	20	*Eisenia andrei*	--
Hexachlorobenzene	--	--	--

[a] Benchmark based on multiple studies of *Aporrectodea caliginosa, Eisenia andrei, Eisenia fetida, Dendrobaena rubida,* and *Lubricus rubellas.*

[b] Benchmark based on multiple studies of *Allolobophora caliginosa, Allolobophora chlorotica, Eisenia fetida, Lubricus rubellus, Aporrectodea caliginosa, Dendrobaena rubida, Eisenia andrei,* and *Octolasium cyaneum.*

[c] Combined inorganicand organic froms of mercury.

[d] Benchmark based on multiple studies of *Eisenia andrei, Eisenia fetida, Aporrectodea rosea, Lumbricus rubellus, Aporrectodea caliginosa,* and *Allolobophora caliginosa*.

[e] Benchmark based on multiple studies of *Eisenia andrei, Eisenia fetida, Eisenia eugeniae, Lumbricus terrestris,* and *Lumbricus rubellus.*

References

Efroymson, R.A., M.E. Will, and G.W. Suter, II. 1997a. Toxicological benchmarks for contaminants of potential concern for effects on soil and litter invertebrates and heterotrophic process: 1997 Revision. ES/ER/TM-126/R2. U.S. Department of Energy.

Efroymson, R.A., M.E. Will, G.W. Suter, II, and A.C. Wooten. 1997b. Toxicological benchmarks for screening contaminants of potential concern for effects on terrestrial plants: 1997 Revision. ES/ER/TM-85/R3. U.S. Department of Energy.

Algorithms Used in Food-Web Models

Hazard Quotient

$$\mathrm{HQ} = \frac{\mathrm{Exposure}}{\mathrm{TRV}}$$

where:

HQ = hazard quotient

Exposure = estimated exposure

TRV = toxicity reference value.

Total Daily Ingested Dose

$$\mathrm{D}_{\mathrm{chemical}} = \frac{\sum_{\mathrm{i}} \left(\mathrm{C}_{\mathrm{i}} \times \mathrm{M}_{\mathrm{i}} \times \mathrm{A}_{\mathrm{i}} \times \mathrm{F}_{\mathrm{i}} \right)}{\mathrm{W}}$$

where:

$\mathrm{D}_{\mathrm{chemical}}$ = daily ingested dose of chemical from all dietary components (mg/kg-body weight/day)

C_{i} = concentration of the chemical in dietary component i (mg/kg)

M_{i} = rate of ingestion of dietary component i (kg/day)

A_{i} = relative gastrointestinal absorption efficiency for the chemical in dietary component i (fraction)

F_{i} = area use factor; portion of the daily intake of dietary component i derived from the investigation area (fraction)

W = body weight of receptor species (kg).

Food Ingestion Rate

Generic Mammal: $\text{FIR} = 0.235 \times \text{BW}^{0.822}$

Rodents: $\text{FIR} = 0.621 \times \text{BW}^{0.564}$

Herbivores: $\text{FIR} = 0.577 \times \text{BW}^{0.727}$

Generic Bird: $\text{FIR} = 0.648 \times \text{BW}^{0.651}$

Passerines: $\text{FIR} = 0.398 \times \text{BW}^{0.850}$

Non-Passerines: $\text{FIR} = 0.301 \times \text{BW}^{0.751}$

Seabirds: $\text{FIR} = 0.495 \times \text{BW}^{0.704}$

where:

FIR = food ingestion rate (g/day, dry-weight basis)

BW = body weight (g).

Drinking Water Ingestion Rate

Generic Mammal: $\text{DIR} = 0.099 \times \text{BW}^{0.90}$

Generic Bird: $\text{DIR} = 0.059 \times \text{BW}^{0.67}$

where:

DIR = drinking water ingestion rate (L/day)

BW = body weight (kg).

Table C-1. Mammalian toxicity reference values[a]

Chemical	ORNL TRV (mg/kg-day)	NOAEL/ LOAEL	Test Species	Chemical Form
Aluminum	1.93 [b]	NOAEL	Mouse	Aluminum chloride
	19.3	LOAEL	Mouse	Aluminum chloride
Antimony	0.125 [b]	NOAEL	Mouse	Antimony potassium tartrate
	1.25	LOAEL	Mouse	Antimony potassium tartrate
Arsenic	0.126 [b]	NOAEL	Mouse	Arsenite
	1.26	LOAEL	Mouse	Arsenite
Barium	5.1	NOAEL	Rat	Barium chloride
	19.8 [c]	LOAEL	Rat	Barium chloride
Benzene	26.36	NOAEL	Mouse	Benzene
	263.6	LOAEL	Mouse	Benzene
Benzo[a]pyrene	1 [b]	NOAEL	Mouse	Benzo[a]pyrene
	10	LOAEL	Mouse	Benzo[a]pyrene
Beryllium	0.66	NOAEL	Rat	Beryllium sulfate
Boron	28	NOAEL	Rat	Boric acid (Borax)
	93.6	LOAEL	Rat	Boric acid (Borax)
Cadmium	1	NOAEL	Rat	Cadmium chloride
	10	LOAEL	Rat	Cadmium chloride
Chromium (trivalent)	2,737	NOAEL	Rat	Chromium(III) oxide
Chromium (hexavalent)	3.28	NOAEL	Rat	Chromium(VI) chromate
	13.14 [c]	LOAEL	Rat	Chromium(VI) chromate
Cobalt	--	--		
Copper	11.7	NOAEL	Mink	Copper sulfate
	15.14	LOAEL	Mink	Copper sulfate
Cyanide	68.7	NOAEL	Rat	Potassium cyanide
Lead	8	NOAEL	Rat	Lead acetate
	80	LOAEL	Rat	Lead acetate
Manganese	88	NOAEL	Rat	Manganese oxide
	284	LOAEL	Rat	Manganese oxide
Mercury	1	NOAEL	Mink	Mercuric chloride
	13.2	NOAEL	Mouse	Mercuric sulfide
Methylmercury	0.015 [c]	NOAEL	Mink	Methylmercury chloride
	0.025 [c]	LOAEL	Mink	Methylmercury chloride
	0.032	NOAEL	Rat	Methylmercury chloride
	0.16	LOAEL	Rat	Methylmercury chloride
Nickel	40	NOAEL	Rat	Nickel sulfate hexahydrate
	80	LOAEL	Rat	Nickel sulfate hexahydrate
Strontium	263	NOAEL	Rat	Strontium chloride
Thallium	0.0074 [b]	NOAEL	Rat	Thallium sulfate
	0.074	LOAEL	Rat	Thallium sulfate
Tin	23.4	NOAEL	Mouse	bis (Tributyltin) oxide
	35	LOAEL	Mouse	bis (Tributyltin) oxide

Table C-1. (cont.)

