SEVIEW

Groundwater and Vadose Transport
With AT123D and SESOIL

Version 7.3
August 2022

User's Guide

for
Microsoft® Windows

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About the Author and Developer

Robert Schneiker has been involved in the groundwater consulting industry since 1982. His project experience includes vadose zone and groundwater modeling, risk-based evaluations, remedial investigations, geophysical exploration and groundwater resources exploration.

He modeled the migration of petroleum compounds in the unsaturated soil zone using SESOIL for the Wisconsin Department of Natural Resources (WDNR). The results were used to establish the minimum baseline compound-specific soil cleanup standards protective of groundwater quality for the WDNR NR 700 Rule Series regulations. He has presented full-day seminars on the development of site-specific cleanup objectives, risk-based evaluations and remediation through natural attenuation.

Since 1985 he has also been a computer consultant and software developer. Mr. Schneiker has a Master of Science degree in Geology/Geophysics from the University of Wisconsin-Milwaukee.

Preface

SEVIEW was designed to provide environmental professionals with the tools used to evaluate environmental risks to groundwater quality. The overall goal of SEVIEW was to simplify transport and fate modeling to the point where any environmental professional could do it, not just the modelers. This was accomplished by simplifying the model setup process and by producing automated reports. Design specifications for SEVIEW were based on requirements identified during the development of the baseline cleanup standards for the Wisconsin Department of Natural Resources (WDNR). SEVIEW was also designed to meet the general modeling requirements identified in the Fundamentals of Ground-Water Modeling, (US EPA, 1992), Assessment Framework for Ground-Water Model Applications (US EPA, 1994) and Applied Groundwater Modeling (Anderson and Woessner, 1992). Additional design specifications were based on numerous modeling projects by consultants using SEVIEW.

I decided to write SEVIEW in 1993, after performing over 700 SESOIL model simulations used by the WDNR to establish default soil cleanup objectives. Modeling was performed using the General Science Corporation RISKPRO system to setup and run SESOIL. RISKPRO proved adequate for setting up and running SESOIL (although, I had to keep track of my modeling activities in an external spreadsheet). However, it provided limited capabilities for documenting the model results. In particular, there was no way of knowing what SESOIL had predicted and how the model scenarios related to each other. So, I decided to write a program that extracted the contaminant mass that volatilized to the atmosphere and the concentration leaching to groundwater. Using this program and a spreadsheet, I was finally able to produce graphs and tables that displayed multiple model results.

To evaluate results from numerous model scenarios, the program summarized the results into several database tables. These tables were later converted into a spreadsheet format and were used to produce most of the figures in the Groundwater Contamination Susceptibility Evaluation, SESOIL Modeling report (Ladwig and Hensel, 1993). This approach not only simplified modeling, it allowed my portion of the project to be completed substantially under budget.

Since that time, contaminant transport and fate modeling has become increasingly important as regulatory agencies move toward the establishment of site-specific cleanup objectives based upon risks to human health and the environment. The reasons for this shift are varied and include the financial stability of the reimbursement programs, the increasing discouragement for the disposal of contaminated soil in the limited landfill space, the limited effectiveness of current remedial actions, and the realization that soil types and other site-specific conditions may provide for natural protection of human health and the environment.

There have been six previous versions of SEVIEW available for sale (several other versions were only used internally or by specific clients). The first two versions (2.1 and 2.5) only worked with the SESOIL vadose zone model. These versions simplified model setup and provided tools to extract SESOIL results. Version 2.6 provided a link between the SESOIL vadose zone model and the BIOSCREEN groundwater model. Version 5.0 provided significant enhancements. It included the addition of the AT123D groundwater model, modeling reports, and a simplified model setup. SEVIEW version 5.0 also included both chemical and climatic databases. SEVIEW 6 included numerous significant improvements including the ability to simulate load to AT123D as a mass or concentration, further simplification of the model setup, and, resizable windows.

Version 7.1 of SEVIEW continues to expand both SESOIL and AT123D capabilities. Enhancements to 7.1 include:

- Simulation of multiple contaminant sources,
- Enhanced Area, Centerline and POC reports with provisions to toggle on/off select contaminant loads,
- Use of long file names, and
- POC results with averaged groundwater concentrations.

Version 7.3 of SEVIEW builds on features and capabilities to 7.1 include:

- Simulation of 999 years of load to SESOIL
- Updated and expanded climate database
- Updated and expanded chemical database
- Addition of a soil database
- Ability to simulate multiple chemicals in a single AT123D run
- Enhanced BIOSCREEN link
- Ability to import groundwater contaminant loads from other models
- Base map scale based on distance

Need to add info on the import AT123D loads.
Delete the obvious dups in the climate file and update count.

Many of the features are only available in SEVIEW.

Acknowledgments

Many people helped to make SEVIEW Version 7.1 a reality; SEVIEW and this User's Guide are dedicated to them. My thanks to Bill Bristol of the Wisconsin State Geological Survey for long discussions regarding program development and to his sister Deb Radder, President of Engineered Plastics Corporation, for providing a work environment where I could refine my programming skills. I wish to thank my cousin Bill Hood who introduced me to numerous programming languages as we traded Commodore 64 programs as though they were baseball cards. Finally, there is Mike Barden of GeoScience Resources, Ltd. in Albuquerque, New Mexico, who provided technical support on many aspects regarding the development of all versions of SEVIEW.

Beta copies of SEVIEW 7.3 were distributed to several users. Their feedback and patience is appreciated. SEVIEW became a better program because of their input. Several users' who deserve recognition are:

Liliana Cecan	InterBrain, LLC
Michael J. Barden	GeoScience Resources Ltd.
David Lawton	Brownfield Restoration Group, LLC

Marc Bonazountas and Janet Wagner deserve thanks for developing SESOIL and David Hetrick for enhancing the SESOIL model. A special thank you to Michael Kulbersh of the U.S. Army Corps of Engineers for providing me with opportunity of develop the multiple source version of AT123D. Thanks to G. T. Yeh for developing AT123D. Additional thanks to John A. Hoopes, Howard Trussel and everyone at the University of Wisconsin-Madison and the WDNR who helped to improve AT123D. Finally, many thanks to Liliana Cecan for assisting me in creating the SESOIL to MODFLOW/MT3D link.

Robert A. Schneiker

August 2022

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2 Getting Started

2.1 Introduction

Welcome to SEVIEW 7.3, a powerful integrated contaminant transport and fate modeling system. As with previous versions SEVIEW links the SESOIL vadose zone model to the AT123D groundwater model. SEVIEW simplifies transport and fate modeling by graphically displaying contaminant sources and points of compliance (POCs) on a base map. By establishing contaminant sources and POCs on a base map SEVIEW provides a visual representation of spatial relationships. SEVIEW can now be used for groundwater modeling with or without any soil contamination. SEVIEW further extends modeling capabilities with the addition of multiple contaminant sources.

This SEVIEW 7.3 User's Guide contains detailed descriptions of all model input parameters as well as background information on the models.

New features:

- Simulation of 999 years of load to SESOIL
- Ability to simulate multiple chemicals in a single AT123D run
- Enhanced BIOSCREEN link
- Updated and expanded climate database
- Updated and expanded chemical database
- Addition of a soil database
- Ability to import groundwater contaminant loads from other models
- Base map scale based on distance

SEVIEW was designed to help you setup, run and evaluate model results and to document modeling activities. This includes reports that document model mass balance, mass fate, and water balance results. SEVIEW provides a link between SESOIL/AT123D and word processing, spreadsheet, graphical presentation and database programs.

☞ *SEVIEW allows you to focus on modeling not on how to use the models.*

SEVIEW Reports
SEVIEW includes graphical reports for SESOIL and At123D. Some including the SESOIL mass balance and fate are unique to SEVIEW.

2.1.1 SEVIEW Models

SEVIEW includes enhanced versions of the SESOIL and AT123D transport and fate models. SESOIL is an unsaturated (vadose) zone model. AT123D is a groundwater model. A brief description of each model is provided below. A detailed description of SESOIL and AT123D are provided in Appendices A and B respectively.

Although modifications have been made to both SESOIL and AT123D over the years the version numbers have remained almost unchanged. This has led to confusion as to which is the latest version. To simplify matters and remove confusion version numbers were modified to match the current version of SEVIEW. Modifications to version 7.3 of the models is outlined below.

2.1.1.1 SESOIL

SESOIL is a one-dimensional vertical transport screening-level model for the unsaturated (vadose) zone. It simulates contaminant transport and fate based on diffusion, adsorption, volatilization, biodegradation, and hydrolysis. SESOIL is an acronym for the **Seasonal Soil** compartment model. It is designed to simultaneously model contaminant, soil water and sediment transport in the soil. Its ability to simulate seasonal climatic variation is what sets SESOIL apart and makes it one of the best vadose zone models. SESOIL was developed for the EPA's Office of Water and the Office of Toxic Substances in 1981 by Bonazountas and Wagner, then at Arthur D. Little, Incorporated. SESOIL is a public domain program written in FORTRAN. SESOIL has been updated several times.

The version of SESOIL included with SEVIEW includes modifications made in 1997 by M. J. Barden then at the Wisconsin Department of Natural Resources to correct a mass balance error. SESOIL was further modified by R. A. Schneiker to run to 999 years. Version 7.3 was modified to allow for up to 999 years of contaminant load. Version 6 of SESOIL was enhanced to provide a separate load to each of the up to 40 sub-layers. Version 6 also included the water diffusion coefficient. This parameter is not used by SESOIL and is simply passed on to the AT123D model.

2.1.1.2 AT123D

AT123D is an acronym for **Analytical Transient 1-, 2-, and 3-Dimensional Simulation of Waste Transport in the Aquifer System**. It is a generalized three-dimensional groundwater transport and fate model. AT123D was developed by G. T. Yeh in 1981, at Oak Ridge National Laboratory. The AT123D program is written in FORTRAN. Significant modifications were made by John Seymor (1982), Darryl Holman (1984) and Howard Trussell, (1986) of the University of Wisconsin-Madison. AT123D was further modified by Robert A. Schneiker (1997) at Environmental Software Consultants Inc. LLC, Version 6.0 of AT123D can simulate up to 999 years of contaminant transport when linked to SESOIL and contains a correction to the steady state algorithm.

The AT123D model was developed to simulate contaminant transport under one-dimensional groundwater flow. Results can be used to estimate how far a contaminant plume will migrate and can be compared to groundwater standards to evaluate risk at specific locations and times. Transport and fate processes simulated by AT123D include advection, dispersion, sorption and biological decay.

Starting with SEVIEW version 6 of AT123D contaminant load can be entered as either a concentration or a mass. Version 6 also included input parameters for the organic carbon adsorption coefficient (K_{oc}) and soil organic carbon content.

Version 7.1 of AT123D simulates contaminant load from up to 15 separate sources. This means that AT123D can now be used to simulate complex release scenarios that in the past could only be evaluated using numerical models such as MODFLOW / MT3D. Version 7.3 was modified to simulate multiple chemicals in a single model scenario.

2.1.2 SEVIEW Goals

SEVIEW Version 7.1 was designed to meet the following goals:

- Multiple sources
- Addition of POCs
- Simplify setup
- Project files
- Easier access to report data

2.1.2.1 Multiple Sources

You can simulate up to 15 separate contaminant releases in SEVIEW. Sources can be either a SESOIL vadose zone release or an AT123D groundwater plume.

2.1.2.2 Observation Well POCs

AT123D groundwater concentrations are now produced at Points of Compliance (POCs) also known as Observation Wells. Analytical models produced results at specific points (typically the top of the water table). In SEVIEW POC results are produced at specific depth and are then averaged for comparison with measured groundwater concentrations. The depth interval is typically based on existing groundwater monitoring well or piezometer specifications.

2.1.2.3 Simplified Setup

SEVIEW includes a sophisticated input interface in which all SESOIL and/or AT123D input parameters are presented in one window. Input parameters are presented in tab-organized input screens which are linked to model input files. Changes are made by simply entering data on the screen. Changes are automatically saved by closing the model setup window. Modifications to model setup in version 7.1 include elimination of the output file designations, as the files are now saved within the project file. The simulation time in years is now entered on the SEVIEW toolbar.

2.1.2.4 Project Files

Separate project files can now be created and opened in SEVIEW 7.3. Project files contain all input and output data and can be transferred from computer to computer. SEVIEW 7.1 project files are automatically converted to the 7.3 format.

☞ *SEVIEW 7.3 project files are not compatible with SEVIEW 7.1.*

2.2 How to Use This Manual

This User's Guide is organized to help you get started and to describe SEVIEW's operation.

Typographical Conventions
This document utilizes the following typographical conventions:

Italic Text	Indicates user data to be entered. For example, "Type *a:setup* and press <ENTER>".
Bold Text	Indicates title, command or emphasized information
<ENTER>	Keyboard and/or mouse keys are bracketed within < >.
+	A plus sign indicates that both keys must be pressed simultaneously. For example, <CTRL + W>.
Go To DOS	Underlined letters indicate keyboard short cut commands, used with the <Alt> key. Example: <Alt + F> followed by a <D> to open a DOS window.

2.3 Learn by Doing

The tutorials in Chapter 4 provide an easy way to learn the basic SEVIEW commands. Using example input data you will perform SESOIL, and AT123D modeling. You may also want to review the tutorials if you have not used SEVIEW for a while.

3 Installation

This section provides important information about SEVIEW 7.3 including the installation process. This section is also designed to help you configure SESOIL and AT123D. The SEVIEW program consists of the sev73.exe file that contains SEVIEW, SESOIL, and AT123D.

3.1 System Requirements

SEVIEW 7.3 works with any version of Microsoft Windows XP or higher including Windows 8, Windows 10 and Windows 11. Microsoft Excel including Microsoft Graph must be installed to use the BIOSCREEN link and to produce the SEVIEW graphs.

3.2 Installing SEVIEW

Installing SEVIEW is quick and easy. To install SEVIEW follow these steps.

☞ *This procedure should take less than ten minutes to complete.*

1. Download SEVIEW 7.3 at www.seview.com.
2. Run the download and follow the instructions in the dialog boxes displayed on the screen.

3.3 Running / Activating SEVIEW

To activate SEVIEW click on the SEVIEW 7.3 shortcut. The first time you run SEVIEW, the SEVIEW Registration form will be displayed on the screen. You will need to fill out the form and activate SEVIEW before you can use it. SEVIEW can be activated in either the standard or trial modes. These modes are identical except that the trial mode will stop working after three days.

☞ *If SEVIEW does not activate, call and we will provide you with an updated Activation Code. Call ESCI between 9:30 AM and 4:30 PM CST at (608) 240-9878 or request an Activation Code via email to seview@seview.com.*

3.3.1 Standard Mode

The standard mode provides full access to the SEVIEW help file and to this SEVIEW 7.3 User's Guide. The help file and User's Guide includes detailed information on model input parameters. In addition this guide includes background information on the SESOIL and AT123D models.

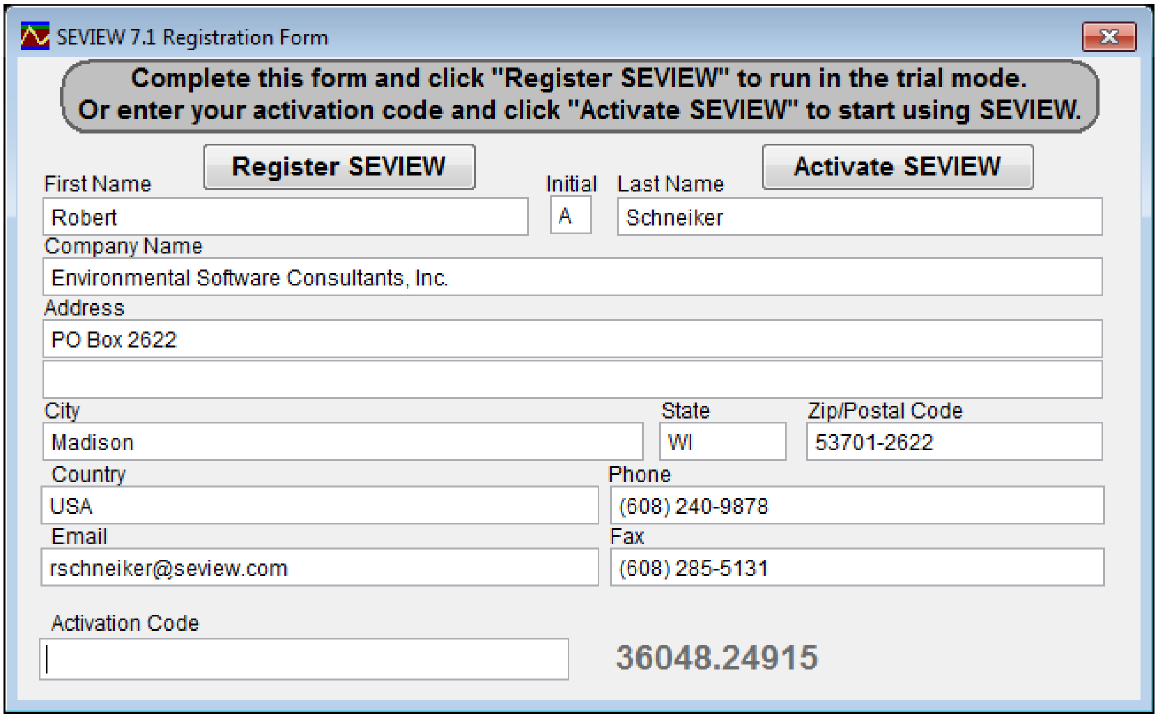
3.3.2 Trial Mode

SEVIEW 7.3 can be run in a trial mode for three days. The trial mode is identical to the full version of SEVIEW except that it will stop working after three days. As with the standard mode the trial mode provides full access to the SEVIEW help file and to this SEVIEW User's Guide. The help file and User's Guide include detailed information on model input parameters. In addition the User's Guide contains background information on the SESOIL and AT123D models.

☞ *You can run SEVIEW in the trial mode by registering SEVIEW via the Internet. Once registered you will receive an email containing the activation code.*

☞ *Although provided for free in the SEVIEW trial mode the SEVIEW User's Guide and the SEVIEW help and User's Guide are copyrighted by ESCI.*

☞ ***SEVIEW is a copyrighted software package. Only <u>one</u> active copy may be installed on one computer.***



SEVIEW 7.1 Registration Form

Complete this form and click "Register SEVIEW" to run in the trial mode.
Or enter your activation code and click "Activate SEVIEW" to start using SEVIEW.

First Name: Robert
Initial: A
Last Name: Schneiker
Company Name: Environmental Software Consultants, Inc.
Address: PO Box 2622
City: Madison
State: WI
Zip/Postal Code: 53701-2622
Country: USA
Phone: (608) 240-9878
Email: rschneiker@seview.com
Fax: (608) 285-5131
Activation Code:
36048.24915

☞ *If the SEVIEW registration screen extends off the bottom of your screen simply resize the screen until it fits.*

☞ *As part of the activation process SEVIEW will decode the climatic and chemical databases.*

3.3.3 Running SEVIEW

SEVIEW will shut down following the activation process. You can start it again by clicking on the SEVIEW 7.3 icon on your desktop. A base map including the commands used to setup and run the models will be displayed.

Although the use of SEVIEW is intuitive, it is recommended that you first proceed to the tutorials in Section 4 of this SEVIEW User’s Guide prior to modeling (a copy of the User’s Guide can be found using the SEVIEW menu Help option). By working through the tutorials you will become familiar with the basic SEVIEW functions and utilities.

4 SEVIEW Tutorials

There are a total of five SEVIEW tutorials. They are divided in to two for SESOIL, two for AT123D and one for BIOSCREEN. The tutorials contain information of how to setup and run the models, and how to view the results.

4.1 SESOIL Tutorials

This section contains two SESOIL tutorials. These tutorials are designed to familiarize you with the basic features of setting up and running SESOIL. The tutorials describe the procedures used to modify SESOIL input files, run SESOIL and produce reports. Upon completing the tutorials you should be able to use the basic SESOIL commands. However, SEVIEW is a feature-filled program and these tutorials do not describe all of them.

4.1.1 Tutorial One -- Create and Run a SESOIL Source

As part of this tutorial you will setup and run SESOIL. The SESOIL model uses a total of four input data files. The input data files contain information pertaining to the climatic, chemical, soil, and soil column (application) parameters for each SESOIL source. In this tutorial you will learn how to modify the climate data and run SESOIL. An overview of the steps for creating a SESOIL source within SEVIEW are outlined below.

1. Start SEVIEW
2. Open a base map, scale and rotate
3. Create a SESOIL source
4. Modify the SESOIL parameters
5. Run SESOIL

Step 1 **Start SEVIEW**

Start SEVIEW by double clicking on the SEVIEW icon on the desktop, or by selecting SEVIEW on the Start menu.

Step 2 **Open a base map, scale and rotate**

Click on the **Base Map** command on the **Side Toolbar**. Select the *"Figure 4.bmp"* file. Then click on the **Set Scale** command on the **Side Toolbar**.