Chemical	ORNL TRV (mg/kg-day)	NOAEL/ LOAEL	Test Species	Chemical Form
Vanadium	0.21 [b]	NOAEL	Rat	Sodium metavanadate
	2.1	LOAEL	Rat	Sodium metavanadate
Vinyl chloride	0.17 [b]	NOAEL	Rat	Vinyl chloride
	1.7	LOAEL	Rat	Vinyl chloride
Xylene (mixed isomers)	2.1	NOAEL	Mouse	Xylene (mixed isomers)
	2.6	LOAEL	Mouse	Xylene (mixed isomers)
Zinc	160	NOAEL	Rat	Zinc oxide
	320	LOAEL	Rat	Zinc oxide

Note: LOAEL - lowest-observed-adverse-effect level
NOAEL - no-observed-adverse-effect level
ORNL - Oak Ridge National Laboratory
TRV - toxicity reference value

[a] Sample et al. (1996).

[b] The chronic NOAEL was estimated by multiplying a chronic LOAEL by a LOAEL–NOAEL uncertainty factor of 0.1.

[c] Chronic values were estimated by multiplying a subchronic LOAEL and NOAEL by a subchronic to chronic uncertanty factor of 0.1.

Table C-2. Avian toxicity reference values[a]

Chemical	ORNL TRV (mg/kg-day)	NOAEL/ LOAEL	Test Species	Chemical Form
Aluminum	109.7	NOAEL	Ringed dove	Aluminum sulfate
Arsenic	2.46	NOAEL	Brown-headed cowbird (males only)	Copper acetoarsenite
	7.38	LOAEL	Brown-headed cowbird (males only)	Copper acetoarsenite
	5.14	NOAEL	Mallard duck	Sodium arsenite
	12.84	LOAEL	Mallard duck	Sodium arsenite
Barium	20.8 [b]	NOAEL	1-day-old chick	Barium hydroxide
	41.7	LOAEL	1-day-old chick	Barium hydroxide
Boron	28.8	NOAEL	Mallard duck	Boric acid (Borax)
	100	LOAEL	Mallard duck	Boric acid (Borax)
Cadmium	1.45	NOAEL	Mallard duck	Cadmium chloride
	20	LOAEL	Mallard duck	Cadmium chloride
Chromium (hexavalent)	1	NOAEL	Black duck	Chromium potassium sulfate
	5	LOAEL	Black duck	Chromium potassium sulfate
Copper	47	NOAEL	1-day-old chick	Copper oxide
	61.7	LOAEL	1-day-old chick	Copper oxide
Lead	3.85	NOAEL	American kestrel	Metallic lead
	1.13	NOAEL	Japanese quail	Lead acetate
	11.3	LOAEL	Japanese quail	Lead acetate
Manganese	977	NOAEL	Japanese quail	Manganese oxide
Mercury	0.45	NOAEL	Japanese quail	Mercuric chloride
	0.9	LOAEL	Japanese quail	Mercuric chloride
Methylmercury	0.0064 [c]	NOAEL	Mallard duck	Methylmercury dicyandiamide
	0.064 [c]	LOAEL	Mallard duck	Methylmercury dicyandiamide
Nickel	77.4	NOAEL	Mallard duckling	Nickel sulfate
	107	LOAEL	Mallard duckling	Nickel sulfate
Tin	6.8	NOAEL	Japanese quail	bis(tributyltin) oxide
	16.9	LOAEL	Japanese quail	bis(tributyltin) oxide
Vanadium	11.4	NOAEL	Mallard duck	Vanadyl sulfate
Zinc	131	LOAEL	White leghorn hen	Zinc sulfate
	14.5	NOAEL	White leghorn hen	Zinc sulfate

Note: LOAEL - lowest-observed-adverse-effect level
NOAEL - no-observed-adverse-effect level
ORNL - Oak Ridge National Laboratory
TRV - toxicity reference value

[a] Sample et al. (1996).

[b] The chronic NOAEL was estimated by multiplying the chronic LOAEL by a LOAEL–NOAEL uncertainty factor of 0.1.

[c] Chronic values were estimated by multiplying the subchronic LOAEL and NOAEL by a subchronic to chronic uncertanty factor of 0.1.