☞ *You may need to use the scroll bars and/or "-/+" commands to view the scale on the base map.*

☞ *The scale can be set by entering the horizontal distance in meters between any two points.*

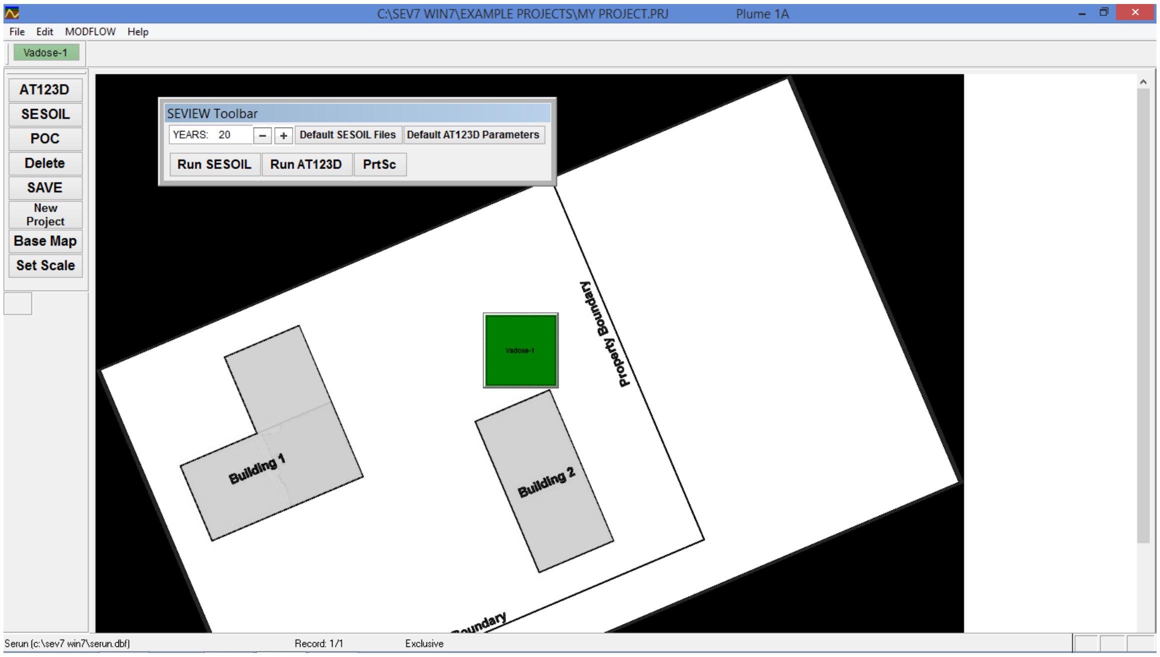
Right Click on the base map itself and enter the number of degrees required to rotate it such that groundwater flow is from left to right across the screen.

To match this example you need to rotate the Figure 4.bmp base map 17.0 degrees.

Step 3 **Create a SESOIL source**

Click on the **SESOIL** command on the **Side Toolbar**. Answer "Yes" when asked if you want to add a SESOIL vadose zone source. A red square that follows the mouse will appear. Move the red source to the desired location on the base map and **Single Click** the source to drop it. The source will turn green.

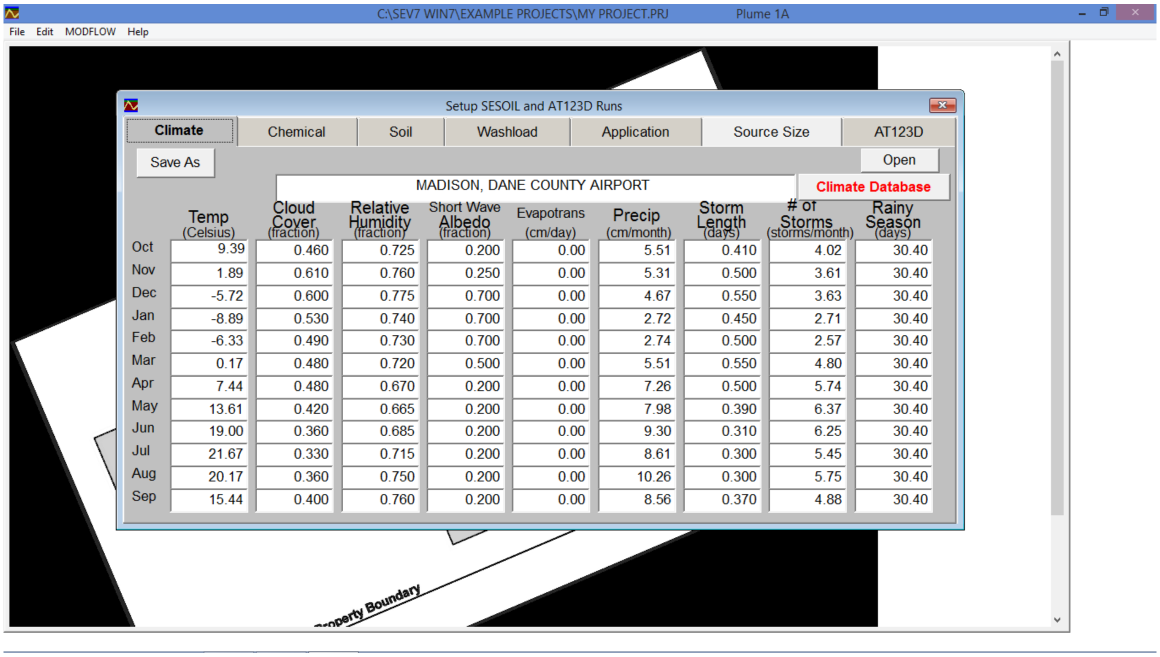
*You can **Right Click** on the source to move it.*



Step 4 **Modify the SESOIL parameters**

Single Click on the green source and a window displaying the SESOIL input parameters will be opened.

*You could also **Click** the green SESOIL source on the **Source Toolbar**.*



MADISON, DANE COUNTY AIRPORT

	Temp (Celsius)	Cloud Cover (fraction)	Relative Humidity (fraction)	Short Wave Albedo (fraction)	Evapotrans (cm/day)	Precip (cm/month)	Storm Length (days)	# of Storms (storms/month)	Rainy Season (days)
Oct	9.39	0.460	0.725	0.200	0.00	5.51	0.410	4.02	30.40
Nov	1.89	0.610	0.760	0.250	0.00	5.31	0.500	3.61	30.40
Dec	-5.72	0.600	0.775	0.700	0.00	4.67	0.550	3.63	30.40
Jan	-8.89	0.530	0.740	0.700	0.00	2.72	0.450	2.71	30.40
Feb	-6.33	0.490	0.730	0.700	0.00	2.74	0.500	2.57	30.40
Mar	0.17	0.480	0.720	0.500	0.00	5.51	0.550	4.80	30.40
Apr	7.44	0.480	0.670	0.200	0.00	7.26	0.500	5.74	30.40
May	13.61	0.420	0.665	0.200	0.00	7.98	0.390	6.37	30.40
Jun	19.00	0.360	0.685	0.200	0.00	9.30	0.310	6.25	30.40
Jul	21.67	0.330	0.715	0.200	0.00	8.61	0.300	5.45	30.40
Aug	20.17	0.360	0.750	0.200	0.00	10.26	0.300	5.75	30.40
Sep	15.44	0.400	0.760	0.200	0.00	8.56	0.370	4.88	30.40

You can grab the edge of the window and resize it to fit your display.

Now click on the **Climate Database** command to open the SEVIEW climatic database.

Again you can grab the edge of the Climate Database window and resize it to fit your display.

Select a location in the **View** option on the Climate Database. Then select the closest location to your site. Next click on the **Save As** command to create the input file. Then click **Yes** to log the new input file. This step will replace and log the new climate file for your source.

Step 5 **Run SESOIL**

Close the SESOIL setup Window. This will take you back to the base map. Click on the **Run SESOIL** command on the **SEVIEW Toolbar**. You should now see the message “SESOIL BEGINS” followed by hydrologic cycle and other monthly information.

Now proceed to Section 4.1.2 to produce reports for your SESOIL scenario. At this point you have setup and run SESOIL and completed the first SEVIEW tutorial. You can now stop working in the tutorial if you wish, or you can continue and view the SESOIL results.

4.1.2 Tutorial Two – View SESOIL Results

This tutorial will demonstrate how to view reports for a SESOIL source. An overview of the steps for this session are outlined below.

1. Initiate SEVIEW
2. Open the model results window
3. View a climatic report
4. View a profile and load report
5. View a hydrologic cycle report
6. View a pollutant cycle report
7. View a SESOIL output file
8. Quit SEVIEW

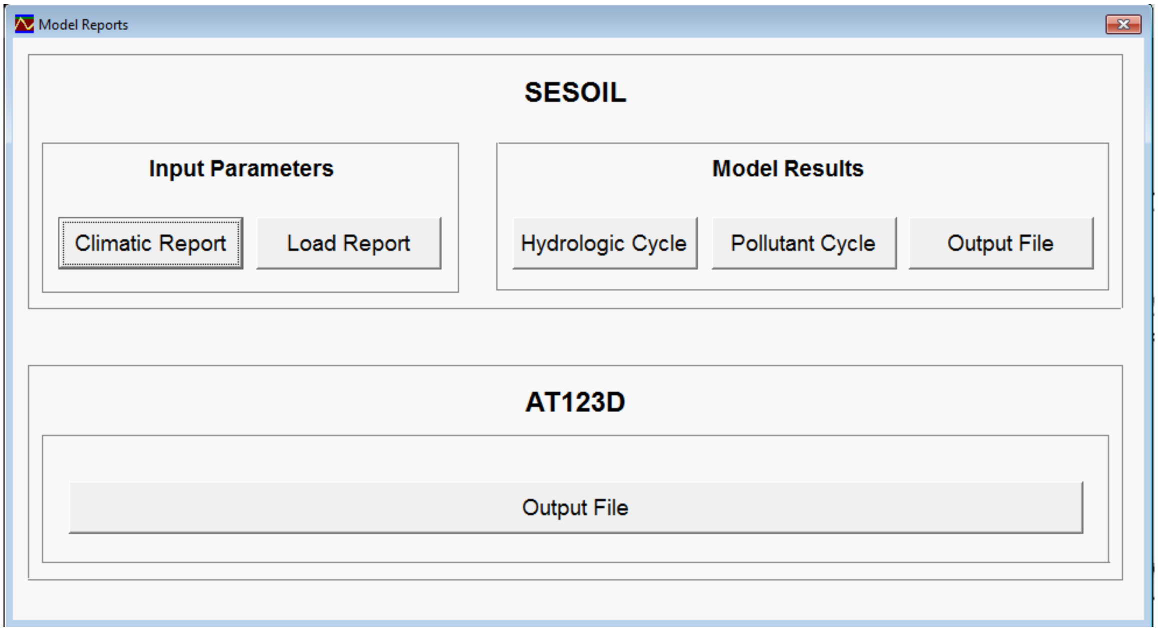
Step 1 **Initiate SEVIEW**

Initiate SEVIEW by double clicking on the SEVIEW icon, or select SEVIEW on the Start menu.

Step 2 **Open model reports window**

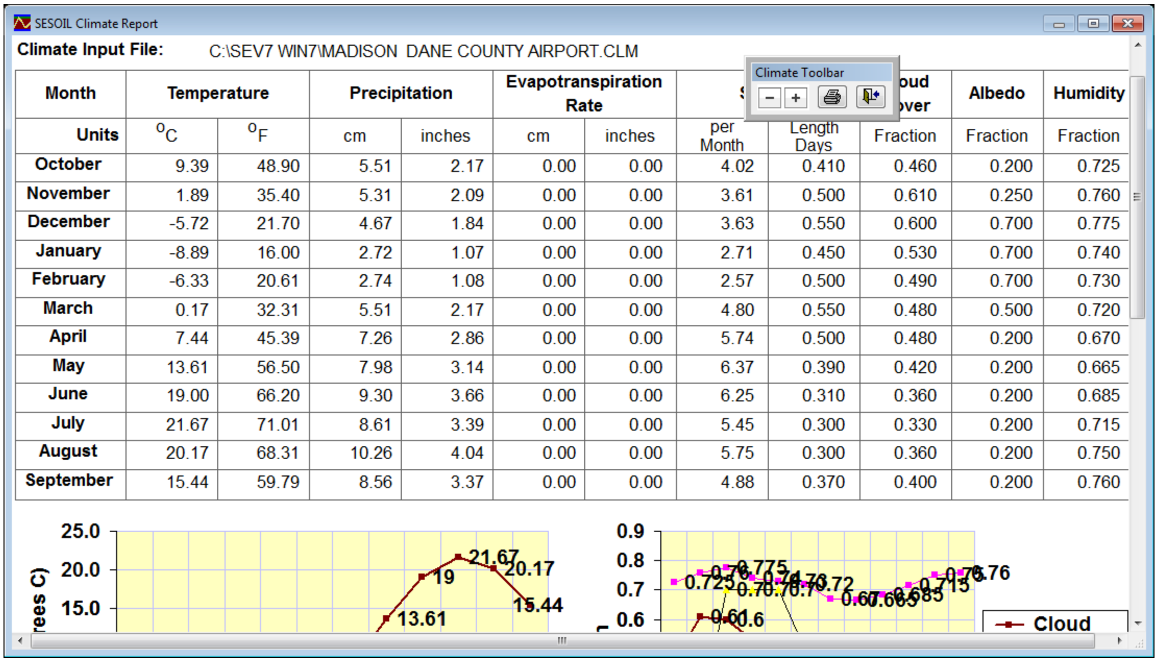
Double Click on the green source on the base map to open the **Model Reports** window.

☞ *You could also* ***Double Click*** *the green SESOIL source on the* ***Source Toolbar****.*



Step 3 View a Climatic Report

Click on the **Climatic Report** command to view it. This report documents the climatic input data used in the SESOIL source. Additional information on the Climatic Report is presented in Section 6.



Climate Input File: C:\SEV7 WIN7\MADISON DANE COUNTY AIRPORT.CLM

Month	Temperature		Precipitation		Evapotranspiration Rate		S		oud over	Albedo	Humidity
Units	°C	°F	cm	inches	cm	inches	per Month	Length Days	Fraction	Fraction	Fraction
October	9.39	48.90	5.51	2.17	0.00	0.00	4.02	0.410	0.460	0.200	0.725
November	1.89	35.40	5.31	2.09	0.00	0.00	3.61	0.500	0.610	0.250	0.760
December	-5.72	21.70	4.67	1.84	0.00	0.00	3.63	0.550	0.600	0.700	0.775
January	-8.89	16.00	2.72	1.07	0.00	0.00	2.71	0.450	0.530	0.700	0.740
February	-6.33	20.61	2.74	1.08	0.00	0.00	2.57	0.500	0.490	0.700	0.730
March	0.17	32.31	5.51	2.17	0.00	0.00	4.80	0.550	0.480	0.500	0.720
April	7.44	45.39	7.26	2.86	0.00	0.00	5.74	0.500	0.480	0.200	0.670
May	13.61	56.50	7.98	3.14	0.00	0.00	6.37	0.390	0.420	0.200	0.665
June	19.00	66.20	9.30	3.66	0.00	0.00	6.25	0.310	0.360	0.200	0.685
July	21.67	71.01	8.61	3.39	0.00	0.00	5.45	0.300	0.330	0.200	0.715
August	20.17	68.31	10.26	4.04	0.00	0.00	5.75	0.300	0.360	0.200	0.750
September	15.44	59.79	8.56	3.37	0.00	0.00	4.88	0.370	0.400	0.200	0.760

☞ *Use the -/+ commands on the toolbar to zoom in or out on the report.*

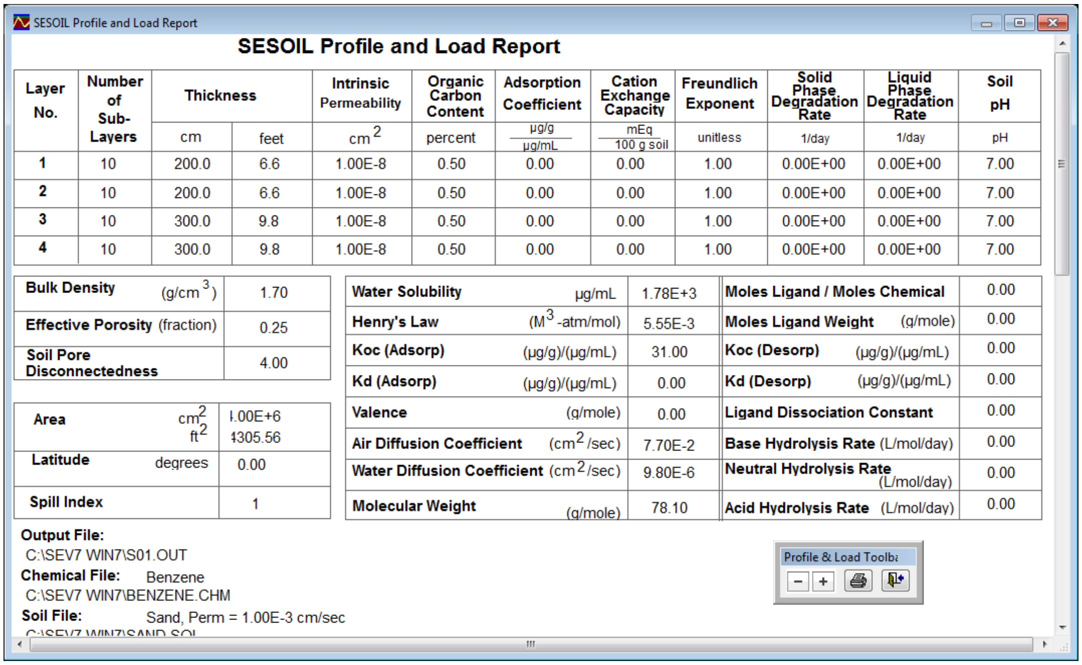
☞ *Use the 🖶 command on the toolbar to print the report.*

☞ ***Double Click** on a graph, then **Double Click** the graph again to open Microsoft Graph. You can use this option to copy and paste the graph or graph data to some other application such as Excel.*

After viewing the **Climatic Cycle Report** close the window and return to the **Model Results** window.

Step 4 View a Profile and Load Report

Click on the **Load Report** command to view it. This report documents the chemical, soil and application data used in the SESOIL source. Additional information on the Load Report is presented in Section 6.



SESOIL Profile and Load Report

Layer No.	Number of Sub-Layers	Thickness		Intrinsic Permeability	Organic Carbon Content	Adsorption Coefficient	Cation Exchange Capacity	Freundlich Exponent	Solid Phase Degradation Rate	Liquid Phase Degradation Rate	Soil pH
		cm	feet	cm^2	percent	µg/g / µg/mL	mEq / 100 g soil	unitless	1/day	1/day	pH
1	10	200.0	6.6	1.00E-8	0.50	0.00	0.00	1.00	0.00E+00	0.00E+00	7.00
2	10	200.0	6.6	1.00E-8	0.50	0.00	0.00	1.00	0.00E+00	0.00E+00	7.00
3	10	300.0	9.8	1.00E-8	0.50	0.00	0.00	1.00	0.00E+00	0.00E+00	7.00
4	10	300.0	9.8	1.00E-8	0.50	0.00	0.00	1.00	0.00E+00	0.00E+00	7.00

Bulk Density (g/cm^3)	1.70
Effective Porosity (fraction)	0.25
Soil Pore Disconnectedness	4.00

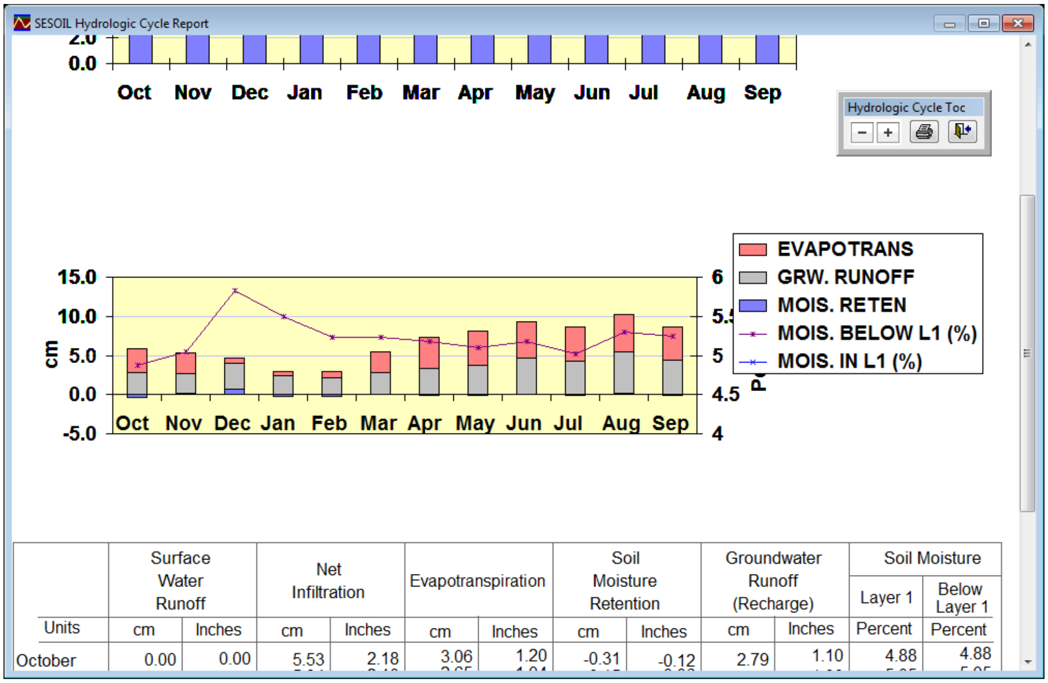
Area cm^2 ft^2	4.00E+6 4305.56
Latitude degrees	0.00
Spill Index	1

Water Solubility µg/mL	1.78E+3	**Moles Ligand / Moles Chemical**	0.00
Henry's Law (M^3-atm/mol)	5.55E-3	**Moles Ligand Weight** (g/mole)	0.00
Koc (Adsorp) (µg/g)/(µg/mL)	31.00	**Koc (Desorp)** (µg/g)/(µg/mL)	0.00
Kd (Adsorp) (µg/g)/(µg/mL)	0.00	**Kd (Desorp)** (µg/g)/(µg/mL)	0.00
Valence (g/mole)	0.00	**Ligand Dissociation Constant**	0.00
Air Diffusion Coefficient (cm^2/sec)	7.70E-2	**Base Hydrolysis Rate** (L/mol/day)	0.00
Water Diffusion Coefficient (cm^2/sec)	9.80E-6	**Neutral Hydrolysis Rate** (L/mol/day)	0.00
Molecular Weight (g/mole)	78.10	**Acid Hydrolysis Rate** (L/mol/day)	0.00

Output File:
C:\SEV7 WIN7\S01.OUT
Chemical File: Benzene
C:\SEV7 WIN7\BENZENE.CHM
Soil File: Sand, Perm = 1.00E-3 cm/sec
C:\SEV7 WIN7\SAND.SOI

Step 5 View a Hydrologic Cycle Report

Click on the **Hydrologic Cycle** command to view the hydrologic cycle report. As the hydrologic cycle report is being created SEVIEW will display information at the bottom of the screen. This is used to indicate that the program is actively scanning the SESOIL output file. Additional information on the SESOIL Hydrologic Cycle Report is presented in Section 6.



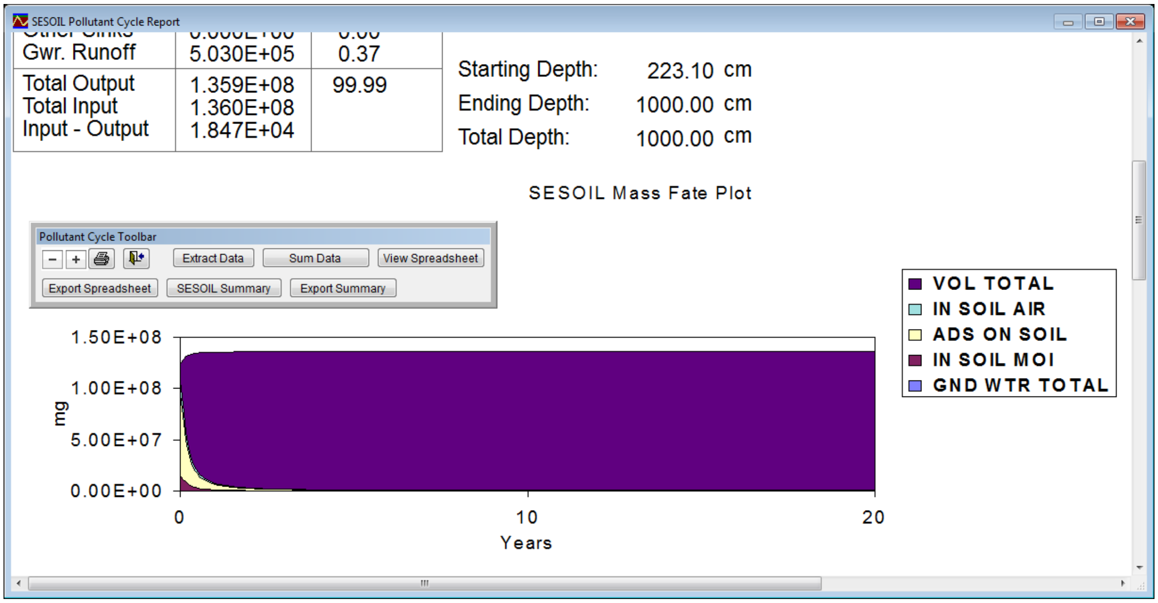
	Surface Water Runoff		Net Infiltration		Evapotranspiration		Soil Moisture Retention		Groundwater Runoff (Recharge)		Soil Moisture	
											Layer 1	Below Layer 1
Units	cm	Inches	cm	Inches	cm	Inches	cm	Inches	cm	Inches	Percent	Percent
October	0.00	0.00	5.53	2.18	3.06	1.20	-0.31	-0.12	2.79	1.10	4.88	4.88

After previewing the Hydrologic Cycle Report on the screen close the window and return to the SESOIL Reports window.

The Hydrologic Cycle Report includes soil moisture.

Step 6 View a Pollutant Cycle Report

Click on the **Pollutant Cycle** command to view the report. As the pollutant cycle report is being created SEVIEW will display information at the bottom of the screen. The information is used to indicate that the program is actively scanning the SESOIL output file. SEVIEW first will display **SESOIL Output** and the number of lines in the SESOIL output file along with the current line number. SEVIEW will then display the following description as the pollutant cycle report is created: **Summing Data, Transferring Data, Mass Balance, Updating Concentration Plot, Updating Mass Fate Plot, Updating Depth Plot** and **Updating SESOIL Depth Profile**. SEVIEW will then present results of Pollutant Cycle. Additional information on the Pollutant Cycle Report is presented in Section 6.


SESOIL Pollutant Cycle Report

Gwr. Runoff	5.030E+05	0.37
Total Output	1.359E+08	99.99
Total Input	1.360E+08	
Input - Output	1.847E+04	

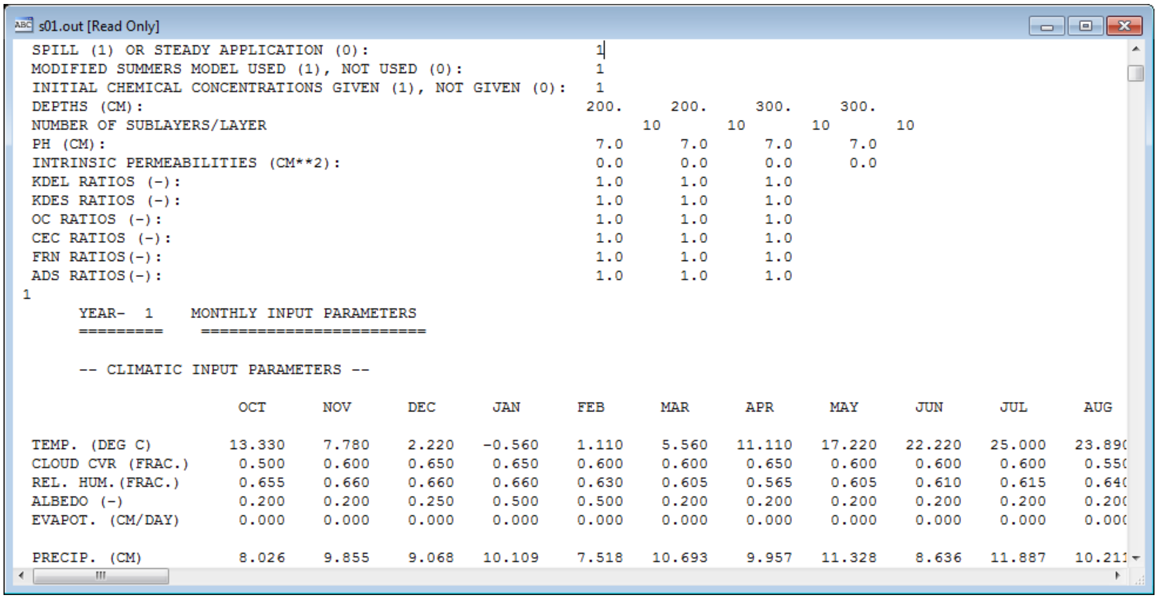
Starting Depth: 223.10 cm
Ending Depth: 1000.00 cm
Total Depth: 1000.00 cm

SESOIL Mass Fate Plot

After reviewing the Pollutant Cycle Report close the window and return to the Model Results window.

Step 7 View a SESOIL output file

Click on the **Output File** command to view the ASCII text results. Viewing this file is useful as it can display errors and warning messages produce by SESOIL. These messages can be useful in debugging modeling errors. Additional information on the Pollutant Cycle Report is presented in Section 6.



```
 SPILL (1) OR STEADY APPLICATION (0):                        1
 MODIFIED SUMMERS MODEL USED (1), NOT USED (0):              1
 INITIAL CHEMICAL CONCENTRATIONS GIVEN (1), NOT GIVEN (0):   1
 DEPTHS (CM):                                               200.     200.     300.     300.
 NUMBER OF SUBLAYERS/LAYER                                        10       10       10       10
 PH (CM):                                                    7.0      7.0      7.0      7.0
 INTRINSIC PERMEABILITIES (CM**2):                           0.0      0.0      0.0      0.0
 KDEL RATIOS (-):                                            1.0      1.0      1.0
 KDES RATIOS (-):                                            1.0      1.0      1.0
 OC RATIOS (-):                                              1.0      1.0      1.0
 CEC RATIOS (-):                                             1.0      1.0      1.0
 FRN RATIOS(-):                                              1.0      1.0      1.0
 ADS RATIOS(-):                                              1.0      1.0      1.0
1
      YEAR-  1    MONTHLY INPUT PARAMETERS
      =========    ========================

      -- CLIMATIC INPUT PARAMETERS --

                       OCT      NOV      DEC      JAN      FEB      MAR      APR      MAY      JUN      JUL      AUG

 TEMP. (DEG C)        13.330    7.780    2.220   -0.560    1.110    5.560   11.110   17.220   22.220   25.000   23.89
 CLOUD CVR (FRAC.)     0.500    0.600    0.650    0.650    0.600    0.600    0.650    0.600    0.600    0.600    0.55
 REL. HUM.(FRAC.)      0.655    0.660    0.660    0.660    0.630    0.605    0.565    0.605    0.610    0.615    0.64
 ALBEDO (-)            0.200    0.200    0.250    0.500    0.500    0.200    0.200    0.200    0.200    0.200    0.20
 EVAPOT. (CM/DAY)      0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.000    0.00

 PRECIP. (CM)          8.026    9.855    9.068   10.109    7.518   10.693    9.957   11.328    8.636   11.887   10.21
```

After viewing the SESOIL output file close the window and return to the Model Results window.

Step 8 **Exit SEVIEW**

To end your SEVIEW session, select the **File** option on the main menu, then select **Exit** or simply close the window.

Congratulations, you have completed both SESOIL tutorials and have become familiar with some of the basic features of SEVIEW. If you have not used SEVIEW for a while or have forgotten how to use it, you may want to review these tutorials. The next section provides two tutorials on using AT123D in SEVIEW.

4.2 AT123D Tutorials

This section contains two AT123D tutorials. It is assumed that you have completed the SESOIL tutorials (Section 4.1). These tutorials are designed to familiarize you with the basic features of setting up and running AT123D in SEVIEW. Upon completing these tutorials you should be able to execute the basic SEVIEW commands necessary to run AT123D and document the results. However, SEVIEW is a feature-filled program and these tutorials do not describe all of the features.

4.2.1 Tutorial Three -- Setup and Run AT123D

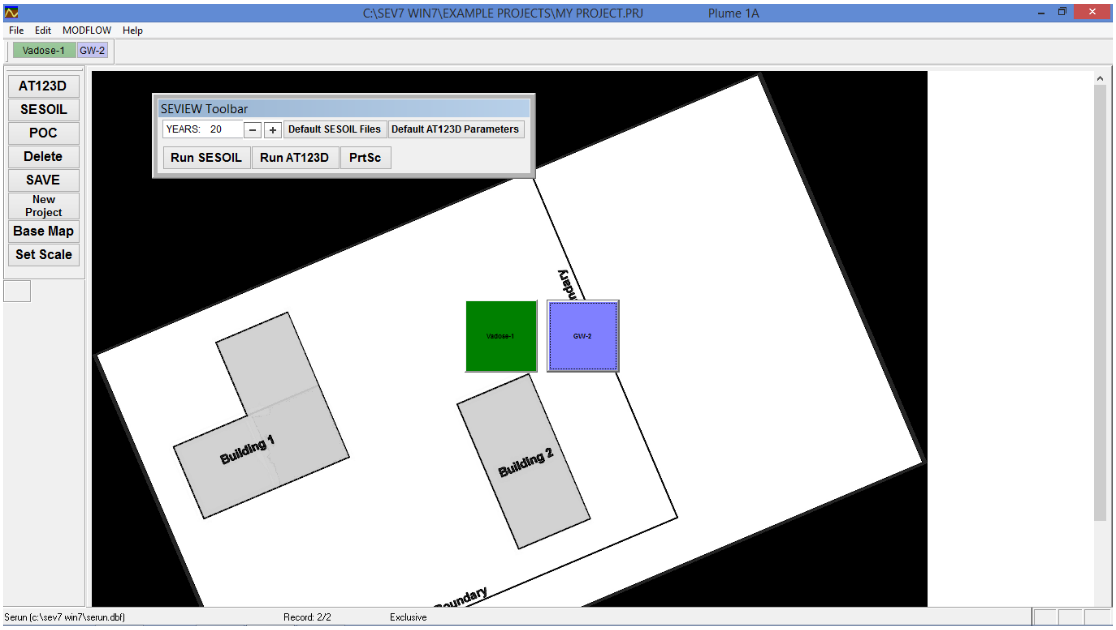
As part of this tutorial you will setup and run the AT123D groundwater model. An overview of the steps for creating a groundwater plume source and running AT123D from within SEVIEW are outlined below.

1. Initiate SEVIEW
2. Create a AT123D source
3. Modify the AT123D parameters
4. Add a point of compliance (POC)
5. Run AT123D

Step 1 **Initiate SEVIEW**
Initiate SEVIEW by double clicking on the SEVIEW icon, or select SEVIEW on the Start menu.

Step 2 **Create an AT123D source**
Click on the **AT123D** command on the **Side Toolbar**. Answer "Yes" when asked if you want to add a AT123D groundwater source. A red square that follows the mouse will appear. Move the red source to the desired location on the base map and **Single Click** the source to drop it. The source will turn blue.

*You can **Right Click** on the source to move it.*



C:\SEV7 WIN7\EXAMPLE PROJECTS\MY PROJECT.PRJ Plume 1A

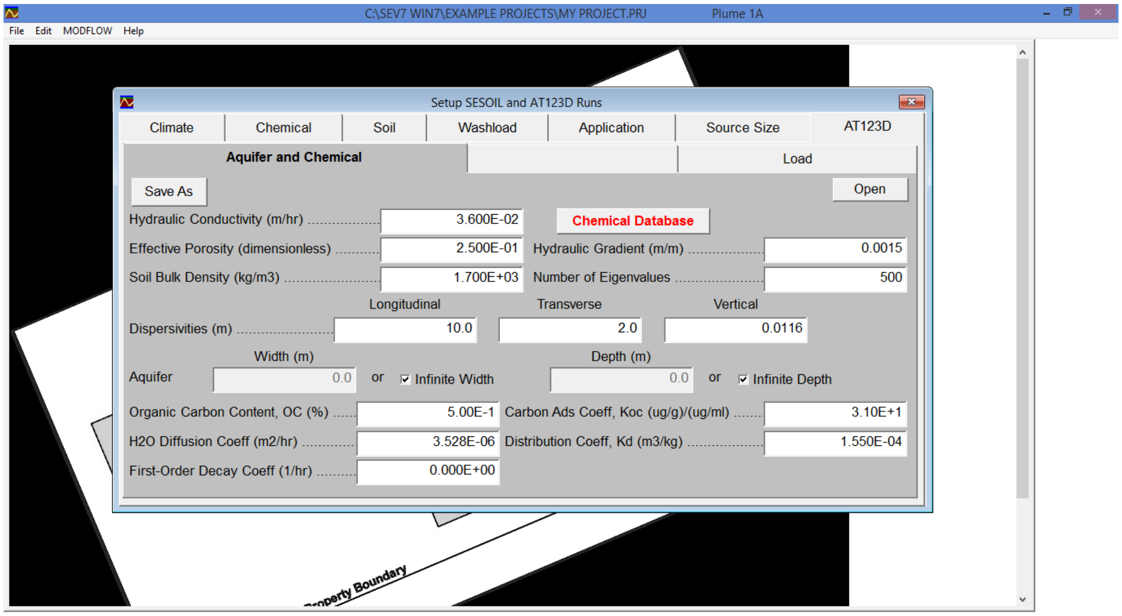
YEARS: 20

Serun (c:\sev7 win7\serun.dbf) Record: 2/2 Exclusive

Step 3 **Modify AT123D Parameters**

Single Click on the blue source and a window displaying the AT123D input parameters will be opened. Click on the **Load** tab and set the **Initial Concentration** to *“0.01”* mg/L.

☞ *You could also **Click** the blue AT123D source on the **Source Toolbar**.*



Hydraulic Conductivity (m/hr) 3.600E-02

Effective Porosity (dimensionless) 2.500E-01

Soil Bulk Density (kg/m3) .... 1.700E+03

Hydraulic Gradient (m/m) 0.0015

Number of Eigenvalues 500

Dispersivities (m) ....: Longitudinal 10.0, Transverse 2.0, Vertical 0.0116

Aquifer Width (m) 0.0 or ☑ Infinite Width

Depth (m) 0.0 or ☑ Infinite Depth

Organic Carbon Content, OC (%) 5.00E-1

H2O Diffusion Coeff (m2/hr) 3.528E-06

First-Order Decay Coeff (1/hr) .... 0.000E+00

Carbon Ads Coeff, Koc (ug/g)/(ug/ml) .... 3.10E+1

Distribution Coeff, Kd (m3/kg) 1.550E-04

☞ *A detailed description of the AT123D input parameters within SEVIEW are presented in Section 7. A complete list of all AT123D parameters including a description is presented in Appendix B.*

☞ *You can set the default AT123D parameters (see Section 7).*

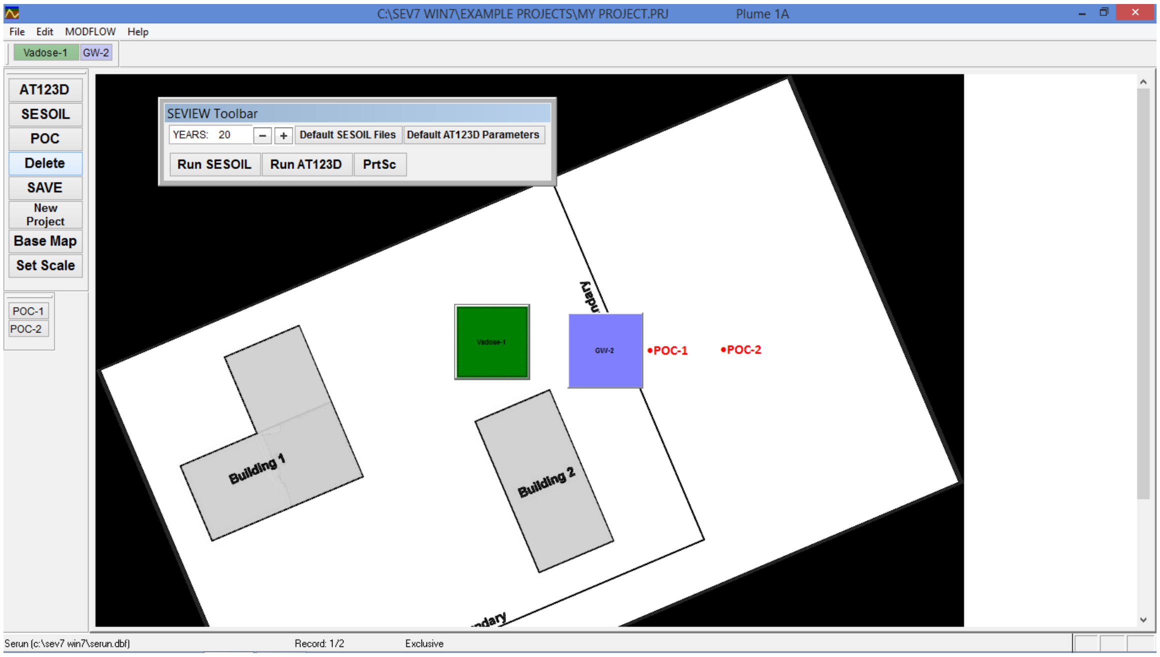
Step 4 **Add a point of compliance (POC)**

Click on the **POC** command on the **Side Toolbar**. Answer “Yes” when asked if you want to add a POC. A grey POC that follows the mouse will appear. Move the mouse to place the POC slightly east (downgradient) of the blue AT123D source on the base map. **Single Click** the POC to drop it. The **POC-1** will turn red.

Step 5 **Add a second point of compliance (POC)**

Click on the **POC** command on the **Side Toolbar**. Answer “Yes” when asked if you want to add a POC. A grey POC that follows the mouse will appear. Move the mouse to place the POC slightly east (downgradient) of the first POC on the base map. **Single Click** the POC to drop it. The **POC-2** will turn red.

☞ *You can **Right Click** on the POC to move it.*



Step 5 **Run AT123D**

Close the AT123D setup Window. This will take you back to the base map. Click on the **Run AT123D** command on the **SEVIEW Toolbar**. You should now see the message "AT123D STARTS" followed by years and source information.

AT123D can run very quickly and it may be difficult to observe it running.

Now proceed to Section 4.2.2 to view results for the AT123D source.

You have now setup and run AT123D and completed the first AT123D tutorial. You can now stop working in the tutorial if you wish, or you can continue and evaluate the AT123D output file you generated. If you continue you will learn how to view AT123D results in the tutorial below.

4.2.2 Tutorial Four – View AT123D Results

This tutorial demonstrates how to view the AT123D results. An overview of the steps for this SEVIEW session are outlined below.