Table C-3. Dietary uptake factors

Analyte	Earthworm Uptake Factors[a,b]	Small Mammal Uptake Factors[c,d]	Benthic Invertebrate Uptake Factors[e,f]	Plant Uptake Factors[g]
Metals and Cyanide				
Aluminum	0.053	0.0263	log(benthos) = 0.2092 + 0.365*(log[sediment])[h]	0.0032
Antimony	ln(earthworm) = –1.421 + 0.706*(ln[soil])[i]	ln(mammal) = –4.8471 + 0.8188*(ln[soil])[i]	log(benthos) = –0.292 + 0.754*(log[sediment])[i]	0.0102
Arsenic	ln(earthworm) = –1.421 + 0.706*(ln[soil])	ln(mammal) = –4.8471 + 0.8188*(ln[soil])	log(benthos) = –0.292 + 0.754*(log[sediment])	ln(plant) = –1.992 + 0.564*(ln[soil])
Barium	N/A	ln(mammal) = –1.412 + 0.7*(ln[soil])	log(benthos) = 0.0395 + 0.692*(log[sediment])[j]	0.213
Beryllium	N/A	N/A	log(benthos) = 1.8 + 0.208*(log[sediment]) [k]	N/A
Boron	N/A	N/A	N/A	N/A
Cadmium	ln(earthworm) = 2.114 + 0.795*(ln[soil])	ln(mammal) = –0.4306 + 0.4865*(ln[soil])	log(benthos) = 0.0395 + 0.692*(log[sediment])	ln(plant) = –0.476 + 0.546*(ln[soil])
Chromium	ln(earthworm) = 2.481 – 0.067*(ln[soil])	ln(mammal) = –1.4599 + 0.7338*(ln[soil])	log(benthos) = 0.2092 + 0.365*(log[sediment])	0.0653
Cobalt	ln(earthworm) = 3.677 – 0.26*(ln[soil])[l]	ln(mammal) = –4.4599 + 1.307*(ln[soil])	log(benthos) = 1.48 – 0.425*(log[sediment])	0.0115
Copper	ln(earthworm) = 1.675 + 0.264*(ln[soil])	ln(mammal) = 2.042 + 0.1444*(ln[soil])	log(benthos) = 1.089 + 0.278*(log[sediment])	ln(plant) = 0.669 + 0.394*(ln[soil])
Cyanide	N/A	N/A	N/A	N/A
Lead	ln(earthworm) = –0.218 + 0.807*(ln[soil])	ln(mammal) = 0.0761 + 0.4422*(ln[soil])	log(benthos) = –0.776 + 0.801*(log[sediment])	ln(plant) = –1.328 + 0.561*(ln[soil])
Manganese	ln(earthworm) = –0.809 + 0.682*(ln[soil])	0.0205	N/A	0.113
Mercury/methylmercury	ln(earthworm) = –0.684 + 0.118*(ln[soil])	ln(mammal) = –4.8666 – 2.2764*(ln[soil])	log(benthos) = –0.67 + 0.327*(log[sediment])	ln(plant) = –0.996 + 0.544*(ln[soil])
Nickel	ln(earthworm) = 3.677 – 0.26*(ln[soil])	ln(mammal) = –0.2462 + 0.4658*(ln[soil])	log(benthos) = 1.48 – 0.425(log[sediment])	ln(plant) = –2.224 + 0.748*(ln[soil])
Strontium	N/A	N/A	N/A	N/A
Thallium	ln(earthworm) = 0.218 + 0.807*(ln[soil])	0.1124	log(benthos) = –0.776 + 0.801*(log[sediment])[m]	N/A
Tin	N/A	N/A	N/A	N/A
Vanadium	0.039	0.0123	No uptake factor available[i]	0.00548
Zinc	ln(earthworm) = 4.449 + 0.328*(ln[soil])	ln(mammal) = 4.4713 + 0.0738*(ln[soil])	log(benthos) = 1.8 + 0.208*(log[sediment])	ln(plant) = 1.575 + 0.555*(ln[soil])
Semivolatile Organic Compounds				
Benzo[a]pyrene	22.2	1.78	0.023	N/A
Vinyl chloride	N/A	N/A	N/A	N/A
Volatile Organic Compounds				
Benzene	N/A	N/A	N/A	N/A
Xylene (mixed isomers)	N/A	N/A	N/A	N/A

Note: COC - contaminant of concern
UCL - upper confidence limit

[a] Sample et al. (1998a).

[b] COCs for which adequate uptake factors were not available were provided default values of 22.2 as a conservative overestimation (O'Brien & Gere 1999).

[c] Sample et al. (1998b).

[d] COCs for which adequate uptake factors were not available were provided default values of 1.78 as a conservative overestimation (O'Brien & Gere 1999).

[e] Bechtel Jacobs (1998a).

[f] Corps (1999).

[g] Bechtel Jacobs (1998b).

[h] No factor available. Regression used for chromium based on similar valence.

[i] No factor available. Regression used for arsenic based on similar valence.

[j] No factor available. Regression used for cadmium based on similar valence.

[k] No factor available. Regression used for zinc based on same valence.

[l] No factor available. Regression used for nickel as a surrogate.

[m] No factor available. Regression used for lead based on same valence.

Table C-4. Example exposure parameters for screening-level ecological risk calculations

Receptor Common Name	Receptor Scientific Name	Body Weight (kg)	Primary Dietary Components	Percent of Diet from Study Area	Food Ingestion Rate (kg/day dry weight)	Water Ingestion Rate (L/day)	Sediment/Soil Ingestion Rate (% food ingestion dry weight)	Foraging Range (km^2)
White-tailed deer	*Odocoileus virginianus*	33.1 [a]	vegetation (herbaceous and woody plants)	100	1.11	0.615	2.0 [b]	2.59 [c]
Raccoon	*Procyon lotor*	3.67 [d]	vegetation (herbaceous plants, roots, berries), insects, earthworms, aquatic invertebrates, some fish	100	0.200	0.141	9.4 [b]	0.39 [e]
Short-tailed shrew	*Blarina brevicauda*	0.015 [f]	insects, earthworms	100	0.01601	0.0166	10.0 [g]	0.0039 [h]
Red fox	*Vulpes vulpes*	3.94 [i]	small mammals	100	0.212	0.148	2.8 [b]	19.67 [j]
Muskrat	*Ondatra zibethicus*	0.837 [k]	vegetation (aquatic and wetland plans)	100	0.07	0.0524	9.4 [g]	0.0017 [l]
American woodcock	*Scolopax minor*	0.134 [m]	earthworms	100	0.0157	0.0153	10.4 [b]	0.736 [n]
Red-tailed hawk	*Buteo jamaicensis*	1.22 [o]	small mammals	100	0.0662	0.0674	3.0 [p]	6.97 [o]
Northern bobwhite	*Colinus virginianus*	0.154 [q]	vegetation (seeds)	100	0.0172	0.0168	9.3 [r]	0.167 [s]
River otter	*Lutra canadensis*	5 [t]	fish	100	0.258	0.1734	1.0 [u]	4 [v]
Belted kingfisher	*Ceryle alcyon*	0.136 [w]	fish	100	0.0159	0.0155	1.0 [x]	2.19 [y]
Great blue heron	*Ardea herodias*	2.2 [z]	fish, aquatic invertebrates, some small mammals	100	0.0972	0.1001	2.0 [aa]	0.084 [ab]

Table C-4. (cont.)