1. Initiate SEVIEW
2. Produce a Point of Compliance report
3. Exit SEVIEW

Step 1 **Initiate SEVIEW**

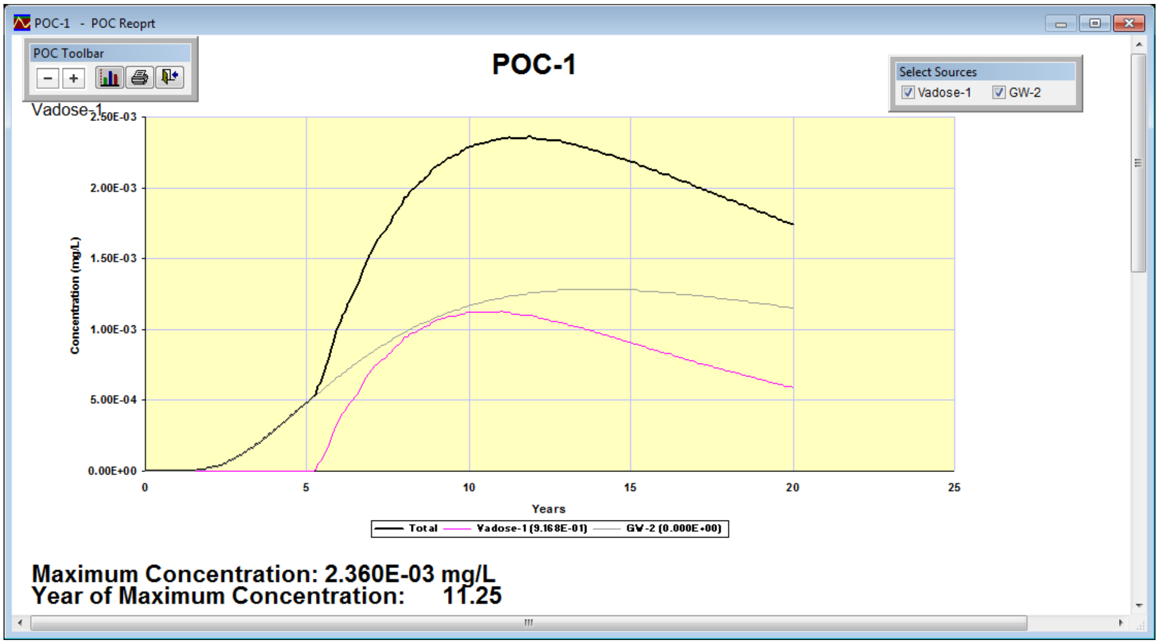
Initiate SEVIEW by double clicking on the SEVIEW icon, or select SEVIEW on the Start menu.

Step 2 **View a point of compliance report**

Double Click the POC. SEVIEW will display results at the location of the POC. The POC report displays contaminant concentrations through time at a specific point. This can be thought of as displaying monthly concentrations through time in a monitoring well. A copy of the POC report is presented below.

*You could also **Double Click** the POC source on the **POC Toolbar**.*

This is essentially the same as an observation well in MT3D.



Maximum Concentration: 2.360E-03 mg/L
Year of Maximum Concentration: 11.25

This POC report displays results for both the SESOIL vadose zone source and the AT123D groundwater source. You can use the **Select Sources Toolbar** to determine which sources to display on the report. For instance if you uncheck the **Vadose-1** source and click on the graph update command. SEVIEW will only display results for the AT123D source.

The dark black line on the POC graph is the cumulative concentration from all of the sources.

You can double click on the graph to open Microsoft Graph.

Step 5 **Exit SEVIEW**

To end your SEVIEW session, select the **File** option on the main menu, then select **Exit** or close the window.

Congratulations, you have completed both AT123D tutorials and have become familiar with the basic features of running and evaluating AT123D using SEVIEW. If you have not used SEVIEW for a while or have forgotten how to use it, you may want to review these tutorials.

The next section provides one tutorial on using BIOSCREEN in SEVIEW.

4.3 BIOSCREEN Tutorials

As part of this tutorial you will use BIOSCREEN to setup and run the AT123D groundwater model. An overview of the steps for linking BIOSCREEN to AT123D are outlined below.

1. Initiate Excel and open BIOSCREEN
2. Initiate SEVIEW
3. Click "Get BIOSCREEN Data"
4. Run AT123D

4.3.1 Tutorial Five – BIOSCREEN Link

Step 1 **Initiate Excel and open BIOSCREEN**
Initiate Excel and open BIOSCREEN.

☞ *You can find BIOSCREEN spreadsheet in* ***augfix***

Step 2 **Initiate SEVIEW**
Initiate SEVIEW by double clicking on the SEVIEW icon, or select SEVIEW on the Start menu.

Step 3 **Get BIOSCREEN Data**
Click on the **Get BIOSCREEN Data** command on the **SEVIEW Toolbar**.

Step 4 **Run AT123D**

Click on the **Run AT123D** command on the **SEVIEW Toolbar**. You should now see the message "AT123D STARTS" followed by years and source information.

☞ *AT123D can run very quickly and it may be difficult to observe it running.*

Now proceed to Section 4.3.2 to view results for the AT123D source.

You have now setup and run AT123D and completed the first AT123D tutorial. You can now stop working in the tutorial if you wish, or you can continue and evaluate the AT123D output file you generated. If you continue you will learn how to view AT123D results in the tutorial below.

4.3.2 Tutorial Six – View AT123D Results

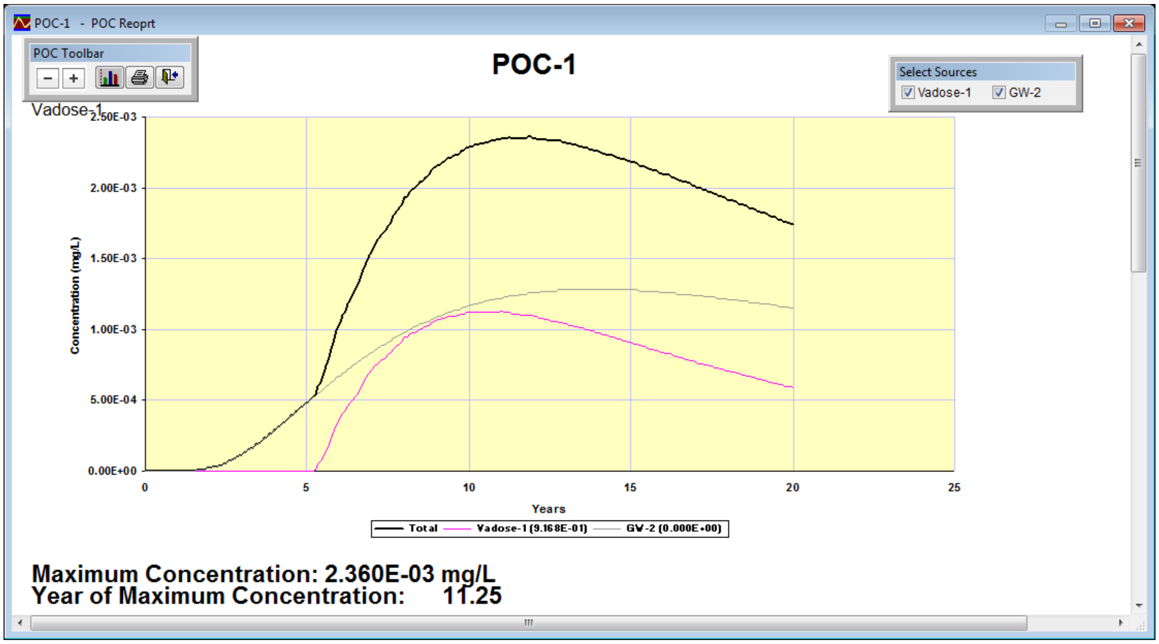
Step 1 **View a point of compliance report**

Double Click the POC. SEVIEW will display results at the location of the POC. The POC report displays contaminant concentrations through time at a specific point. This can be thought of as displaying monthly concentrations through time in a monitoring well. A copy of the POC report is presented below.

☞ *You could also **Double Click** the POC source on the **POC Toolbar**.*

☞ *This is essentially the same as an observation well in MT3D.*

Update this figure to use one produced by the BIOSCREEN link



Maximum Concentration: 2.360E-03 mg/L
Year of Maximum Concentration: 11.25

☞ *The dark black line on the POC graph is the cumulative concentration from all of the sources.*

☞ *You can double click on the graph to open Microsoft Graph.*

Step 5 **Exit SEVIEW**

To end your SEVIEW session, select the **File** option on the main menu, then select **Exit** or close the window.

Congratulations, you have completed both AT123D tutorials and have become familiar with the basic features of running and evaluating AT123D using SEVIEW. If you have not used SEVIEW for a while or have forgotten how to use it, you may want to review these tutorials.

The following sections of this user’s guide present in-depth information about SEVIEW.

5 Using SEVIEW

This section presents a detailed description of all SEVIEW commands and options. When you start the program you will see a base map, toolbar, and program menu that provide access to the SEVIEW commands and options. The base map displays a graphical representation of the model release scenario. The **SEVIEW Toolbar** provides options to set default parameters and run the models. The **Side Toolbar** provides options to setup the model scenario. The program menu you can select sub-menus containing SEVIEW commands.

5.1 The Side Toolbar

The **Side Toolbar** displays the basic commands to setup the models.

Command	Description
AT123D	Use this command to add an AT123D groundwater plume source to the base map.
SESOIL	Use this command to add a SESOIL vadose zone source to the base map.
POC	Use this command to add a POC to the base map.
Delete	Use this command to remove sources and/or POCs.
Save	Click to save any changes to the current project file. The changes will be saved without asking.
New Project	Use this command to start a new SEVIEW project. Clicking it will remove all sources and POCs.
Base Map	Click this command to insert a new base map. You can select any .jpg, .bmp, .png or .tif file.
Set Scale	Used to establish a base map scale.

5.1.1 AT123D

Use the **AT123D** command to add a groundwater source to the base map. Click **AT123D** and move the mouse over the base map and a red square will follow it. Move the red source to the desired location on the base map and **Single Click** the source to drop it. The source will then turn blue.

☞ *You can **Right Click** on the source if you need to move it again.*

You can set the AT123D model parameters by **Clicking** on the source. AT123D results can be displayed by **Double Clicking** on a POC on the base map. Additional AT123D results can be displayed by **Double Clicking** on the AT123D source.

5.1.2 SESOIL

Use this command to add a SESOIL vadose zone source to the base map. Click **SESOIL** and move the mouse over the base map and a red square will follow it. Move the red source to the desired location on the base map and **Single Click** the source to drop it. The source will turn green.

☞ *You can **Right Click** on the source if you need to move it again.*

You can set the SESOIL model parameters by **Clicking** on the source. SESOIL results can be displayed by **Double Clicking** on the SESOIL source.

5.1.3 POC

Use the **POC** command to add a point of compliance. Click **POC** and move the mouse over the base map and a grey POC will follow it. Move the POC to the desired location on the base map and **Single Click** the POC to drop it. The POC will turn red.

☞ *You can **Right Click** on the POC if you need to move it again.*

AT123D results can be displayed by **Double Clicking** on a POC on the base map.

☞ *You can **Double Click** the POC on the POC toolbar.*

5.1.4 Delete

Use the **Delete** command to remove a AT123D or SESOIL source. You can also use this commend to remove a POC.

☞ *You can delete a source or POC on the Sources and POC toolbars.*

5.1.5 Save

Click the **Save** command to save any changes to the current SEVIEW project. Please note that SEVIEW will not ask prior to saving the file.

☞ *The changes will be saved without asking.*

☞ *Be sure to save your project often.*

5.1.6 New Project

Use the **New Project** command to start a new SEVIEW project. Clicking **New Project** will remove all SESOIL and AT123D sources along with all POCs. This data will be lost unless you have already saved the SEVIEW project file.

5.1.7 Base Map

Click the **Base Map** command to open a new base map. You can select any .jpg, .bmp, .png or .tif file.

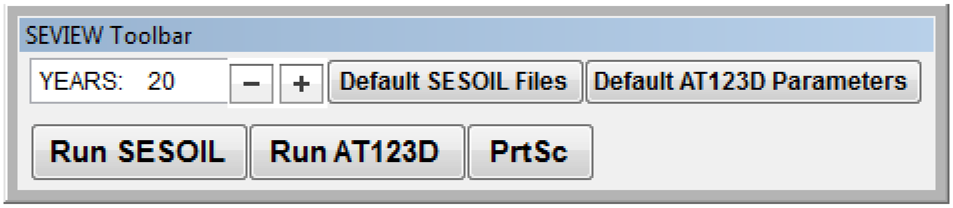
5.1.8 Set Scale

The **Set Scale** option is used to establish the scalar distances on the base map. When you **click** on the **Set Scale** command the mouse pointer on the base map will change to a crosshair with a P1 designation. **Click** on the first point on the base map and the mouse pointer designation will change to a crosshair with a P2 designation. Next **click** on the second point on the base map. Then enter the distance in meters in the input field that appears.

5.2 The SEVIEW Toolbar

The **SEVIEW Toolbar** displays the commands to run the models. It also provides access to the default model parameters.

Add Get BIOSCREEN data to the figure



Command	Description
Years	Sets the number of years that the models will simulate. The value can range from 2 to 999 years.
-/+	Use this command to zoom in or out on the base map.
Default SESOIL Files	Click this command to establish the default input files used by the SESOIL model.
Default AT123D parameters	Click this command to establish the default AT123D input parameters.

Run SESOIL	Click this command to run the SESOIL model.
Run AT123D	Click this command to run the AT123D model. Please note that you will need to first run the SESOIL model if you have any vadose zone sources.
PrtSc	Click this command to grab a snapshot of the current screen.
Get BIOSCREEN Data	

5.2.1 Years

The **Years** field is used to set the total number of years to be simulated by SESOIL and/or AT123D. The value can range from 2 to 999 years.

5.2.2 Zoom

The − + commands are used to zoom in or out on the base map.

5.2.3 Default SESOIL Files

Click this command to establish the default input files used by the SESOIL model.

5.2.4 Default AT123D Parameters

Click this command to establish the default AT123D input parameters.

5.2.5 Run SESOIL

The **Run SESOIL** command will run the SESOIL model.

5.2.6 Run AT123D

The **Run AT123D** command will run the AT123D model. Please note that you will need to first run the SESOIL model if you have any vadose zone sources.

5.2.7 PrtSc

Click the **PrtSc** command to grab a snapshot of the current screen. You can use the image as part of your report.

☞ *SEVIEW will temporally remove the Side and SEVIEW toolbars prior to taking the snapshot.*

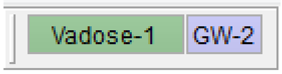
☞ *You may want to use a screen capture utility to crop the captured image.*

5.2.8 Get BIOSCREEN Data

Click the **Get BIOSCREEN Data** command to import a BIOSCREEN **scenario**.

5.3 The Source Toolbar

The **Source Toolbar** is displayed at the top of the screen. Clicking on a source will open the properties for that source.



Command	Description
Green	SESOIL vadose zone source.
Blue	AT123D groundwater source.

5.3.1 Green SESOIL Source

Single Click on a **green** source to open a window displaying the SESOIL input parameters. **Double Click** to view the results.

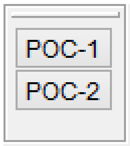
☞ *Clicking a source on the toolbar does the same thing as clicking on the source on the base map. This option can be used to set parameters for sources that may not be visible on the base map.*

5.3.2 Blue AT123D Source

Single Click on a **blue** source to open a window displaying the AT123D input parameters. **Double Click** to view the output file.

5.4 The POC Toolbar

The **POC Toolbar** is displayed at the below the **Side Toolbar**. **Single Clicking** on a POC will open the parameters for that POC.



☞ *Clicking a POC on the toolbar does the same thing as clicking on the POC on the base map. This option can be used to set parameters for POCs that may not be visible on the base map.*

5.5 SESOIL Source Mouse Click Commands

Command	Description
Click	Used to set the parameters of the SESOIL model. This includes the climate, chemical, soil and application files for the selected source.
Double Click	Presents results of the SESOIL model. This includes the Climatic, Load, Hydrologic Cycle, and Pollutant Cycle reports.
Right Click	Used to move the SESOIL source. Drop the SESOIL source by **Clicking** it again.

5.6 AT123D Source Mouse Click Commands

Command	Description
Click	Used to set the parameters of the AT123D model for the selected source.
Double Click	Used to view the AT123D ASCII output file. Additional AT123D results are displayed by clicking on a POC.
Right Click	Used to move the AT123D source. Drop the AT123D source by **Clicking** it again.

5.7 POC Mouse Click Commands

Command	Description
Click	Used to set the parameters of the POC. In addition to the x and y coordinates you can establish up to 10 points along the z-axis (depth) for each POC. SEVIEW averages the groundwater concentration over the depth interval for each POC.
Double Click	Opens the POC report that presents groundwater concentration results at the location. You can select any combination of the sources.
Right Click	Used to move the POC. Drop the POC by **Clicking** it again.

5.8 Base Map Mouse Click Commands

Command	Description

Right Click	Used to set the base map rotation angle. This is used to establish groundwater flow such that it moves from left to right.

5.9 Using the SEVIEW Main Menu

SEVIEW contains an easy to use menu.

Starting SEVIEW

Double Click on the SEVIEW icon. When SEVIEW is started the following menu is displayed.

File Edit MODFLOW Help

The **File** option provides access to the project files, printer setup and a way to quit SEVIEW. The **Edit** sub-menu provides access to the basic Windows edit, cut and paste commands. The **MODFLOW** menu option is used to set the default MODFLOW parameters. The **Help** sub-menu provides access to on-line help, this User's Guide, and the About SEVIEW display. A detailed description of each menu option is presented below.

5.9.1 File Commands

File commands are used open and save SEVIEW project files, open A DOS window, setup the printer , and to quit SEVIEW.

File Edit SESOIL AT123D MODFLOW Help
Open a SEVIEW Project
Save as SEVIEW Project
Go To DOS
Close
Save
Save as...
Print
Printer Setup
Exit

5.9.1.1 Open a SEVIEW Project

Use the **Open a SEVIEW Project** command to open an existing model project. When selected this option, SEVIEW will ask if you want to save changes to the current project. If you click yes SEVIEW will prompt you for a project file name.

☞ *You can open defaults SEVIEW projects contain in the **Example Projects** subfolder.*

☞ *Be careful not to over right your current file.*

☞ *If you do not choose a project file (Cancel is selected, the <ESCAPE> key is pressed, or the window is closed) the current project will be retained.*

☞ *Version 7.1 project files will be automatically be converted to version 7.3 project files.*

5.9.1.2 Save as SEVIEW Project

Use the **Save as SEVIEW Project** command to save your model project. When selected this option, SEVIEW will ask if you want to save changes to the current project. If you click yes SEVIEW will prompt you for a project file name. You can take the default option to save the data to the current project.

☞ *Please note that version 7.3 project files are not compatible with SEVIEW 7.1. Once saved there is no going back.*

☞ *Be sure to save your data often.*

5.9.1.3 Go To DOS

There is no need to quit SEVIEW to access DOS or to run a DOS program. The **Go To DOS** option provides easy access to DOS without closing SEVIEW. This command is simply a short cut to opening a DOS window.

☞ *As with any DOS window, type exit and press enter to close it.*

☞ *This option can be used to help debug SESOIL and AT123D scenarios. Unlike the **Run SESOIL** and **Run AT123D** commands, this DOS window will not close once SESOIL has run. Allowing you to view any error messages.*

5.9.1.4 Close

The **File, Close** option is used to close the currently opened file. If the file has been modified you will be prompted if the changes should be saved.

5.9.1.5 Save

The **File, Save** option is used to save the currently opened file. If the file has been modified the changes will be saved.

5.9.1.6 Save As

The **File, Save As** option is used to save the currently opened file as a new file. If the new file already exists the user will be asked if the file should be overwritten.

5.9.1.7 Print

The **File, Print** option is used to print a SESOIL or AT123D input file. The **Print** option can also be used to print a text file or the contents of the clipboard.

5.9.1.8 Printer Setup

The **File, Printer Setup** option is used to select the default printer and the paper size and orientation. Specific options presented are determined by your printer.

5.9.1.9 Exit

Use the **File, Exit** menu to quit SEVIEW. This option should only be used when you have completed all of your modeling and SEVIEW data management tasks. Keep in mind that there is no need to quit SEVIEW to run SESOIL, AT123D or to use any other DOS or Windows programs.

5.9.2 Edit

The **Edit** command options are used when editing or searching text files.

File **Edit** **SESOIL** **AT123D** **MODFLOW** **Help**

- **Undo**
- **Redo**
- **Cut**
- **Copy**
- **Paste**
- **Select All**
- **Goto Line**
- **Find**
- **Find Again**

5.9.2.1 Undo

Undo reverses the last action performed on any text. If you repeatedly select **Undo**, your actions will be reversed all the way to the start of the current editing session. The <CONTROL + Z> short cut keys can also be used to execute the **Undo** command.

5.9.2.2 Redo

Redo restores the action previously reversed with the **Undo** command. The **Redo** command is the opposite of the **Undo** command. The **Redo** command is used if you change your mind after using the **Undo** command. If you repeatedly select **Redo**, your **Undo** actions will be restored in the order they were undone. The <CONTROL + R> short cut keys can also be used to execute the **Redo** command.

5.9.2.3 Cut

The **Cut** command removes selected text and places it in the Windows clipboard. The **Cut** command is used when you want to move text from one location to a new location. The **Paste** command is used to insert the text. The <CONTROL + X> short cut keys can be used to execute the **Cut** command.

5.9.2.4 Copy

The **Copy** command places a duplicate copy of the selected text into the clipboard. The **Copy** command is used when you want to move copies of text and place it in a new location. The **Paste** command is used to insert the text. The <CONTROL + C> short cut keys can also be used to execute the **Copy** command.

5.9.2.5 Paste

The **Paste** command inserts a copy of the clipboard into the current file at the cursor location. To copy text to the clipboard, see the **Cut** and **Copy** commands above. The <CONTROL + V> short cut keys can also be used to execute the **Paste** command.

5.9.2.6 Select All

The **Select All** command highlights all text to be copied, cut or deleted.

5.9.2.7 Go to Line

The **Go to Line** command moves the cursor to the beginning of the selected line number.

5.9.2.8 Find

The **Find** command searches for text within the document. The <CONTROL + F> short cut keys can also be used to execute the **Find** command.

5.9.2.9 Find Again

The **Find Again** command repeats the last find. The <CONTROL + G> short cut keys can be used to execute the **Find Again** command.

5.9.3 MODFLOW

The **MODFLOW** command option is used to set parameters for the SESOIL to MODFLOW link.

File Edit SESOIL AT123D **MODFLOW** Help
Set MODFLOW Parameters

5.9.3.1 Set MODFLOW Parameters

This command is used to establish default parameters for the MODFLOW link. The link data is created whenever you print or preview a **SESOIL Pollutant Report**. A description of the parameters is presented in Section 8.

5.9.4 Help

The **Help** command options are used when editing or searching text.

File Edit SESOIL AT123D MODFLOW **Help**
SEVIEW Help
SEVIEW User's Guide
About SEVIEW

5.9.4.1 SEVIEW Help

Click on the **SEVIEW Help** command to view the on-line Help.

5.9.4.2 SEVIEW User's Guide

Opens a pdf version of the SEVIEW User's Guide (this document).

5.9.4.3 About SEVIEW

The **About SEVIEW** command provides information on the current version of SEVIEW.

6 SESOIL Parameter Specifications

6.1 Introduction

This section provides a detailed description of each SESOIL input parameter. You will need to create a SESOIL source prior to modifying the parameters. SESOIL data files can be entered in any order. SESOIL input files contain data that describe the physical and chemical characteristics of the source release. These input parameters can be obtained from laboratory analysis, field investigations, and values cited in reference literature.

At a minimum, four input data files are required to run SESOIL. The four data sets are contained in the climate, soil, chemical, and application files. A fifth data set, the washload file, is optional and rarely used.

6.2 The SEVIEW Input Screen

Click on a green SESOIL source to open the **Setup SESOIL and AT123D Runs** input screen. This screen provides easy access to all model input parameters. The input screen is divided into tab organized parameters.

6.2.1 Model Parameters

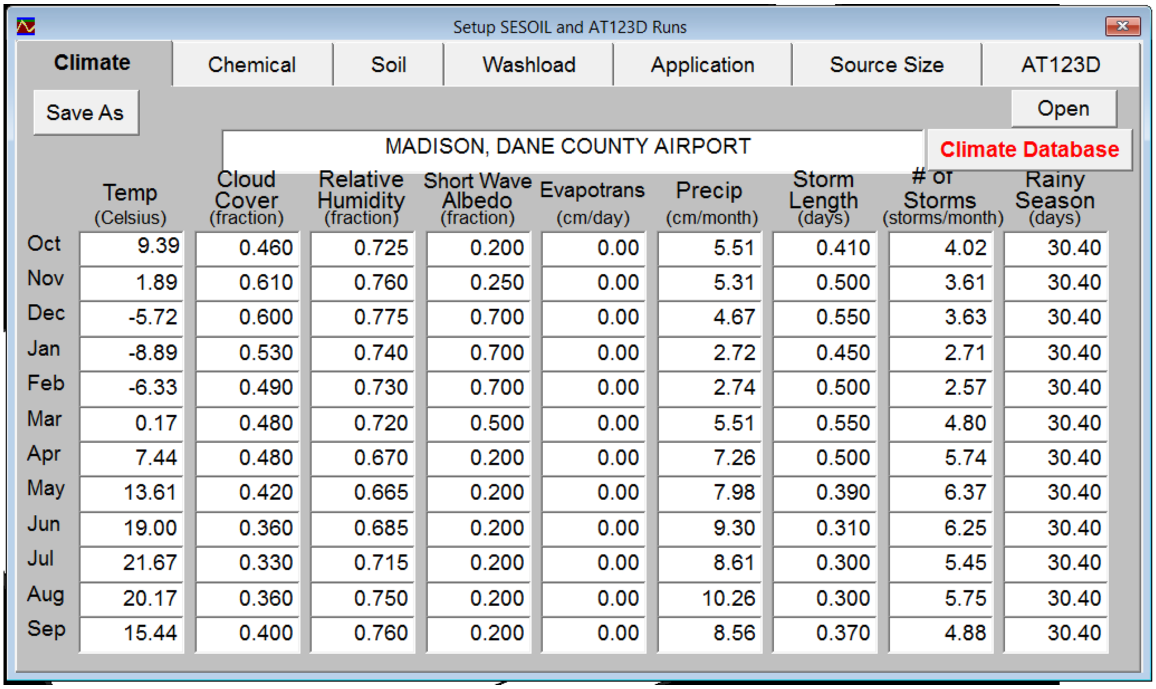
The SEVIEW input screen contains tabs that provide access to all of the SESOIL and AT123D input parameters. To modify model input data simply enter the new values into the appropriate parameter fields.

☞ *New input files are created by clicking on the **Save As** command displayed on each input tab. Next save the input data to a new file. Finally you will be asked if you want to log the new input file into the journal. If you click yes SEVIEW will replace the current input file with the new one.*

*For instance if I wanted to create a clay soil input file I would first save the sand.soi as "clay.soi". This will create a clay.soi text file on the computer. However the clay.soi file will not be used unless you log it. You open and log the file by clicking on the **Open** command.*

6.3 Climate File Input Parameters

The SESOIL climate data set contains information describing the specifics of the local climate. This includes: air temperature, cloud cover, relative humidity, short wave albedo, mean evapotranspiration rate, monthly precipitation, length of precipitation events, number of precipitation events per month and the distribution of precipitation events throughout the month. Users can custom-fit data for a particular scenario. A detailed description of each input parameter is provided below.



MADISON, DANE COUNTY AIRPORT

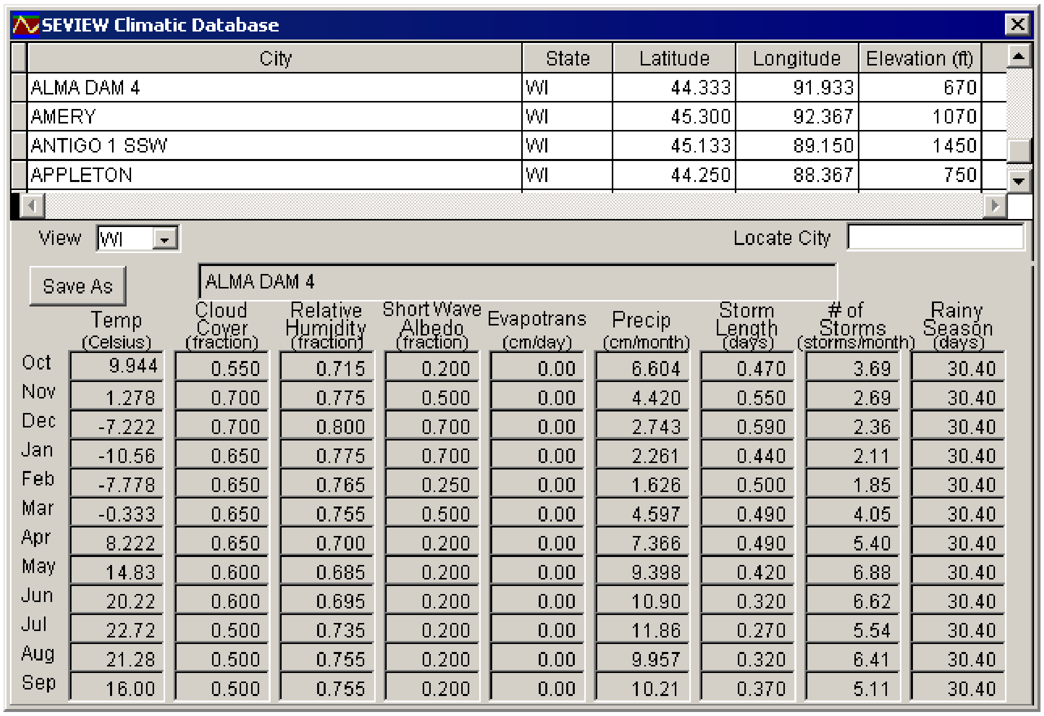
	Temp (Celsius)	Cloud Cover (fraction)	Relative Humidity (fraction)	Short Wave Albedo (fraction)	Evapotrans (cm/day)	Precip (cm/month)	Storm Length (days)	# of Storms (storms/month)	Rainy Season (days)
Oct	9.39	0.460	0.725	0.200	0.00	5.51	0.410	4.02	30.40
Nov	1.89	0.610	0.760	0.250	0.00	5.31	0.500	3.61	30.40
Dec	-5.72	0.600	0.775	0.700	0.00	4.67	0.550	3.63	30.40
Jan	-8.89	0.530	0.740	0.700	0.00	2.72	0.450	2.71	30.40
Feb	-6.33	0.490	0.730	0.700	0.00	2.74	0.500	2.57	30.40
Mar	0.17	0.480	0.720	0.500	0.00	5.51	0.550	4.80	30.40
Apr	7.44	0.480	0.670	0.200	0.00	7.26	0.500	5.74	30.40
May	13.61	0.420	0.665	0.200	0.00	7.98	0.390	6.37	30.40
Jun	19.00	0.360	0.685	0.200	0.00	9.30	0.310	6.25	30.40
Jul	21.67	0.330	0.715	0.200	0.00	8.61	0.300	5.45	30.40
Aug	20.17	0.360	0.750	0.200	0.00	10.26	0.300	5.75	30.40
Sep	15.44	0.400	0.760	0.200	0.00	8.56	0.370	4.88	30.40

The following parameter descriptions are provided as a guideline for each of the climate parameters used in SESOIL.

The following descriptions also apply to the climatic database. The climatic database is opened by clicking on the Climate Database *command displayed in the SESOIL climate input screen tab. A copy of the climatic database screen is presented below.*

I need to update the figure to include the 1971-2000 and 1991-2020 data.

The climate database now contains climatic data for over 22,355 climate stations. There are 15,615 stations for the 1991 – 2020 data and 6,740 stations for the 1971 – 2000 data.



City	State	Latitude	Longitude	Elevation (ft)
ALMA DAM 4	WI	44.333	91.933	670
AMERY	WI	45.300	92.367	1070
ANTIGO 1 SSW	WI	45.133	89.150	1450
APPLETON	WI	44.250	88.367	750

ALMA DAM 4

	Temp (Celsius)	Cloud Cover (fraction)	Relative Humidity (fraction)	Short Wave Albedo (fraction)	Evapotrans (cm/day)	Precip (cm/month)	Storm Length (days)	# of Storms (storms/month)	Rainy Season (days)
Oct	9.944	0.550	0.715	0.200	0.00	6.604	0.470	3.69	30.40
Nov	1.278	0.700	0.775	0.500	0.00	4.420	0.550	2.69	30.40
Dec	-7.222	0.700	0.800	0.700	0.00	2.743	0.590	2.36	30.40
Jan	-10.56	0.650	0.775	0.700	0.00	2.261	0.440	2.11	30.40
Feb	-7.778	0.650	0.765	0.250	0.00	1.626	0.500	1.85	30.40
Mar	-0.333	0.650	0.755	0.500	0.00	4.597	0.490	4.05	30.40
Apr	8.222	0.650	0.700	0.200	0.00	7.366	0.490	5.40	30.40
May	14.83	0.600	0.685	0.200	0.00	9.398	0.420	6.88	30.40
Jun	20.22	0.600	0.695	0.200	0.00	10.90	0.320	6.62	30.40
Jul	22.72	0.500	0.735	0.200	0.00	11.86	0.270	5.54	30.40
Aug	21.28	0.500	0.755	0.200	0.00	9.957	0.320	6.41	30.40
Sep	16.00	0.500	0.755	0.200	0.00	10.21	0.370	5.11	30.40

As you can see this window looks very much like the climate input screen with the addition of the city, state, latitude, longitude, and elevation fields. ***Click*** *on the* ***Save As*** *command to create a new SESOIL climatic input from the database. If you do not want to update the SESOIL climate file simply close the window.*

You can use the View and Locate City commands to find locations in the climate database.

Parameter	**Description of the Climatic Data Set**
SESOIL Variable	TITLE
Description	Description used to identify the climatic data set. Limited to a maximum of 48 characters in length.

Parameter	**Air Temperature**
Units	degrees Celsius
SESOIL Variable	TA
Description	An array of the monthly mean air temperature for each month of the year (in degrees Celsius). The air temperature is used to determine the monthly evapotranspiration rates and soil temperatures. If the actual monthly evapotranspiration rates are known [i.e. non-zero values entered for evapotranspiration rates (REP)], then air temperature is not used to calculate evapotranspiration. However, air temperature is always used to

	calculate soil temperature.
Source of Data	NOAA

Parameter	**Cloud Cover**
Units	fraction
SESOIL Variable	NN
Description	An array of the monthly mean cloud cover fraction for each month of the year (dimensionless fraction ranging from 0.0 to 1.0) used to calculate evapotranspiration rates. If the monthly evapotranspiration rates are known [i.e. non-zero values entered for evapotranspiration rates (REP)] then the percent cloud cover is not used.
Source of Data	NOAA

Parameter	**Relative Humidity**
Units	fraction
SESOIL Variable	S
Description	An array of the monthly mean relative humidity for each month of the year (dimensionless fraction ranging from 0.0 to 1.0) used to calculate evapotranspiration rates. If the monthly evapotranspiration rates are [i.e. non-zero values entered for evapotranspiration rates (REP)], then the percent relative humidity is not used.
Source of Data	NOAA

<table>
<tr><th>Parameter</th><th>Short Wave Albedo</th></tr>
<tr><td>Units</td><td>Fraction</td></tr>
<tr><td>SESOIL Variable</td><td>A</td></tr>
<tr><td>Description</td><td>The albedo fraction is the ratio of the reflective short wave energy to the incoming energy. An array of the short wave albedo fraction for each month of the year (dimensionless fraction ranging from 0.0 to 1.0) used determine soil temperature which is used to calculate evapotranspiration rates. If the monthly evapotranspiration rates are known [i.e. non-zero values entered for evapotranspiration rates (REP)], then the short wave albedo fractions not used.</td></tr>
<tr><td>Source of Data</td><td>Table 1 Short Wave Albedo Values
<table>
<tr><th>Surface</th><th>Range</th><th>Typical Values</th></tr>
<tr><td>Soil and Bedrock</td><td></td><td></td></tr>
<tr><td>Dark moist soil with high humus content</td><td>0.05 - 0.15</td><td>0.10</td></tr>
<tr><td>Gray moist soil</td><td>0.10 - 0.20</td><td>0.15</td></tr>
</table>
</td></tr>
</table>

Dry desert soil	0.20 - 0.35	0.30
Sand, wet	0.20 - 0.30	0.25
Sand, light dry	0.30 - 0.40	0.35
Soil (black, moist)	0.05 - 0.10	- -
Soil (black, dry)	0.10 - 0.15	- -
Desert	0.25 - 0.40	0.37
Desert, clayey	0.29 - 0.31	- -
Granite	0.12 - 0.18	- -
Rocks in general	0.12 - 0.15	- -
Sand, wet	0.15 - 0.25	- -
Snow		
Fresh dry snow	0.70 - 0.90	0.80
Old snow	0.60 - 0.75	0.70
Dirty snow	0.40 - 0.75	- -
Thawing snow	0.35 - 0.65	0.50
Vegetation		
Grasses	0.15 - 0.30	0.20
Green grass	0.18 - 0.27	- -
Green vegetation (short)	0.10 - 0.20	0.17
Grassland parched	0.16 - 0.30	- -
Grassland, dry	0.25 - 0.30	- -
Dry vegetation	0.20 - 0.30	0.25
Forests	0.05 - 0.20	- -
Coniferous forest	0.10 - 0.15	0.12
Green deciduous forest	0.15 - 0.25	0.17
Yellow deciduous forest (autumn)	0.33 - 0.38	- -
Man Made Surfaces		
Concrete	0.15 - 0.35	0.20
Asphalt	0.05 - 0.10	0.07

Parameter	**Evapotranspiration Rate**
Units	cm/day
SESOIL Variable	REP
Description	An array of the monthly mean evapotranspiration rate (cm/day) for each month of the year. If 0.0 is entered, SESOIL will calculate evapotranspiration based on air temperature, percent cloud cover, percent relative humidity, and short wave albedo fraction, soil type and depth to groundwater. If a non-zero positive value is entered for the daily evapotranspiration rate, SESOIL will ignore the values for air temperature, cloud cover, relative humidity, and short wave albedo.
Typical Values	Daily evapotranspiration rate is typically set to 0.0. By doing so SESOIL will establish evapotranspiration rates based on climatic data, soil properties and depth to groundwater.
Source of Data	Site-specific

☞ *Be careful if you enter an evapotranspiration rate as the units are in cm/day not cm/month!*

Parameter	**Precipitation**
Units	cm/month
SESOIL Variable	MPM
Description	An array of the total rain precipitation per month (cm/month).
Source of Data	NOAA

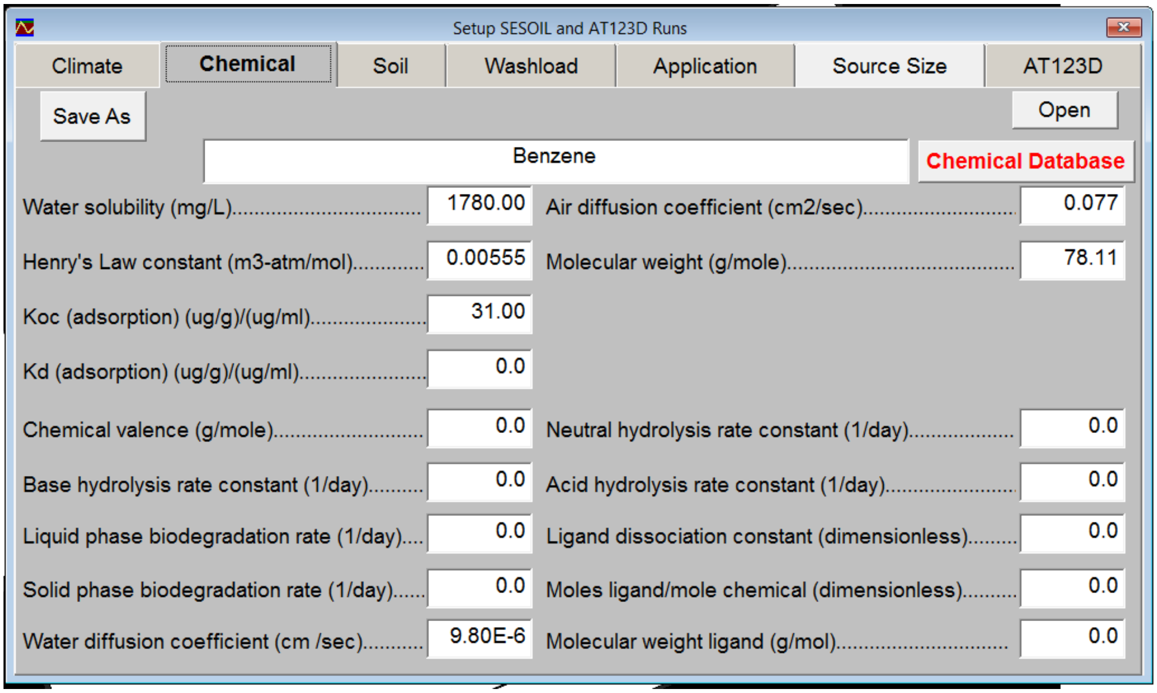
Parameter	**Duration of Individual Storm Events**
Units	days
SESOIL Variable	MTR
Description	An array of the mean duration of individual storm events in days, for each month of the year.
Source of Data	NOAA
Parameter	**Number of Storm Events**
Units	storm events/month
SESOIL Variable	MN
Description	An array of the number of storm events per month for each month of the year.
Source of Data	NOAA

Parameter	**Length of Rainy Season**
Units	Days
SESOIL Variable	MT
Description	An array of the length of the rainy season (in days) for each month of the year. For most regions in the United States, this parameter should be set to 30.4 (the default value) for all months, since rain events may occur throughout the entire month.
Source of Data	NOAA

☞ *SESOIL calculates the amount of precipitation that enters the soil column (infiltration) and the amount in the surface water runoff. Water entering the soil column may either, return to the atmosphere by the process of evapotranspiration, remain in soil moisture and/or percolate through the soil* *column to enter groundwater as recharge. Climatic parameters are used by SESOIL to simulate these processes. Air temperature, cloud cover, humidity, and albedo, are used to estimate evapotranspiration (REP), if a value for this parameter is not provided. If a value for evapotranspiration rate is provided, the model will use that value and will not compute the estimate.*

6.4 Chemical File Input Parameters

The chemical input file contains information describing the chemical and physical properties of the contaminant released or applied to the soil column. This information includes water solubility, air diffusion coefficient, Henry's Law constant, organic carbon adsorption coefficient, soil partition coefficient, molecular weight, valence of the compound, acid, base and neutral hydrolysis rate constants, liquid and solid phase biodegradation rates, ligand stability constant, moles ligand per mole compound, and the molecular weight of the ligand. A copy of the chemical input screen tab and a description of the input parameters are presented below.