Receptor Common Name	Receptor Scientific Name	Body Weight (kg)	Dietary Composition	Percent of Diet from Study Area	Food Ingestion Rate (kg/day dry weight)	Water Ingestion Rate (L/day)	Sediment/Soil Ingestion Rate (% food ingestion dry weight)	Foraging Range (km^2)
Spotted sandpiper	*Actitis macularia*	0.0379 [ac]	benthic invertebrates	100	0.0069	0.0066	18.4 [b,ad]	0.0025 [ac]
Lesser scaup	*Aythya affinis*	0.77 [ae]	benthic invertebrates	100	0.0491	0.0495	11.0 [b,af]	0.89 [ag]
Mallard	*Anas platyrhynchos*	1.04 [ah]	vegetation (aquatic and wetland plants), some insects	100	0.0597	0.0606	3.3 [b]	6.2 [ai]
Bald eagle	*Haliaeetus leucocephalus*	3 [aj]	small mammals, fish	100	0.1189	0.1232	3.0 [ak]	7 [al]

[a] Silva and Downing (1995).

[b] Beyer et al. (1994).

[c] NJDFW (2002).

[d] Johnson (1970, as cited by U.S. EPA 1993).

[e] Lotze (1979, as cited by U.S. EPA 1993).

[f] Schlesinger and Potter (1974).

[g] Estimated from racoon based on Beyer et al. (1994).

[h] Buckner (1966, as cited by U.S. EPA 1993).

[i] Storm et al. (1976, as cited by U.S. EPA 1993).

[j] Jones and Theberge (1982, as cited by U.S. EPA 1993).

[k] Reeves and Williams (1956, as cited by U.S. EPA 1993).

[l] Proulx and Gilbert (1983, as cited by U.S. EPA 1993).

[m] Dwyer et al. (1988, as cited by U.S. EPA 1993).

Table C-4. (cont.)

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[n] Hudgins et al. (1985, as cited by U.S. EPA 1993).

[o] Craighead and Craighead (1956).

[p] Estimated from Beyer et al. (1994).

[q] Guthery et al. (1988, as cited by U.S. EPA 1993).

[r] Estimated from wild turkey based on Beyer et al. (1994).

[s] Urban (1972, as cited in U.S. EPA 1993).

[t] Melquist and Dronkert (1987).

[u] Best professional judgment based on U.S. EPA (1993).

[v] Foy (1984, as cited by U.S. EPA 1993).

[w] Brooks and Davis (1987).

[x] NYSDEC (2001).

[y] Brooks and Davis (1987). Note: This is the linear shoreline distance in km.

[z] Hartman (1961).

[aa] Best professional judgement, based on Eckert and Karalus (1983).

[ab] Bayer (1978, as cited by U.S. EPA 1993).

[ac] Maxson and Oring (1980, as cited by U.S. EPA 1993).

[ad] Estimated from least, western, and semipalmatred sandpipers.

[ae] Nelson and Martin (1953, as cited by U.S. EPA 1993).

[af] Estimated from wood duck.

[ag] Hammel (1973, as cited by U.S. EPA 1993).

[ah] Nelson and Martin (1953).

[ai] Kirby et al. (1985, as cited by U.S. EPA 1993).

[aj] Wiemeyer (1991, pers. comm., as cited by U.S. EPA 1993).

[ak] Estimated from red fox, based on Beyer et al. (1994).

[al] Craig et al. (1988, as cited by U.S. EPA 1993). Note: This foraging distance is a linear distance in km.

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Example 1: White-Tailed Deer Exposure to Lead

Scenario:

Site soils are contaminated with lead. A population of white-tailed deer is known to forage on the site. Using the information in Appendices B and C, perform a worst-case risk calculation for dietary exposure of deer to lead, then consider the effect of site size on probable exposure and risk.

Key Input Assumptions:

Site size	=	100 acres
Maximum soil lead concentration	=	12,000 mg/kg
Maximum surface water lead concentration	=	0.003 mg/L
Deer diet	=	100 percent vegetation
Body weight	=	33.1 kg (Silva and Downing 1995)
Soil ingestion rate	=	2 percent of food ingestion rate (Beyer et al. 1994)
NOAEL TRV	=	8 mg/kg body wt/day (Sample et al. 1996)

Step 1: Estimate the maximum lead concentration in vegetation using a soil-to-plant uptake factor (see Table C-3).

$$\mathrm{Ln}[\mathrm{vegetation}_{\mathrm{lead}}] = \mathrm{B0} + \mathrm{B1} \times \ln[\mathrm{soil}_{\mathrm{lead}}]$$

where:

$\mathrm{B0} = -1.328$

$\mathrm{B1} = 0.561$

$[\mathrm{soil}_{\mathrm{lead}}] = 12{,}000$ mg/kg.

$$[\mathrm{vegetation}_{\mathrm{lead}}] = e^{(-1.328 + 0.561 \times \ln[12{,}000])}$$

$$[\mathrm{vegetation}_{\mathrm{lead}}] = 51.5 \text{ mg/kg}$$

Step 2: Estimate the food ingestion rate (FIR) for a deer using the allometric food ingestion model for herbivorous mammals (see Appendix B).

$$FIR = 0.577 \times BW^{0.727}$$

where:

BW = body weight = 33.1 kg = 33,100 g

$$FIR = 0.577 \times 33{,}100^{0.727}$$
$$FIR = 1{,}114.5 \text{ g/day} = 1.11 \text{ kg/day}$$

Step 3: Estimate the soil ingestion rate (SIR) for a deer.

$$SIR = 2\% \times FIR$$
$$SIR = 0.02 \times 1.11 \text{ kg/day}$$
$$SIR = 0.0223 \text{ kg/day}$$

Step 4: Estimate the drinking water ingestion rate (DIR) for a deer, using the allometric water ingestion model for mammals (see Appendix B).

$$DIR = 0.099 \times BW^{0.90}$$

where:

BW = 33.1 kg

$$DIR = 0.099 \times 33.1^{0.90}$$
$$DIR = 2.31 \text{ L/day}$$

Step 5: Estimate maximum lead exposure from ingested vegetation, soil, and water.

$$\text{Food exposure} = FIR \times [\text{vegetation}_{\text{lead}}]$$
$$\text{Food exposure} = 1.11 \text{ kg/day} \times 51.5 \text{ mg/kg}$$
$$\text{Food exposure} = 57.2 \text{ mg/day}$$

$$\text{Soil exposure} = SIR \times \text{maximum soil lead concentration}$$
$$\text{Soil exposure} = 0.0223 \text{ kg/day} \times 12{,}000 \text{ mg/kg}$$
$$\text{Soil exposure} = 267.6 \text{ mg/day}$$

$$\text{Water exposure} = DIR \times \text{maximum water lead concentration}$$
$$\text{Water exposure} = 2.31 \text{ L/day} \times 0.003 \text{ mg/L}$$
$$\text{Water exposure} = 0.00693 \text{ mg/day}$$

Step 6: Estimate maximum total dietary lead exposure.