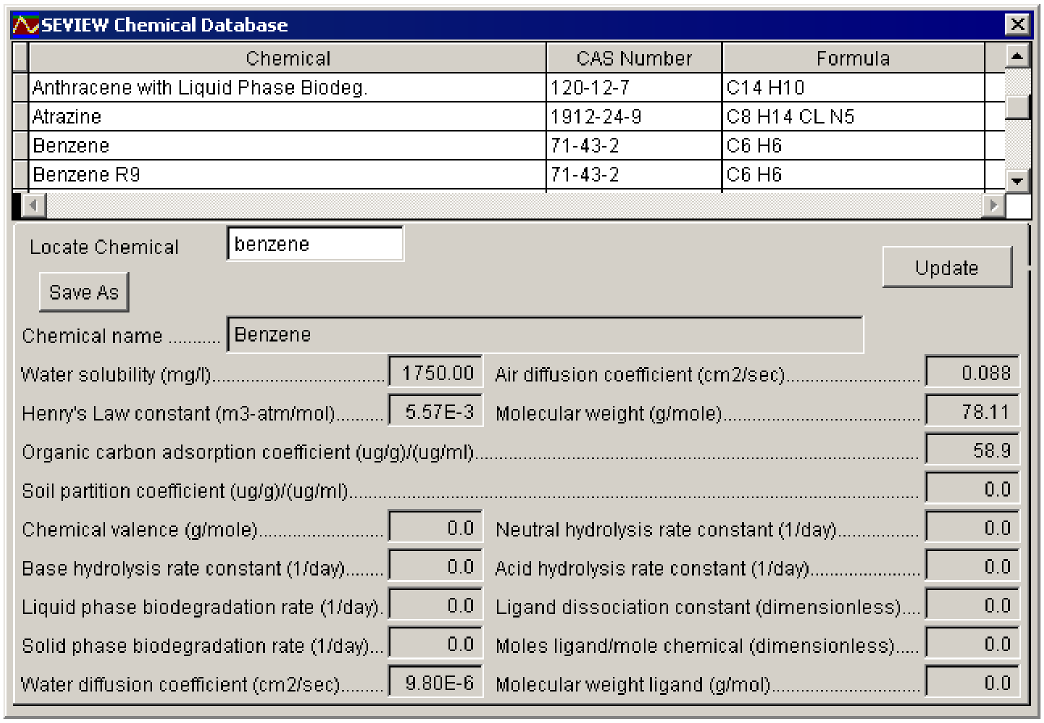


Benzene

Water solubility (mg/L) 1780.00
Air diffusion coefficient (cm2/sec) 0.077
Henry's Law constant (m3-atm/mol) 0.00555
Molecular weight (g/mole) 78.11
Koc (adsorption) (ug/g)/(ug/ml) 31.00
Kd (adsorption) (ug/g)/(ug/ml) 0.0
Chemical valence (g/mole) 0.0
Neutral hydrolysis rate constant (1/day) 0.0
Base hydrolysis rate constant (1/day) 0.0
Acid hydrolysis rate constant (1/day) 0.0
Liquid phase biodegradation rate (1/day) 0.0
Ligand dissociation constant (dimensionless) 0.0
Solid phase biodegradation rate (1/day) 0.0
Moles ligand/mole chemical (dimensionless) 0.0
Water diffusion coefficient (cm /sec) 9.80E-6
Molecular weight ligand (g/mol) 0.0

The following parameter descriptions are provided as a guideline for each of the chemical parameters used in SESOIL.

The following descriptions also apply to the chemical database. The chemical database is opened by clicking on the Chemical Database *command displayed in the SESOIL chemical input screen tab. A copy of the chemical database screen is presented below.*



Chemical	CAS Number	Formula
Anthracene with Liquid Phase Biodeg.	120-12-7	C14 H10
Atrazine	1912-24-9	C8 H14 CL N5
Benzene	71-43-2	C6 H6
Benzene R9	71-43-2	C6 H6

Locate Chemical: benzene

Chemical name: Benzene

Water solubility (mg/l)	1750.00	Air diffusion coefficient (cm2/sec)	0.088
Henry's Law constant (m3-atm/mol)	5.57E-3	Molecular weight (g/mole)	78.11
Organic carbon adsorption coefficient (ug/g)/(ug/ml)			58.9
Soil partition coefficient (ug/g)/(ug/ml)			0.0
Chemical valence (g/mole)	0.0	Neutral hydrolysis rate constant (1/day)	0.0
Base hydrolysis rate constant (1/day)	0.0	Acid hydrolysis rate constant (1/day)	0.0
Liquid phase biodegradation rate (1/day)	0.0	Ligand dissociation constant (dimensionless)	0.0
Solid phase biodegradation rate (1/day)	0.0	Moles ligand/mole chemical (dimensionless)	0.0
Water diffusion coefficient (cm2/sec)	9.80E-6	Molecular weight ligand (g/mol)	0.0

As you can see this window looks very much like the input screen with the addition of the chemical, CAS number and formula fields. To copy the data to the SESOIL chemical input file move to the desired chemical and click on the Save As *command and close the database window. If you do not want to update the SESOIL chemical file simply close the window.*

Parameter	**Description of the Chemical Data Set / Chemical Name**
SESOIL Variable	TITLE
Description	Description used to identify the chemical data set. Limited to a maximum of 48 characters in length.

Parameter	**Water Solubility**
Units	(mg/L)
SESOIL Variable	SL
Description	The solubility of the compound in water at 25° C.
Source of Data	Chemical reference literature.

☞ *SESOIL requires a water solubility value for the chemical. If the water solubility is unknown and migration to groundwater is the concern, then an estimated value that is somewhat high should be used. This will ensure that the estimates of chemical of chemical leaching are conservative.*

<table>
<tr><th>Parameter</th><th>Air Diffusion Coefficient</th></tr>
<tr><td>Units</td><td>cm^2/sec</td></tr>
<tr><td>SESOIL Variable</td><td>DA</td></tr>
<tr><td>Description</td><td>The diffusion coefficient in air, used by SESOIL to calculate volatilization.</td></tr>
<tr><td>Source of Data</td><td>Chemical reference literature, or air diffusion coefficient can be estimated using the following relationship:

$$DA = DA'\sqrt{\frac{MWT'}{MWT}}$$

where:
<table>
<tr><th>Parameter</th><th>Description</th></tr>
<tr><td>DA</td><td>Air diffusion coefficient of the current compound,</td></tr>
<tr><td>DA'</td><td>A diffusion coefficient for a reference compound,</td></tr>
<tr><td>MWT'</td><td>Molecular weight of the reference compound, and</td></tr>
<tr><td>MWT</td><td>Molecular weight of the current compound.</td></tr>
</table>
☞ <i>The diffusion coefficient (0.083 cm^2/sec) and molecular weight (131.5 g/mole) for trichloroethylene can be used as the reference compound.</i></td></tr>
</table>

Parameter	Henry's Law Constant
Units	M^3-atm/mol
SESOIL Variable	H
Description	Dimensional form of Henry's Law constant (m^3-atm/mole), used in Equations (A7), (A11), and (A13) in Appendix A.
Source of Data	Chemical reference literature.

Parameter	Organic Carbon Adsorption Coefficient, K_{oc}
Units	(μg/g)/(μg/ml)
SESOIL Variable	KOC
Description	The adsorption coefficient of the compound on organic carbon. If the adsorption coefficient on the soil K_d, is used, a zero should be entered for organic carbon adsorption coefficient, as it will not be used.
Source of Data	Chemical reference literature.

☞ *Values entered for K_{oc}, soil partition coefficient (K), liquid phase biodegradation rate, and solid phase biodegradation rate are for the uppermost soil layer and are used as a reference point for the other layers. The layer-specific ratios can be specified in the application file (see Section 6.7).*

Parameter	**Distribution Coefficient, K_d**
Units	(µg/g)/(µg/ml)
SESOIL Variable	K
Description	The distribution coefficient of the compound on soil. If a non-zero value is entered for the soil partition coefficient (K_d), SESOIL will use this value as the adsorption coefficient. If a zero is entered for the distribution coefficient, SESOIL will calculate K_d by multiplying the organic carbon adsorption coefficient (K_{oc}) times the soil organic carbon content, (OC in the soil input file) see Appendix A, Section A2.5.4.
Source of Data	Chemical reference literature.

☞ *Adsorption in SESOIL can be represented either by the overall distribution coefficient (K), which is often labeled K_d in the literature, or by the organic carbon:water partitioning coefficient, K_{oc}. If a value for the overall distribution coefficient is unknown, this parameter should be entered as zero. In this case, SESOIL uses the product of K_{oc} and the organic carbon fraction to produce an estimated value for the distribution coefficient (K). If the user enters a measured value for the distribution coefficient, SESOIL will not perform the estimation.*

☞ *Values entered for distribution coefficient (K) and organic carbon adsorption coefficient (K_{OC}) apply to the uppermost soil layer; layer-specific ratios are entered in the application file.*

Parameter	**Molecular Weight**
Units	g/mol
SESOIL Variable	MWT
Description	The molecular weight of the compound.
Source of Data	Chemical reference literature.

☞ *Molecular weight is only used if the complexation or cation exchange algorithms are utilized.*

Parameter	**Valence of the Compound**
Units	g/mol
SESOIL Variable	VAL
Description	The valence of the compound used to calculate cation exchange with soil. A positive integer number should be entered without a sign.
Source of Data	Chemical reference literature.

☞ *VAL is used only if the cation exchange algorithm is used.*

Parameter	**Neutral Hydrolysis Rate Constant**
Units	L/mol/day
SESOIL Variable	KNH
Description	The neutral hydrolysis rate constant (L/mol/day).
Source of Data	Chemical reference literature.

Parameter	**Base Hydrolysis Rate Constant**
Units	L/mol/day
SESOIL Variable	KBH
Description	The base hydrolysis rate constant (L/mol/day).
Source of Data	Chemical reference literature.

Parameter	**Acid Hydrolysis Rate Constant**
Units	l/mol/day
SESOIL Variable	KAH
Description	The acid hydrolysis rate constant (L/mol/day).
Source of Data	Chemical reference literature.

Parameter	**Liquid Phase Biodegradation Rate**
Units	l/day
SESOIL Variable	KDEL

Description	The biodegradation rate of the compound in the liquid phase.
Source of Data	Chemical reference literature.

Parameter	**Solid Phase Biodegradation Rate**
Units	l/day
SESOIL Variable	KDES
Description	The biodegradation rate of the compound in the solid phase.
Source of Data	Chemical reference literature.

Parameter	**Ligand Stability (Dissociation) Constant**
Units	Dimensionless
SESOIL Variable	SK
Description	The stability (dissociation) constant of the compound/ligand complex. A zero should be entered if a ligand compound is not used.
Source of Data	Chemical reference literature.

Parameter	**Moles Ligand per Mole Compound**
Units	Dimensionless
SESOIL Variable	B
Description	The number of moles of ligand per mole of compound complexed. A zero should be entered if a ligand compound is not used.
Source of Data	Chemical reference literature.

Parameter	**Water Diffusion Coefficient**
Units	cm^2/sec
SESOIL Variable	DW
Description	Water diffusion coefficient.
Source of Data	Chemical-specific.
SEVIEW Link	The water diffusion coefficient is not used by SESOIL, however it is passed to AT123D.

Parameter	**Molecular Weight of Ligand**

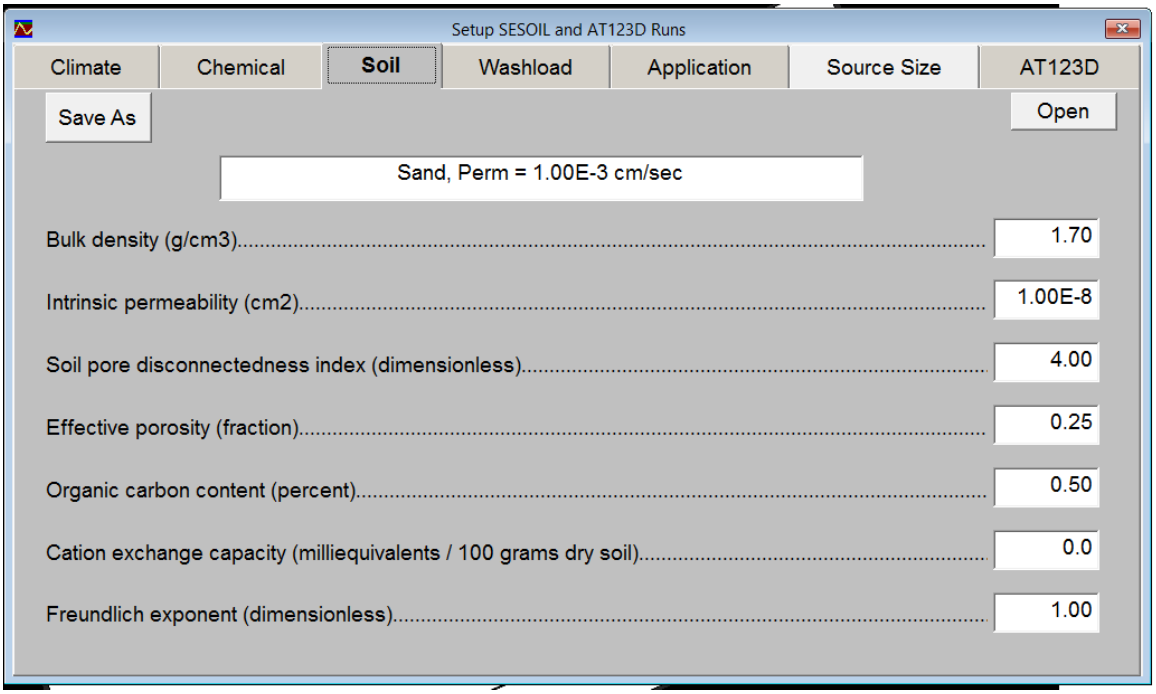
Units	g/mol
SESOIL Variable	MWTLIG
Description	The molecular weight of the ligand (g/mole). A zero should be entered if a ligand compound is not used.
Source of Data	Chemical reference literature.

☞ *Additional processes for handling the binding of a contaminant to soil constituents are included in the cation exchange and complexation options. The molecular weight and valence of the contaminant are used in the cation exchange calculations. Complexation estimation requires the contaminant's molecular weight, the molecular weight of the ligand participating in the complex, the moles of ligand per mole of contaminant in the complex, and the stability constant of the contaminant/ligand complex.*

☞ *Cation exchange and complexation are primarily used for metals. Values for these parameters can be set to zero for most other applications.*

6.5 Soil File Input Parameters

The soil input file specifies information describing the soil properties for a SESOIL column. This information includes: soil bulk density, intrinsic permeability, soil disconnectedness index, effective porosity, organic carbon content, cation exchange capacity and Freundlich exponent. Vertical variation of soil properties for non-uniform soils consisting of 2, 3, or 4 layers is specified in the application file (Section 6.7.2). Variation within the soil column is based on information supplied in the soil file and applied to the uppermost soil layer. A copy of the soil input screen tab and a description of the input parameters are presented below.



Sand, Perm = 1.00E-3 cm/sec

Bulk density (g/cm3)........ 1.70

Intrinsic permeability (cm2)........ 1.00E-8

Soil pore disconnectedness index (dimensionless)........ 4.00

Effective porosity (fraction)........ 0.25

Organic carbon content (percent)........ 0.50

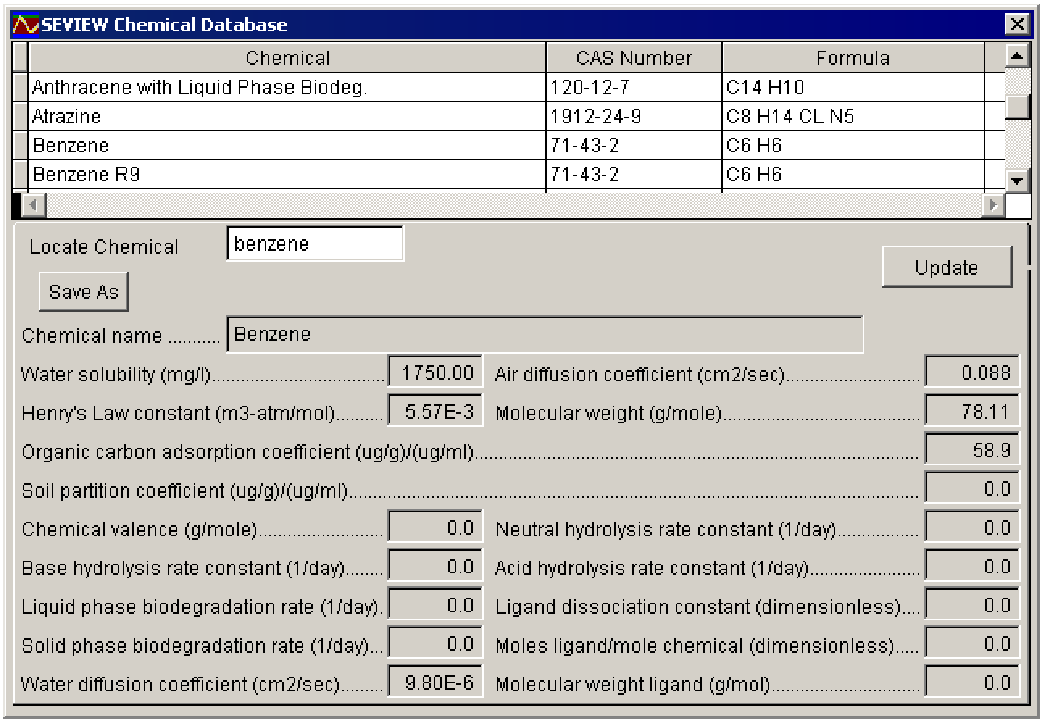
Cation exchange capacity (milliequivalents / 100 grams dry soil)........ 0.0

Freundlich exponent (dimensionless)........ 1.00

☞ *The following parameter descriptions are provided as a guideline for each of the soil parameters used in SESOIL.*

☞ *The following descriptions also apply to the soil database. The soil database is opened by clicking on the* Chemical Database *command displayed in the SESOIL chemical input screen tab. A copy of the soil database screen is presented below.*

I need to replace this figure.



SEVIEW Chemical Database

Chemical	CAS Number	Formula
Anthracene with Liquid Phase Biodeg.	120-12-7	C14 H10
Atrazine	1912-24-9	C8 H14 CL N5
Benzene	71-43-2	C6 H6
Benzene R9	71-43-2	C6 H6

Locate Chemical: benzene

Chemical name .... Benzene

Water solubility (mg/l)........ 1750.00

Air diffusion coefficient (cm2/sec)........ 0.088

Henry's Law constant (m3-atm/mol)........ 5.57E-3

Molecular weight (g/mole)........ 78.11

Organic carbon adsorption coefficient (ug/g)/(ug/ml)........ 58.9

Soil partition coefficient (ug/g)/(ug/ml)........ 0.0

Chemical valence (g/mole)........ 0.0

Neutral hydrolysis rate constant (1/day)........ 0.0

Base hydrolysis rate constant (1/day)........ 0.0

Acid hydrolysis rate constant (1/day)........ 0.0

Liquid phase biodegradation rate (1/day)........ 0.0

Ligand dissociation constant (dimensionless)........ 0.0

Solid phase biodegradation rate (1/day)........ 0.0

Moles ligand/mole chemical (dimensionless)........ 0.0

Water diffusion coefficient (cm2/sec)........ 9.80E-6

Molecular weight ligand (g/mol)........ 0.0

Save As *command and close the database window. If you do not want to update the SESOIL soil file simply close the window.*

Parameter	**Description of Soil Data Set**
SESOIL Variable	TITLE
Description	Description used to identify the soil data set. Limited to a maximum of 48 characters in length.

<table>
<tr><th>Parameter</th><th>Bulk Density</th></tr>
<tr><td>Units</td><td>g/cm^3</td></tr>
<tr><td>SESOIL Variable</td><td>RS</td></tr>
<tr><td>Description</td><td>The average dry soil bulk density (g/cm^3) for the entire soil profile.
Table 2 Typical Soil Bulk Density Values
<table>
<tr><th>Soil Type</th><th>Estimated Bulk Density (g/cm^3)</th></tr>
<tr><td>Sand</td><td>1.18 - 1.58</td></tr>
<tr><td>Silt</td><td>1.29 - 1.80</td></tr>
<tr><td>Clay</td><td>1.40 - 2.20</td></tr>
</table>
</td></tr>
</table>

Source of Data	Geotechnical laboratory analysis or estimated based on soil type.

Parameter	**Intrinsic Permeability**
Units	cm^2
SESOIL Variable	K1
Description	The average soil intrinsic permeability (cm^2) for the entire soil profile. If K1 is zero, then the layer-specific intrinsic permeabilities (K11, K12, K13 and K14) specified in the application data file are used instead.
Source of Data	Field measurements (slug test, pump tests), geotechnical analysis or estimated based on soil type.

Table 3 Default Values For Intrinsic Permeability

(Bonazountas and Wagner, 1984)

USDA Textural Soil Class	Permeability (cm^2)
Clay (very fine)	7.5 X 10^{-11}
Clay (medium fine)	2.5 X 10^{-10}
Clay (fine)	6.0 X 10^{-10}
Silty clay	5.0 X 10^{-11}
Silty clay loam	8.5 X 10^{-11}
Clay loam	6.5 X 10^{-10}
Loam	8.0 X 10^{-10}
Silt loam	3.5 X 10^{-10}
Silt	5.0 X 10^{-11}
Sandy clay	1.5 X 10^{-9}
Sandy clay loam	2.5 X 10^{-9}
Sandy loam	2.0 X 10^{-9}
Loamy sand	5.0 X 10^{-8}
Sand	1.0 X 10^{-8}

☞ ***Caution!*** *The default values for intrinsic permeability may not be appropriate for a given soil or site and should be used with care.*

☞ *SESOIL requires permeability in units of intrinsic permeability in cm^2. Intrinsic permeability can be estimated by multiplying hydraulic conductivity in units of cm/sec by 1.0 X 10^{-5} cm sec.*

☞ *The soil intrinsic permeability (K1) represents the average value for the entire soil column. Intrinsic permeability (K1) should be set to zero in the soil input file, if separate values are entered in the application file, See Section 6.7.2.*

☞ *Intrinsic permeability, soil disconnectedness index, and effective porosity have been found to be sensitive parameters in SESOIL. It is recommended these values be varied to calibrate results to field data at your site (see Appendix A*

Section A2.3.3).

<table>
<tr><th>Parameter</th><th>Soil Pore Disconnectedness Index</th></tr>
<tr><td>Units</td><td>Dimensionless</td></tr>
<tr><td>SESOIL Variable</td><td>C</td></tr>
<tr><td>Description</td><td>The soil pore disconnectedness index for the entire soil profile. Values typically range from 3.7 for sand to 12.0 for fine clay. It relates the soil permeability to the soil moisture content (see Appendix A Section A2.3.3).</td></tr>
<tr><td>Source of Data</td><td>Typically estimated based on soil type.
Table 4 Default Values for Soil Pore Disconnectedness Index (Bonazountas and Wagner, 1984)
<table>
<tr><th>USDA Textural Soil Class</th><th>Soil Pore Disconnectedness Index</th></tr>
<tr><td>Clay (very fine)</td><td>12.0</td></tr>
<tr><td>Clay (medium fine)</td><td>12.0</td></tr>
<tr><td>Clay (fine)</td><td>12.0</td></tr>
<tr><td>Silty clay</td><td>12.0</td></tr>
<tr><td>Silty clay loam</td><td>10.0</td></tr>
<tr><td>Clay loam</td><td>7.5</td></tr>
<tr><td>Loam</td><td>6.5</td></tr>
<tr><td>Silt loam</td><td>5.5</td></tr>
<tr><td>Silt</td><td>12.0</td></tr>
<tr><td>Sandy clay</td><td>6.0</td></tr>
<tr><td>Sandy clay loam</td><td>4.0</td></tr>
<tr><td>Sandy loam</td><td>4.0</td></tr>
<tr><td>Loamy sand</td><td>3.9</td></tr>
<tr><td>Sand</td><td>3.7</td></tr>
</table>
</td></tr>
</table>

☞ *You should not enter value of less than 3.5 for the soil disconnectedness index.*

Parameter	**Effective Porosity**
Units	Fraction
SESOIL Variable	N
Description	The effective porosity for the entire soil profile (unitless). Effective porosity is defined by Eagleson (1978) as; $N = (1 - s_r)\, n_t$ where:

<table>
<tr>
<td></td>
<td>
<table>
<tr><th>Parameter</th><th>Description</th></tr>
<tr><td>n_t</td><td>Total porosity (volume of voids / total volume)</td></tr>
<tr><td>s_r</td><td>The residual medium saturation (volume of water unmoved by natural forces / volume of voids)</td></tr>
<tr><td>N</td><td>Effective porosity</td></tr>
</table>
Effective porosity should generally have a value that is close to the total porosity, and typically ranges from 0.2 to 0.4.
</td>
</tr>
<tr>
<td>Source of Data</td>
<td>
Typically estimated based on soil type.

Table 5 Default Values for Effective Porosity

(Bonazountas and Wagner, 1984)
<table>
<tr><th>USDA Textural Soil Class</th><th>Effective Porosity</th></tr>
<tr><td>Clay (very fine)</td><td>0.20</td></tr>
<tr><td>Clay (medium fine)</td><td>0.20</td></tr>
<tr><td>Clay (fine)</td><td>0.22</td></tr>
<tr><td>Silty clay</td><td>0.25</td></tr>
<tr><td>Silty clay loam</td><td>0.27</td></tr>
<tr><td>Clay loam</td><td>0.30</td></tr>
<tr><td>Loam</td><td>0.30</td></tr>
<tr><td>Silt loam</td><td>0.35</td></tr>
<tr><td>Silt</td><td>0.27</td></tr>
<tr><td>Sandy clay</td><td>0.24</td></tr>
<tr><td>Sandy clay loam</td><td>0.26</td></tr>
<tr><td>Sandy loam</td><td>0.25</td></tr>
<tr><td>Loamy sand</td><td>0.28</td></tr>
<tr><td>Sand</td><td>0.30</td></tr>
</table>
</td>
</tr>
</table>

Although the default values for effective porosity for low permeability soils presented above seem high, Bonazountas and Wagner (1984) found these values to be appropriate for use in the SESOIL model. However, the values for effective porosity should be used with care.

Parameter	**Organic Carbon Content**
Units	Percent
SESOIL Variable	OC
Description	The organic carbon content of the uppermost soil layer. The relative values of organic carbon content for the lower layers are specified in the application data file.
Source of Data	Geotechnical laboratory analysis.

Parameter	**Cation Exchange Capacity**
Units	MEq/100 grams dry soil
SESOIL Variable	CEC
Description	The cation exchange capacity of the uppermost soil layer. The relative values of the cation exchange capacity for the lower layers are specified in the application data file.
Source of Data	Geotechnical laboratory analysis.

☞ *Unless the user has accounted for the combined effects of cation exchange and sorption, these processes should not be used at the same time.*

Parameter	**Freundlich Exponent**
Units	Dimensionless
SESOIL Variable	FRN
Description	The Freundlich Equation Exponent is used to establish the chemical sorption for the top soil layer (see Appendix A, Equation A8). The relative values of Freundlich Equation Exponent for the lower layers are specified in the application data file.
Source of Data	Values of Freundlich Equation Exponent typically range from 0.9 to 1.4. If the value is not known, the default value of 1.0 is recommended.

☞ *Additional soil properties for non-uniform soils are entered in the application file (see Section 6.7.2).*

☞ *Values for bulk density, soil disconnectedness, and effective porosity are specified for the entire soil column. A separate intrinsic permeability can be specified for each layer in the application file Section 6.7.2 (to do this, intrinsic permeability in the soil file must be set to zero). Also, values for organic carbon content, the cation exchange capacity, and the Freundlich exponent may be varied between soil layers by specifying ratios in the application file.*

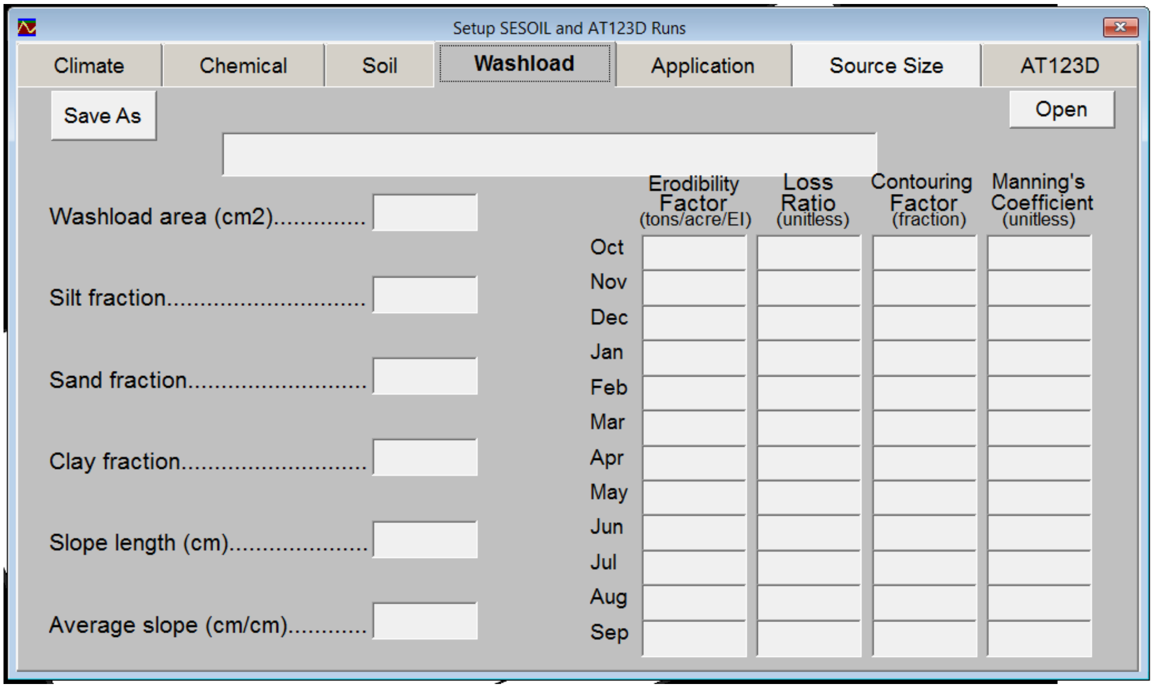
☞ *If separate intrinsic permeabilities are entered in the application file (see Section 6.7.2), a depth weighted average value is calculated for the hydrologic cycle (see Appendix A, Equation (3)). However, the individual values for intrinsic permeability are used for each layer in the pollutant cycle (see Appendix A, Section A2.5.2).*

☞ *The bulk density, intrinsic permeability, and effective porosity are all interrelated* *parameters, yet only the intrinsic permeability can be varied from one layer to the next. Thus, if varying intrinsic permeabilities are used in the application file, the bulk density and effective porosity may not be appropriate for the resultant average permeability (see Equation A3).*

6.6 Washload File Input Parameters

The washload option is rarely if ever used and is typically left blank.

The washload file contains data used by SESOIL to calculate washload transport (the removal of the contaminant adsorbed to eroding soil particles). If you do not wish to simulate washload, you do not need to create the washload file, as this is an optional process.



Note that surface runoff, in which a dissolved contaminant may be transported as part of overland flow of rainwater, is simulated by SESOIL as part of the pollutant cycle only if the index of pollutant transport in surface runoff (ISRM in the application file) does not equal zero. Chemicals with high adsorption coefficients are likely to be transported as part of the eroding soil. A good introductory application may be found in Hetrick & Travis (1988).

Parameter	**Description of the Washload Data Set**
SESOIL Variable	TITLE
Description	Description used to identify the washload data set. Limited to a maximum of 48 characters in length.

Parameters	**Washload Area**
Units	cm^2
SESOIL Variable	AWR
Description	Area of the washload. The washload area should be equal to or less than the application area of the soil column (AR in the application file).
Source of Data	Estimated based on site characteristics.

☞ *The washload area (AWR in the washload file) refers to a patch of topsoil subject to erosion. The areal extent of this patch can be smaller than or equal to the application area for the soil column (AR in the application file). The silt, sand, and clay fractions refer to the layer of topsoil. This topsoil specified in the washload file need not have the same properties as the upper layer of soil of the soil column. The washload option also requires information concerning the land over which the surface runoff and the washload will travel, including the length of the slope between the washload area and a barrier or sink into which the runoff will drain, and the average slope of the land.*

Parameters	**Silt Fraction**
Units	fraction
SESOIL Variable	SLT
Description	The fraction of silt in the washload topsoil.
Source of Data	Estimated based on site characteristics.

Parameters	**Sand Fraction**
Units	fraction
SESOIL Variable	SND
Description	The fraction of sand in the washload topsoil.
Source of Data	Estimated based on site characteristics.

Parameters	**Clay Fraction**
Units	fraction
SESOIL Variable	CLY
Description	The fraction of clay in the washload topsoil.
Source of Data	Estimated based on site characteristics.

☞ *The sum of silt, sand and clay fractions must add up to 1.0.*

Parameters	**Slope Length**
Units	cm
SESOIL Variable	SLEN
Description	The slope length (length of travel) of the representative overland flow profile.
Source of Data	Estimated based on site characteristics.

Parameters	**Land Slope**
Units	cm/cm
SESOIL Variable	SLP
Description	The average slope over the representative overland flow profile.
Source of Data	Estimated based on site characteristics.

Parameters	**Soil Erodibility Factor**
Units	*tons/acre/English EI*
SESOIL Variable	KSOIL
Description	The soil erosion (erodibility) factor (tons/acre/English EI) used in the Universal Soil Loss Equation. This value typically ranges from 0.03 to 0.69; the default value is 0.23.
Source of Data	Estimated based on site characteristics.

Parameters	**Soil Loss Ratio**
Units	unitless
SESOIL Variable	CFACT

Description	The soil loss ratio used in the Universal Soil Loss Equation. The ratio depends on the type of ground cover and land management practices. Typical values range from 0.0001 (well managed land) to 0.94 (tilled soil). The default value of the soil loss ratio is 0.26.
Source of Data	Estimated based on site characteristics.

Parameters	**Contouring Factor**
Units	fraction
SESOIL Variable	PFACT
Description	The contouring factor for agricultural land. Typical contouring factors range from 0.1 (extensive practices) to 1.0 (no supporting practice). The default contouring factor value is 1.0.
Source of Data	Estimated based on site characteristics.

Parameters	**Manning's Coefficient**
Units	unitless
SESOIL Variable	NFACT
Description	Manning's coefficient for overland flow as used in the Universal Soil Loss Equation. This value typically ranges from 0.01 to 0.40; the default value is 0.03.
Source of Data	Estimated based on site characteristics.

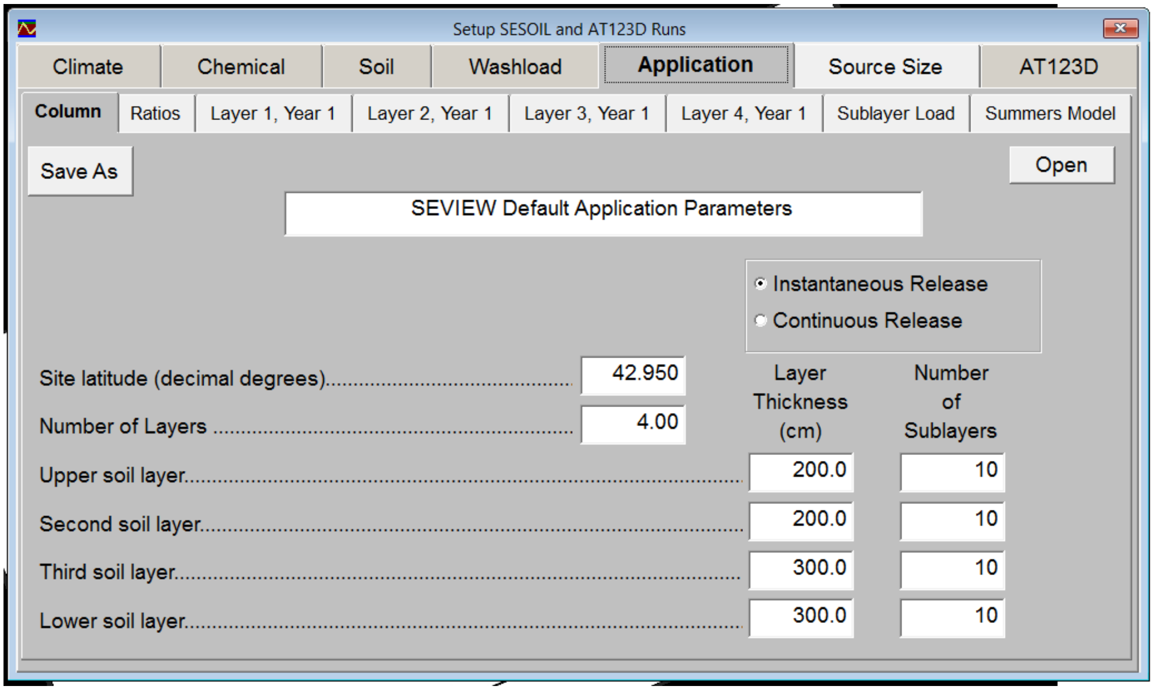
☞ *Examples of the washload parameters can be found in the CREMS model documentation (Knisel, 1980; Foster et al., 1980).*

☞ *If only one year of washload data is entered, it will be used to generate the remaining years. If the number of years of available data is less than the number of years specified for the SESOIL run, the model will automatically use the last year of available data for all remaining years of the simulation.*

6.7 Application File Input Parameters

The application file contains information describing the amount of contaminant released or applied to the soil column. The application file also includes specifications regarding the dimensions of the soil column, the thickness of the soil layers, and additional soil properties beyond those specified in the soil input file (e.g., pH). Vertical variation in soil properties are established as the ratio of the information contained in the soil and chemical files that apply to the uppermost layer.

The user can tailor the application data for a particular site. Several years of chemical loading data may be entered into the soil column or the user may provide one year of data and specify that this year of data is to be used for all remaining years of the simulation. A description of the application input parameters is presented below.



SEVIEW Default Application Parameters

● Instantaneous Release
○ Continuous Release

Site latitude (decimal degrees)........ 42.950
Number of Layers 4.00

	Layer Thickness (cm)	Number of Sublayers
Upper soil layer........	200.0	10
Second soil layer........	200.0	10
Third soil layer........	300.0	10
Lower soil layer........	300.0	10

6.7.1 Column Parameters

Parameter	**Description of the Application Data Set**
SESOIL Variable	TITLE
Description	Description used to identify the application data set. Limited to a maximum of 48 characters in length.

Parameter	**Latitude of Site**

Units	decimal degrees
SESOIL Variable	L
Description	The latitude of the site in decimal degrees. Latitude is used along with the climate parameters of temperature, relative humidity, short wave albedo and percent cloud cover to calculate evapotranspiration.
Source of Data	Set by the latitude of the climate station selected in the climate database. Will revert to 0.0 if a climate file is opened.

☞ *The latitude of the site is used in the calculation of potential solar radiation.*

Parameter	**Continuous / Instantaneous Release (Spill Index)**
Units	unitless
SESOIL Variable	ISPILL
Description	Indicates if a contaminant load is instantaneous or a continuous load over each month. Set the spill index to 1 to model an instantaneous spill occurring at the beginning of the month. Set the spill index to 0 for a continuous loading rate occurring throughout the month.
Source of Data	Site-specific

☞ *If the spill index is to zero, then the monthly load is applied continuously in 30 equal parts, representing the 30 daily time steps of the month. If the spill index is set to 1, the load is applied in the first time step (day) of the month. See Appendix A, Section A2.5.2 for more details.*

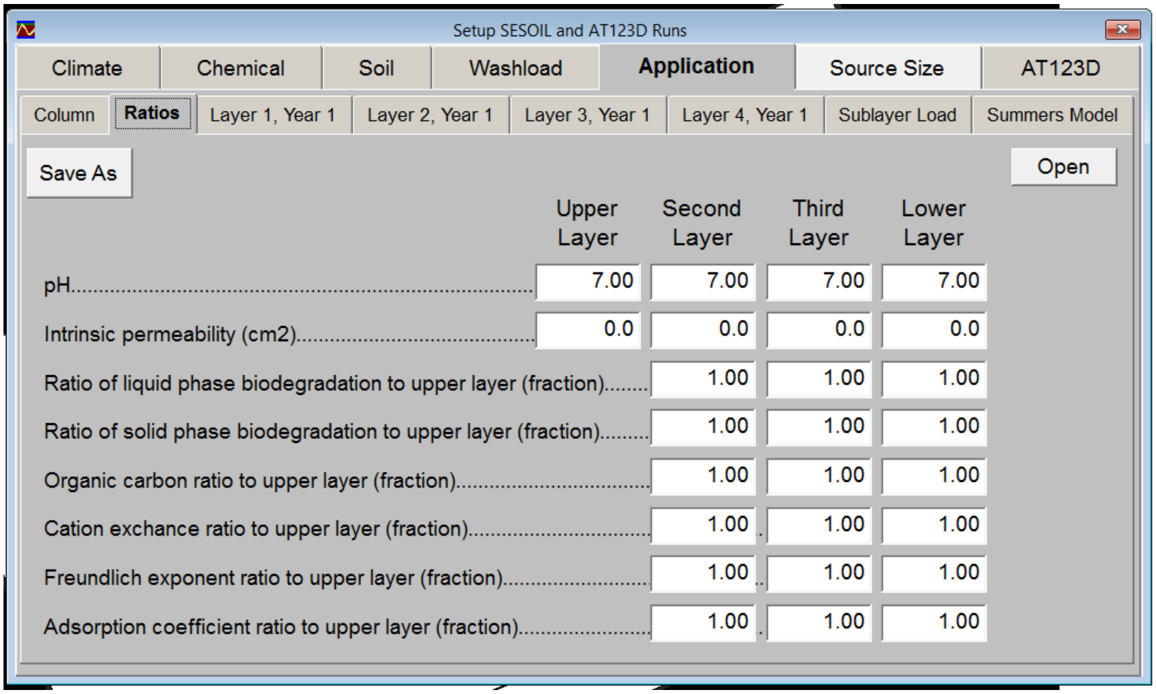
☞ *SESOIL allows the user to specify either continuous or instantaneous release, as discussed above. Instantaneous releases assume that the total mass is loaded during the first day of the month, and can be used to simulate a spill load. However, this option applies only to the first layer. The continuous load (where the load is divided into 30 daily loads, for each month) is always used for layers 2, 3, and/or 4 even if the spill index is set to 1. See Appendix A, Section A2.5.2 for more details.*

Parameter	**Number of Soil Layers**
Units	unitless
SESOIL Variable	ILYS
Description	Establishes the number of soil layers in SESOIL. The number of layers can be set from 2 to 4.
Source of Data	Site-specific.