Total dietary exposure = food exposure + soil exposure + water exposure
Total dietary exposure = 57.2 + 267.6 + 0.00693 mg/day
Total dietary exposure = 324.8 mg/day

Step 7: Calculate body weight normalized daily dose of lead

$$\text{Daily dose} = \frac{\text{total daily exposure}}{\text{body weight}}$$

$$\text{Daily dose} = \frac{324.8\ \text{mg/day}}{33.1\ \text{kg}}$$

Daily dose = 9.81 mg/kg-body weight/day

Step 8: Evaluate the worst case hazard quotient (HQ).

$$\text{HQ} = \frac{\text{Daily dose}}{\text{TRV}}$$

$$\text{HQ} = \frac{9.81\ \text{mg/kg - body weight/day}}{8\ \text{mg/kg - body weight/day}}$$

HQ = 1.2

Step 9: Adjust exposure and risk estimate for probable area use.

$$\text{Area Use Factor} = \frac{\text{Site Area}}{\text{Receptor Forage Range}}$$

$$\text{Area Use Factor} = \frac{100\ \text{acres}}{(2.59\ \text{km}^2) \times (247.1\ \text{acres / km}^2)}$$

Area Use Factor = 0.16

Area Use Adjusted Daily Exposure = maximum dietary exposure × Area Use Factor
Area Use Adjusted Daily Exposure = 9.81 mg/kg-body weight/day × 0.16
Area Use Adjusted Daily Exposure = 1.57 mg/kg-body weight/day

$$\text{Area Use Adjusted HQ} = \frac{1.57\ \text{mg/kg - body weight/day}}{8\ \text{mg/kg - body weight/day}} = 0.2$$

Conclusions:

Use of the maximum site lead concentrations and 100 percent area use by deer (both typical assumptions for screening-level assessments) leads to a prediction that the daily exposure will slightly exceed the NOAEL TRV. In other words, these conservative assumptions suggest that adverse effects to deer from dietary lead exposure are possible. Consideration of the typically large foraging range of deer relative to the site area indicates that adverse effects are highly unlikely, however. Even retaining the maximum site concentrations in the exposure model, the area use adjusted HQ is well below 1, indicating negligible risk to deer from soil lead. In either calculation, the bulk of the estimated lead exposure is driven by direct soil ingestion rather than uptake of lead into vegetation. Drinking water exposure is not a significant pathway under the conditions modeled.

Example 2: Bald Eagle Exposure to Benzo(a)pyrene

Scenario:

Site soils are contaminated with Benzo(a)pyrene (BaP). A stream located onsite has also been contaminated by runoff and the concentration of BaP in fish has been measured empirically. A nesting pair of bald eagles is present near the center of the site. While eagles typically have large forage ranges, field observations indicate that these eagles derive virtually their entire diet from a small area near the nest, foraging on both fish from the stream and small mammals from fields. Using the information in Appendices B and C, perform a worst-case risk calculation for dietary exposure of eagles to BaP.

Key Input Assumptions:

Maximum soil BaP concentration = 5 mg/kg

Maximum surface water BaP concentration = 0.0003 mg/L

Maximum fish BaP concentration = 0.10 mg/kg dry weight

Eagle diet = 50 percent fish and 50 percent small mammals

Body weight = 3 kg (Wiemeyer 1991, pers. comm., as cited by U.S. EPA 1993)

Soil ingestion rate = 3 percent of terrestrial food ingestion rate (Beyer et al. 1994)

Sediment ingestion rate = Zero (no contact with sediment assumed)

Area use factor = 100 percent

NOAEL TRV = 0.143 mg/kg-day (Hough et al. 1993).

Step 1: Estimate the maximum lead concentration in terrestrial prey using a soil to small mammal uptake factor (see Table C-3).

$$[\text{mammal}_{\text{BaP}}] = 1.78 \times [\text{soil}_{\text{BaP}}]$$

where:

$[\text{soil}_{\text{BaP}}]$ = 5 mg/kg.

$$[\text{mammal}_{\text{BaP}}] = 8.90 \text{ mg/kg}$$

Step 2: Estimate the food ingestion rate (FIR) for an eagle using the generic bird allometric food ingestion model (see Appendix A).

$$FIR = 0.648 \times BW^{0.651}$$

where:

BW = body weight = 3 kg = 3,000 g

$$FIR = 0.648 \times 3{,}000^{0.651}$$
$$FIR = 118.9 \text{ g/day} = 0.119 \text{ kg/day}$$

Step 3: Estimate the soil ingestion rate (SIR) for a bald eagle.

$$SIR = 0.03 \times FIR \times 0.5^{*}$$

$$SIR = 0.03 \times 0.119 \times 0.5 \text{ kg/day}$$
$$SIR = 0.00178 \text{ kg/day}$$

[*] Only 50 percent of the total diet is from terrestrial prey:

Step 4: Estimate the drinking water ingestion rate (DIR) for a bald eagle.

$$DIR = 0.059 \times BW^{0.67}$$

where:

BW = 3 kg

$$DIR = 0.059 \times 3^{0.67}$$
$$DIR = 0.123 \text{ L/day}$$

Step 5: Estimate the maximum BaP exposure from food (50 percent small mammals and 50 percent fish), soil, and water.

$$\text{Food exposure}_{\text{mammals}} = FIR \times [\text{mammal}_{\text{BaP}}] \times 0.5$$
$$\text{Food exposure}_{\text{mammals}} = 0.119 \text{ kg/day} \times 8.90 \text{ mg/kg} \times 0.5$$
$$\text{Food exposure}_{\text{mammals}} = 0.530 \text{ mg/day}$$

$$\text{Food exposure}_{\text{fish}} = FIR \times [\text{fish}_{\text{BaP}}] \times 0.5$$
$$\text{Food exposure}_{\text{fish}} = 0.119 \text{ kg/day} \times 0.10 \text{ mg/kg} \times 0.5$$
$$\text{Food exposure}_{\text{fish}} = 0.0060 \text{ mg/day}$$

$$\text{Total food exposure} = \text{food exposure}_{\text{mammals}} + \text{food exposure}_{\text{fish}}$$
$$\text{Total food exposure} = 0.530 \text{ mg/day} + 0.0060 \text{ mg/day}$$
$$\text{Total food exposure} = 0.536 \text{ mg/day}$$

$$\text{Soil exposure} = \text{SIR} \times \text{maximum soil BaP concentration}$$
$$\text{Soil exposure} = 0.00178 \text{ kg/day} \times 5 \text{ mg/kg}$$
$$\text{Soil exposure} = 0.00890 \text{ mg/day}$$

$$\text{Water exposure} = \text{DIR} \times \text{maximum water BaP concentration}$$
$$\text{Water exposure} = 0.123 \text{ L/day} \times 0.0003 \text{ mg/L}$$
$$\text{Water exposure} = 0.0000369 \text{ mg/day}$$

Step 6: Calculate the maximum dietary exposure.

$$\text{Maximum dietary exposure} = \text{total food exposure} + \text{soil exposure} + \text{water exposure}$$
$$\text{Total daily exposure} = 0.536 \text{ mg/day} + 0.00890 \text{ mg/day} + 0.0000369 \text{ mg/day}$$
$$\text{Total daily exposure} = 0.545 \text{ mg/day}$$

Step 7: Calculate body weight normalized daily dose of BaP.

$$\text{Daily dose} = \frac{\text{total daily exposure}}{\text{body weight}}$$

$$\text{Daily dose} = \frac{0.545 \text{ mg/day}}{3 \text{ kg}} = 0.1816 \text{ mg/kg-body weight/day}$$

Step 8: Evaluate the worst case hazard quotient (HQ).

$$\text{HQ} = \frac{\text{Daily dose}}{\text{TRV}}$$

$$\text{HQ} = \frac{0.1816 \text{ mg/kg - body weight/day}}{0.143 \text{ mg/kg - body weight/day}}$$

$$\text{HQ} = 1.27$$

Conclusions:

Use of the maximum site BaP concentrations, 100 percent area use by eagle, and a diet consisting of equal parts fish and terrestrial prey leads to a prediction that the daily exposure will be 127 percent of the NOAEL TRV. In other words, these assumptions suggest a potential risk of adverse effects to an eagle from dietary BaP exposure. The risk driving exposure assumptions are the area use factor of 100 percent, the use of maximum soil concentrations, and the modeled BaP concentration in small mammals (based on maximum soil concentration). Both direct soil exposure and drinking water exposure are negligible compared to food exposure. Refinement of the risk assessment could be accomplished by better characterizing the distribution of soil concentrations in the eagles' terrestrial forage areas, direct measurement of BaP concentrations in small mammal prey species, and/or quantitative study of the eagles' forage patterns and site usage. As in all HQ calculations, the TRV is also a key risk-driving assumption, which should be critically evaluated. The sensitivity of birds to PAHs has not been thoroughly investigated.

Example 3: Belted Kingfisher Exposure to Mercury

Scenario:

A stream located on a site is contaminated with mercury. Fish and sediments from the streams were analyzed and found to contain significant mercury concentrations. The chemical form of the mercury has not been determined, but reducing conditions in the sediments make it likely that at least some of the mercury has been methylated. A nesting pair of belted kingfishers is present at the site. Based on field observations, the belted kingfishers are deriving all of their diet from the fish in the most contaminated portion of the stream. Using the information in Appendices B and C, perform a worst-case risk calculation for dietary exposure of belted kingfishers to mercury.

Key Input Assumptions:

Maximum surface water mercury concentration = 0.003 mg/L
Maximum fish mercury concentration = 3.5 mg/kg dry weight
Maximum sediment mercury concentration = 10 mg/kg

Belted kingfisher diet = 100 percent fish
Body weight = 0.136 kg (Brooks and Davis 1987)
Sediment ingestion rate = 1 percent of food ingestion rate
Area use factor = 100 percent
NOAEL TRV for inorganic mercury = 0.45 mg/kg-day (Sample et al. 1996)
NOAEL TRV for methylmercury = 0.0064 mg/kg-day (Sample et al. 1996)

Step 1: Estimate the food ingestion rate (FIR) for a belted kingfisher using the generic bird allometric food ingestion model (see Appendix A).

$$FIR = 0.648 \times BW^{0.651}$$

where:

BW = body weight = 0.136 kg = 136 g

$$FIR = 0.648 \times 136^{0.651}$$
$$FIR = 5.9 \text{ g/day} = 0.0159 \text{ kg/day}$$

Step 2: Estimate the sediment ingestion rate (SIR) for a belted kingfisher.

$$SIR = 0.01 \times FIR$$
$$SIR = 0.01 \times 0.0159 \text{ kg/day}$$
$$SIR = 0.000159 \text{ kg/day}$$

Step 3: Estimate the drinking water ingestion rate (DIR) for a belted kingfisher.

$$\text{DIR} = 0.059 \times \text{BW}^{0.67}$$

where:

BW = 0.136 kg

$$\text{DIR} = 0.059 \times 0.136^{0.67}$$

$$\text{DIR} = 0.0155 \text{ L/day}$$

Step 4: Estimate the maximum mercury exposure from food (100 percent fish), sediment, and water.

$$\text{Food exposure}_{\text{fish}} = \text{FIR} \times [\text{fish}_{\text{Mercury}}]$$

$$\text{Food exposure}_{\text{fish}} = 0.0159 \text{ kg/day} \times 3.5 \text{ mg/kg}$$

$$\text{Food exposure}_{\text{fish}} = 0.056 \text{ mg/day}$$

$$\text{Sediment exposure} = \text{SIR} \times \text{maximum sediment mercury concentration}$$

$$\text{Sediment exposure} = 0.000159 \text{ kg/day} \times 10 \text{ mg/kg}$$

$$\text{Sediment exposure} = 0.00159 \text{ mg/day}$$

$$\text{Water exposure} = \text{DIR} \times \text{maximum water mercury concentration}$$

$$\text{Water exposure} = 0.0155 \text{ L/day} \times 0.003 \text{ mg/L}$$

$$\text{Water exposure} = 0.0000465 \text{ mg/day}$$

Step 5: Calculate the maximum dietary mercury exposure.

$$\text{Maximum dietary exposure} = \text{food exposure} + \text{sediment exposure} + \text{water exposure}$$

$$\text{Total daily exposure} = 0.056 \text{ mg/day} + 0.00159 \text{ mg/day} + 0.0000465 \text{ mg/day}$$

$$\text{Total daily exposure} = 0.0576 \text{ mg/day}$$

Step 6: Calculate body weight normalized daily dose of mercury.

$$\text{Daily dose} = \frac{\text{total daily exposure}}{\text{body weight}}$$

$$\text{Daily dose} = \frac{0.0576 \text{ mg/day}}{0.136 \text{ kg}}$$

$$\text{Daily dose} = 0.424 \text{ mg/kg-body weight/day}$$

Step 7: Evaluate the hazard quotient (HQ).

The worst case is if all of the detected mercury is in the form of methylmercury.

$$\mathrm{HQ} = \frac{\text{Daily dose}}{\text{TRV}}$$

$$\mathrm{HQ} = \frac{0.424\ \text{mg/kg - body weight/day}}{0.0064\ \text{mg/kg - body weight/day}}$$

$$\mathrm{HQ} = 66.3$$

The best case (given the exposure assumptions above) is that all of the mercury is in inorganic forms.

$$\mathrm{HQ} = \frac{0.424\ \text{mg/kg - body weight/day}}{0.45\ \text{mg/kg - body weight/day}}$$

$$\mathrm{HQ} = 0.94$$

Conclusions:

Under conservative assumptions that maximize exposure of the belted kingfisher to mercury, the total daily exposure exceeds the NOAEL TRV for methylmercury by a significant factor, however it does not exceed the NOAEL TRV for inorganic mercury. The estimated mercury exposure is driven by uptake from fish prey. Direct sediment ingestion and drinking water exposure are not significant pathways under the conditions modeled. Belted kingfishers are highly territorial, and may derive all of their diet from a relatively small area, therefore the assumption of 100% area use may be valid. The primary source of uncertainty in the risk calculation is the chemical form of the mercury ingested by the kingfisher, which has a dramatic influence on the TRV. If little or no methylmercury is included, then risk may be low to negligible. If a significant fraction of the mercury has been methylated, then risk may well be significant. Standard total mercury analyses do not indicate the chemical form present. Refinement of the risk calculation could be accomplished by analyzing site sediments and fish for methylmercury as well as total mercury.

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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

$$MF_i = \frac{C_{soil\ i}}{C_{TPH}} \qquad \text{Q-1}$$

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:

$$HI = \sum_{i=1}^{13} HQ_i = \sum MF_i \frac{SSTL_{TPH}}{SSTL_i} \qquad \text{Q-2}$$

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 $SSTL_{TPH}$

$$SSTL_{TPH} = \frac{HI}{\sum \frac{MF_i}{SSTL_i}} \qquad \text{Q-3}$$

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:

$$HI = \sum_{i=1}^{13} HQ_i = \sum MIN\left[SSTL_{TPH} \frac{MF_i}{SSTL_i}, \frac{C_{sat\,i}}{SSTL_i} \right] \qquad \text{Q-4}$$

$C_{sat\,i}$ = 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

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.

APPENDIX R: REVIEW OF RISK INTEGRATED SOFTWARE FOR CLEANUPS (RISC) V4.0

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R.1 INTRODUCTION TO RISC V4.0

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 for 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 1×10^6 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.

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	✓	✓
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:

1. 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.

2. 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	$4.19\text{x}10^{-9}$	$5.6\text{x}10^{-9}$
5%	$4.02\text{x}10^{-8}$	$3.9\text{x}10^{-8}$
50%	$3.83\text{x}10^{-7}$	$2.3\text{x}10^{-7}$
75%	$4.73\text{x}10^{-7}$	$4.7\text{x}10^{-7}$
90%	$8.88\text{x}10^{-7}$	$8.7\text{x}10^{-7}$
95%	$1.23\text{x}10^{-6}$	$1.2\text{x}10^{-6}$
maximum	$5.59\text{x}10^{-6}$	$7.4\text{x}10^{-6}$

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]	3.23x10^5		
Calculated Value [mg/m^3]	3.23x10^5		
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]	2.27×10^{-3}			
Independent calculation [mg/m^3]	2.27×10^{-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]	2.27×10^{-3}		
Independent calculation [mg/m^3]	2.27×10^{-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.

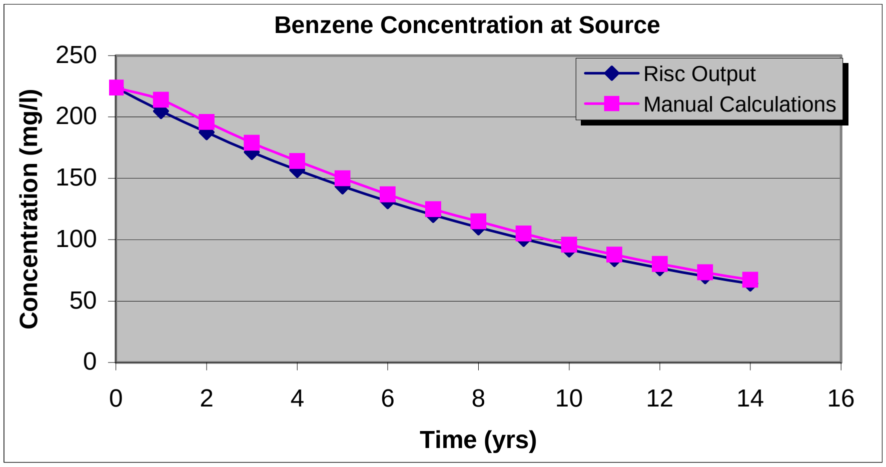

Figure R-1. Benzene Concentration vs Time in the Vadose Zone Source.

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) = $(1- \exp(-4x^2/pi))^{1/2}$, which can have an error of up to 0.7%.

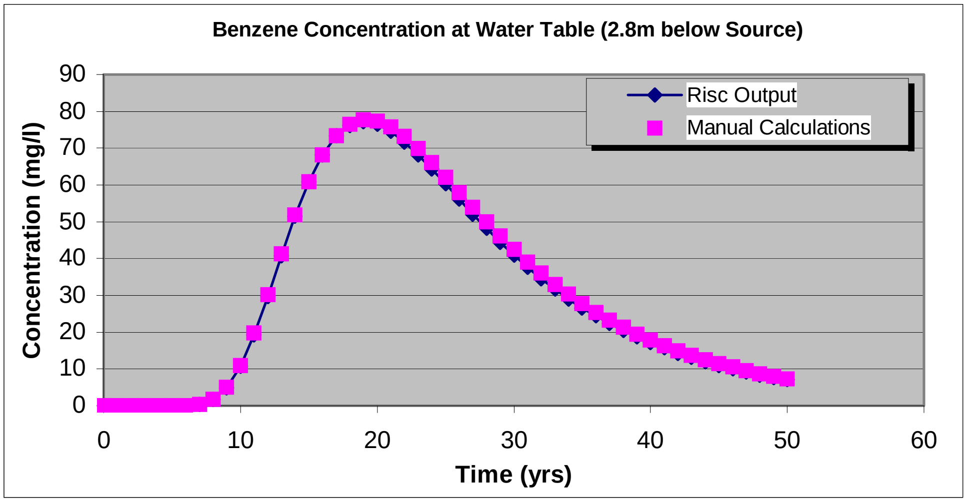

Figure R-2. Benzene Concentration vs Time at the Water Table.

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]	$1.25x10^6$	$1.25x10^6$
Manual Calculation	$1.25x10^6$	$1.25x10^6$
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]	6.85x10^{-6}	6.85x10^{-6}	6.85x10^{-6}	6.85x10^{-6}
CDI (calculated) [mg/kg-d]	6.85x10^{-6}	6.85x10^{-6}	6.85x10^{-6}	6.85x10^{-6}
Cancer Risk (RISC)	4.4x10^{-6}	8.5x10^{-8}	2.1x10^{-5}	0.00
Cancer Risk (calculated)	4.4x10^{-6}	8.51x10^{-8}	2.14x10^{-5}	NQ
Hazard Index (RISC)	2.3x10^{-2}	0.00	0.00	6.8x10^{-5}
Hazard Index (calculated)	2.28x10^{-2}	NQ	NQ	6.85x10^{-5}
Dermal Contact with Soil				
Concentration (mg/kg-soil)	5.00	5.00	5.00	5.00
CDI (RISC) [mg/kg-d]	1.18x10^{-5}	3.94x10^{-5}	3.94x10^{-5}	3.94x10^{-5}
CDI (calculated) [mg/kg-d]	1.18x10^{-5}	3.94x10^{-5}	3.94x10^{-5}	3.94x10^{-5}
Cancer Risk (RISC)	7.6x10^{-6}	4.9x10^{-7}	1.2x10^{-4}	0.00
Cancer Risk (calculated)	7.60x10^{-6}	4.9x10^{-7}	1.2x10^{-4}	NQ
Hazard Index (RISC)	3.9x10^{-2}	0.00	0.00	3.9x10^{-4}
Hazard Index (calculated)	3.94x10^{-2}	NQ	NQ	3.9x10^{-4}
Ingestion of Groundwater				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d]	5.48x10^{-2}	5.48x10^{-2}	5.48x10^{-2}	5.48x10^{-2}
CDI (calculated) [mg/kg-d]	5.48x10^{-2}	5.48x10^{-2}	5.48x10^{-2}	5.48x10^{-2}
Cancer Risk (RISC)	3.5x10^{-2}	6.8x10^{-4}	1.7x10^{-1}	0.00
Cancer Risk (calculated)	3.52x10^{-2}	6.81x10^{-4}	1.71x10^{-1}	NQ
Hazard Index (RISC)	1.8x10^{2}	0.00	0.00	5.5x10^{-1}
Hazard Index (calculated)	1.83x10^{2}	NQ	NQ	5.48x10^{-1}
Dermal Contact in Shower				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d]	1.26x10^{-4}	2.65x10^{-3}	1.51x10^{-1}	1.03x10^{0}
CDI (calculated) [mg/kg-d]	1.26x10^{-4}	2.65x10^{-3}	1.51x10^{-1}	1.03x10^{0}
Cancer Risk (RISC)	8.1x10^{-5}	3.3x10^{-5}	4.7x10^{-1}	0.00
Cancer Risk (calculated)	8.10x10^{-5}	3.29x10^{-5}	4.73x10^{-1}	NQ
Hazard Index (RISC)	4.2x10^{-1}	0.00	0.00	1.0x10^{1}
Hazard Index (calculated)	4.20x10^{-1}	NQ	NQ	1.03x10^{1}
Inhalation in Shower				
Concentration (mg/l-H$_2$0)	2.00	2.00	2.00	2.00
CDI (RISC) [mg/kg-d]	0.00x10^{0}	6.67x10^{-2}	2.34x10^{-4}	4.84x10^{-2}
CDI (calculated) [mg/kg-d]	0.00x10^{0}	6.67x10^{-2}	2.34x10^{-4}	4.84x10^{-2}
Cancer Risk (RISC)	0.00x10^{0}	7.7x10^{-4}	3.1x10^{-4}	0.00
Cancer Risk (calculated)	0.00x10^{0}	7.7x10^{-4}	3.1x10^{-4}	NQ
Hazard Index (RISC)	0.00x10^{0}	0.00	0.00	1.8x10^{-1}
Hazard Index (calculated)	0.00x10^{0}	NQ	NQ	1.8x10^{-1}
Ingestion of Root Vegetables (Soil)				
Concentration (mg/kg)	5.00	5.00	5.00	5.00
CDI (RISC) [mg/kg-d]	1.08x10^{-5}	1.29x10^{-5}	6.05x10^{-7}	4.24x10^{-7}
CDI (calculated) [mg/kg-d]	1.08x10^{-5}	1.29x10^{-5}	6.05x10^{-7}	4.24x10^{-7}
Cancer Risk (RISC)	6.93x10^{-6}	1.61x10^{-1}	1.89x10^{-6}	0.00
Cancer Risk (calculated)	6.93x10^{-6}	1.61x10^{-1}	1.89x10^{-6}	NQ
Hazard Index (RISC)	3.60x10^{-2}	0.00	0.00	4.24x10^{-6}
Hazard Index (calculated)	3.60x10^{-2}	NQ	NQ	4.24x10^{-6}