Parameters	**Layer Thickness**
Units	cm
SESOIL Variables	D1, D2, D3 and D4
Description	Thickness of the SESOIL layers.
Source of Data	Site-specific

Parameters	**Number of Sub-Layers per Layer**
Units	Unitless
SESOIL Variables	NSUB1, NSUB2, NSUB3 and NSUB4
Description	The number of sub-layers in each SESOIL layer. The number of sub-layers can be set from 1 to 10. SESOIL will divide each layer into the appropriate number of sub-layers of equal thickness. Each sub-layer will have the same properties as the layer in it resides.
Source of Data	Site-specific

6.7.2 Ratio Parameters



	Upper Layer	Second Layer	Third Layer	Lower Layer
pH	7.00	7.00	7.00	7.00
Intrinsic permeability (cm2)	0.0	0.0	0.0	0.0
Ratio of liquid phase biodegradation to upper layer (fraction)		1.00	1.00	1.00
Ratio of solid phase biodegradation to upper layer (fraction)		1.00	1.00	1.00
Organic carbon ratio to upper layer (fraction)		1.00	1.00	1.00
Cation exchance ratio to upper layer (fraction)		1.00	1.00	1.00
Freundlich exponent ratio to upper layer (fraction)		1.00	1.00	1.00
Adsorption coefficient ratio to upper layer (fraction)		1.00	1.00	1.00

Parameters	**pH of each Layer**
Units	pH
SESOIL Variables	PH1, PH2, PH3 and PH4

Description	The pH of each SESOIL soil layer.
Source of Data	Geotechnical laboratory analysis.

☞ *The pH parameter is only used if the hydrolysis algorithm is utilized. Thus, if neutral hydrolysis, acid hydrolysis and base hydrolysis rates are set to zero in the chemical input file, you can ignore the pH values for the layers.*

Parameters	**Intrinsic Permeability**
Units	cm^2
SESOIL Variables	K11, K12, K13 and K14
Description	The intrinsic permeability for each SESOIL layer.
Source of Data	Field measurements (slug test, pump tests), geotechnical analysis or estimated based on soil type.

☞ *The intrinsic permeability (K1 in the soil file) must be set to zero, for the varying intrinsic permeabilities entered in the application data to be used. If the intrinsic permeability in the soil data is not zero then the varying intrinsic permeabilities entered in the application data are ignored, and should be set to zero. Refer to Appendix A, Sections A2.3, A2.5.2, and A2.5.9 for a description regarding the uses of permeabilities in SESOIL.*

Parameters	**Ratio of liquid phase biodegradation to upper layer**
Units	fraction
SESOIL Variables	KDEL2, KDEL3 and KDEL4
Description	The ratio of liquid phase biodegradation between the upper soil layer (KDEL in the chemical data) and the lower layers.
Source of Data	Geotechnical analysis or estimated based on site characteristics.

☞ *For most model runs, the user will use 1.0 for the layer ratios of liquid phase biodegradation, solid phase biodegradation, organic carbon content, cation exchange capacity and Freundlich exponent.*

Parameters	**Ratio of solid phase biodegradation to upper layer**
Units	fraction
SESOIL Variables	KDES2, KDES3 and KDES4
Description	The ratio of solid phase biodegradation between the upper soil layer (KDES in the chemical data) and the lower layers.
Source of Data	Geotechnical analysis or estimated based on site characteristics.

☞ *For example, the liquid phase biodegradation in layer 2 is computed as KDEL2 x KDEL where KDEL is input in the chemical file.*

Parameters	**Organic carbon ratio to upper layer**
Units	fraction
SESOIL Variables	OC2, OC3 and OC4
Description	The ratio of the organic carbon content between the upper soil layer (OC in the soil data) and the lower layers.
Source of Data	Geotechnical analysis or estimated based on site characteristics.

☞ *The organic carbon ratios are only used if the soil partition coefficient (K in the chemical file) is set to zero. This causes SESOIL to compute soil the partition coefficient using the organic carbon adsorption coefficient (KOC from the chemical data) and the organic carbon content (OC from the soil file or the ratios in the application data).*

☞ *The organic carbon content of native soil typically decreases with depth.*

Parameters	**Cation exchange ratios to upper layer**
Units	fraction
SESOIL Variables	CEC2, CEC3 and CEC4
Description	The ratio of the cation exchange capacity between the upper soil layer (CEC in the soil data) and the lower layers.
Source of Data	Geotechnical analysis or estimated based on site characteristics.

Parameters	**Freundlich exponent ratio to upper layer**
Units	fraction
SESOIL Variables	FRN2, FRN3 and FRN4
Description	The ratio of the Freundlich exponent between the upper soil layer (FRN in the soil data) and the lower layers.
Source of Data	Geotechnical analysis or estimated based on site characteristics.

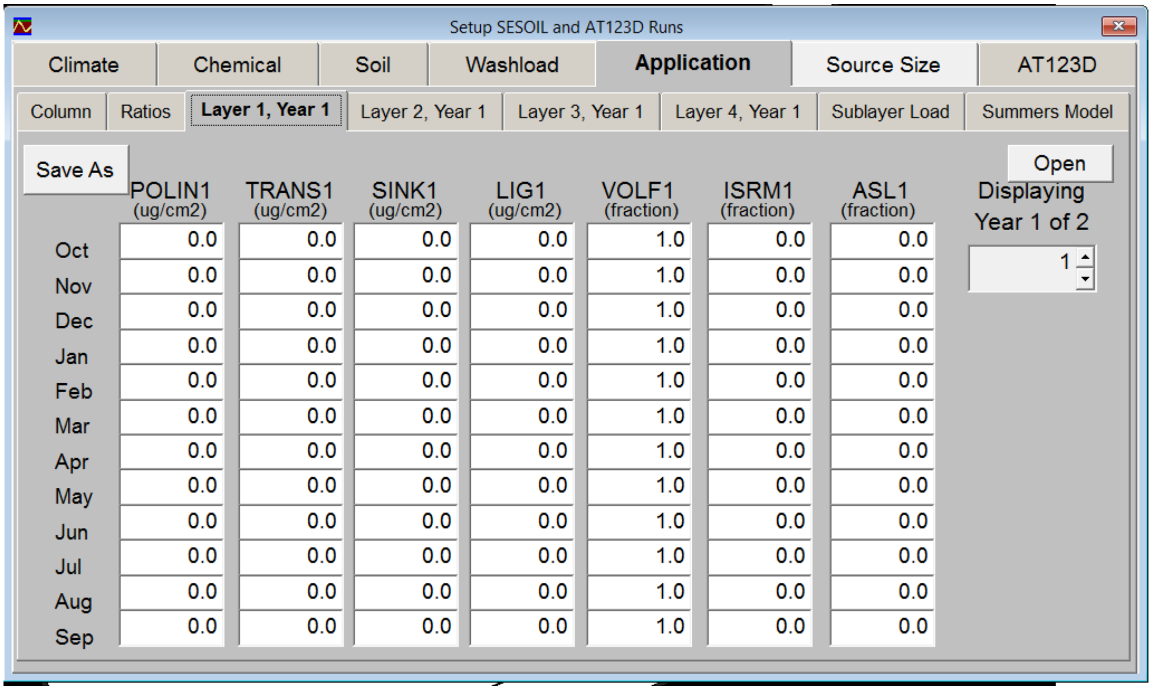
☞ *For example, the Freundlich exponent layer 2 is computed as FRN2 x FRN where FRN is input in the soil file.*

Parameters	**Adsorption coefficient ratio to upper layer**
Units	fraction
SESOIL Variables	ADS2, ADS3 and ADS4

Description	The ratio of the adsorption coefficient between the upper soil layer and the soil partition coefficient (K in the chemical data) and the lower layers.
Source of Data	Geotechnical analysis or estimated based on site characteristics.

If the organic carbon adsorption coefficient (KOC from the chemical file) is used, the adsorption ratios (ADS2, ADS3 and ADS4) should be set to 1.0 since organic carbon adsorption coefficient (K_{oc}) does not change. The calculated soil partition coefficient (K_d) is dependent on the organic carbon content (see OC2, OC3, and OC4 above). If K_d (K from the chemical file) is used, the values can be varied with the ratios ADS2 ADS3, and ADS4.

6.7.3 Contaminant Load Parameters



Displaying Year 1 of 2

1

	POLIN1 (ug/cm2)	TRANS1 (ug/cm2)	SINK1 (ug/cm2)	LIG1 (ug/cm2)	VOLF1 (fraction)	ISRM1 (fraction)	ASL1 (fraction)
Oct	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Nov	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Dec	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Jan	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Feb	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Mar	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Apr	0.0	0.0	0.0	0.0	1.0	0.0	0.0
May	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Jun	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Jul	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Aug	0.0	0.0	0.0	0.0	1.0	0.0	0.0
Sep	0.0	0.0	0.0	0.0	1.0	0.0	0.0

Parameters	**Contaminant Load (POLIN)**
Units	µg/cm^2/month
SESOIL Variables	POLIN# # indicates the layer number
Description	The monthly contaminant load (mass per unit area) entering the top of each soil layer. If an initial soil-sorbed concentration is desired, a contaminant load may be applied at the beginning of the first month of the first year to create the initial condition. The contaminant load is calculated using the following equation:

<table>
<tr><td></td><td>

$$POLIN = CONC \times D \times RS$$

where:

<table>
<tr><th>Parameter</th><th>Description</th></tr>
<tr><td>$POLIN$</td><td>The contaminant load to apply in μg/cm^2/month,</td></tr>
<tr><td>$CONC$</td><td>The concentration sorbed to the soil in μg/g (ppm),</td></tr>
<tr><td>D</td><td>The thickness of the layer in centimeters which the contaminant is applied (D1, D2, D3 and D4), and</td></tr>
<tr><td>RS</td><td>The soil bulk density of the soil in g/cm^3.</td></tr>
</table>

</td></tr>
<tr><td>Source of Data</td><td>Geotechnical analysis or estimated based on site characteristics.</td></tr>
</table>

☞ ***The sub-layer concentration load option is typically used instead.***

☞ *Contaminant loads in each layer are applied to the uppermost sub-layer.*

☞ *Although each sub-layer has the same soil properties as the major soil layer in which they reside, the resulting chemical concentrations in each sub-layer will be different.*

☞ *SESOIL requires that data on contaminant release be expressed as a monthly load. This loading may enter into any of the soil layers, or may enter the uppermost layer via rainfall. When a layer is broken into sub-layers, SESOIL assumes that the chemical loading enters the top sub-layer and is immediately spread throughout this sub-layer. If a layer has only one sub-layer the load is immediately spread throughout the entire layer.*

☞ *See Appendix A, Section A2.5.2 for an explanation of how the contaminant depth is computed after the contaminant is loaded into a sub-layer.*

☞ *If the spill index (ISPILL) is zero, the monthly load is released in 30 equal portions for each day of the month. If the spill index is set to 1, the entire monthly load is released during the first day of the month. See Section A2.5.2 for additional information on the release rates.*

Parameters	**Mass of Contaminant Transformed (TRANS)**
Units	μg/cm^2/month
SESOIL Variables	TRANS# # indicates the layer number
Description	The monthly mass of contaminant transformed in each layer by a process not otherwise included in SESOIL.
Source of Data	Site measurements or estimated based on site characteristics.

☞ *The parameters for contaminant transformed and contaminant removed (TRANS# and SINK#) are means for the user to incorporate transformation and* *transport processes not specifically included in the SESOIL program. These parameters may be specified for each of the soil layers.*

Parameters	**Mass of Contaminant Removed (SINK)**
Units	µg/cm^2/month
SESOIL Variables	SINK# # indicates the layer number
Description	The monthly mass of contaminant removed from each layer by a process not otherwise included in SESOIL. An example could include an estimated of the amount of chemical lost from the soil column due to lateral flow.
Source of Data	Site measurements or estimated based on site characteristics.

Parameters	**Ligand Load (LIG)**
Units	µg/cm^2/month
SESOIL Variables	LIG# # indicates the layer number
Description	The monthly ligand load input into each layer.
Source of Data	Site measurements or estimated based on site characteristics.

☞ *When simulating a contaminant which undergoes complexation, the user must also provide a loading rate for the ligand which becomes part of the complex (LIG#).*

Parameters	**Volatilization / Diffusion Index (VOLF)**
Units	fraction
SESOIL Variables	VOLF# # indicates the layer number
Description	The index of volatilization/diffusion upward from a soil layer. Values range from 0.0 to 1.0. A volatilization index of 0.0 means there will be no volatilization/diffusion upward from the soil layer. A volatilization index of 1.0 means 100 percent of the estimated volatilization/diffusion will simulated for the soil layer. A volatilization index of 0.5 specifies that 50 percent of the estimated volatilization/diffusion will be simulated from the soil layer. See Appendix A, Section A2.5.3 for additional information on volatilization.
Source of Data	Site measurements or estimated based on site characteristics.

Parameters	**Index of Contaminant Transport in Surface Runoff (ISRM)**
Units	fraction
SESOIL Variable	ISRM
Description	The index for contaminant transport in surface runoff. Index values

	may range from 0.0 to 1.0. ISRM is the ratio of the contaminant concentration in the surface runoff to the dissolved concentration in the top sub-layer of the top soil layer. A contaminant transport index of 0.0 means no contaminant transport will occur in the surface runoff. A contaminant transport index of 0.40 specifies that the contaminant concentration in surface runoff is 0.40 times the concentration in the soil moisture of the top soil sub-layer. A contaminant transport index of 1.0 establishes a one to one ratio between the contaminant concentration in surface runoff and soil moisture in the top sub-layer (see the Washload data and Appendix A, Section A2.5.7 for additional information).
Source of Data	Estimated based on site characteristics.

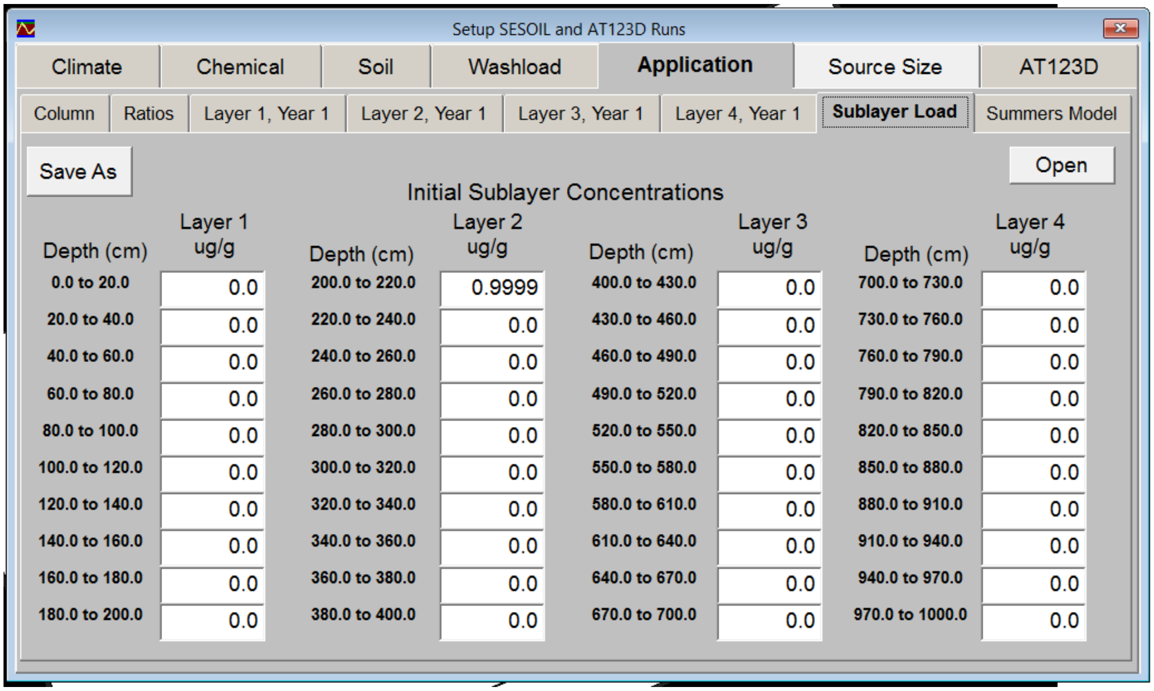
Parameters	**Ratio of Contaminant Concentration in Rain to Water Solubility (ASL)**
Units	fraction
SESOIL Variable	ASL
Description	Contaminant load contained in the monthly precipitation. The load is determined by the ratio of the contaminant concentration in precipitation to the contaminant's maximum solubility in water. The contaminant load to the top soil layer is determined by the contaminant concentration ratio (ASL) multiplied by the water solubility (SL in the chemical data) and the infiltration rate computed by the hydrologic cycle.
Source of Data	Estimated based on site characteristics.

☞ *SESOIL 7.3 was modified to simulate up to 999 years of contaminant load.*

☞ *SEVIEW displays two years of application data. This was done as SESOIL uses the last year of data for all subsequent years of the simulation. Since contaminant load is typically applied for the first month of the first year using this approach no additional contaminant load is applied in the second year and so on.*

☞ *If the organic carbon adsorption coefficient (KOC from the chemical file) is used, the adsorption ratios (ADS2, ADS3 and ADS4) should be set to 1.0 since organic carbon adsorption coefficient (K_{oc}) does not change. The calculated soil partition coefficient (K_d) is dependent on the organic carbon content (see OC2, OC3, and OC4 above). If K_d (K from the chemical file) is used, the values can be varied with the ratios ADS2 ADS3, and ADS4.*

6.7.4 Sub-Layer Load Parameters

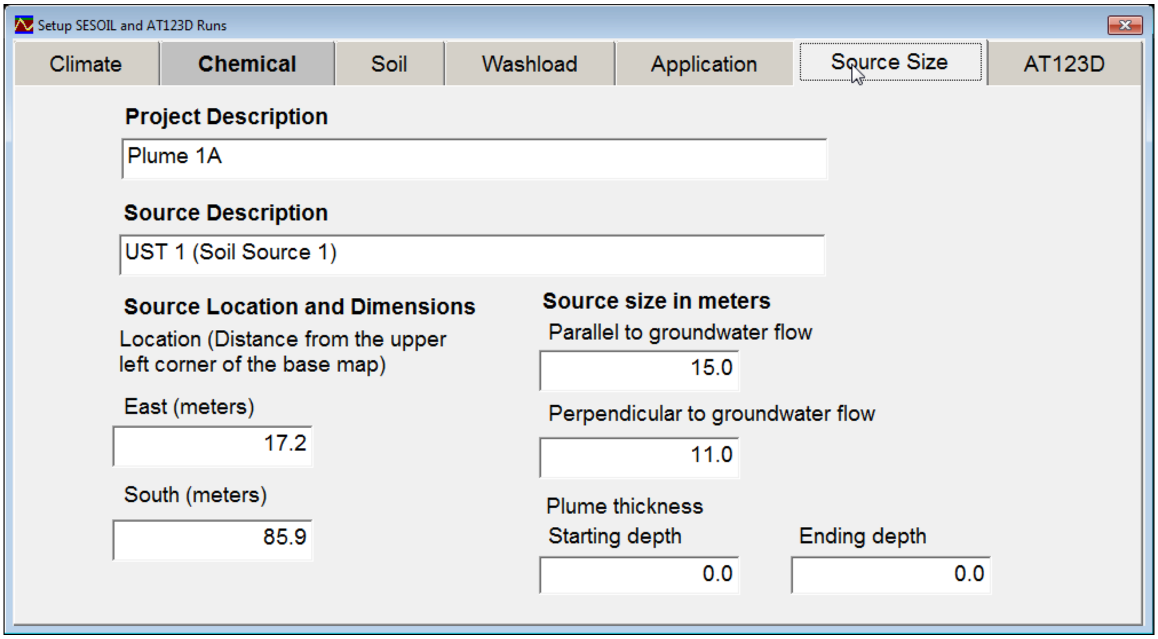


Initial Sublayer Concentrations

Depth (cm)	Layer 1 ug/g	Depth (cm)	Layer 2 ug/g	Depth (cm)	Layer 3 ug/g	Depth (cm)	Layer 4 ug/g
0.0 to 20.0	0.0	200.0 to 220.0	0.9999	400.0 to 430.0	0.0	700.0 to 730.0	0.0
20.0 to 40.0	0.0	220.0 to 240.0	0.0	430.0 to 460.0	0.0	730.0 to 760.0	0.0
40.0 to 60.0	0.0	240.0 to 260.0	0.0	460.0 to 490.0	0.0	760.0 to 790.0	0.0
60.0 to 80.0	0.0	260.0 to 280.0	0.0	490.0 to 520.0	0.0	790.0 to 820.0	0.0
80.0 to 100.0	0.0	280.0 to 300.0	0.0	520.0 to 550.0	0.0	820.0 to 850.0	0.0
100.0 to 120.0	0.0	300.0 to 320.0	0.0	550.0 to 580.0	0.0	850.0 to 880.0	0.0
120.0 to 140.0	0.0	320.0 to 340.0	0.0	580.0 to 610.0	0.0	880.0 to 910.0	0.0
140.0 to 160.0	0.0	340.0 to 360.0	0.0	610.0 to 640.0	0.0	910.0 to 940.0	0.0
160.0 to 180.0	0.0	360.0 to 380.0	0.0	640.0 to 670.0	0.0	940.0 to 970.0	0.0
180.0 to 200.0	0.0	380.0 to 400.0	0.0	670.0 to 700.0	0.0	970.0 to 1000.0	0.0

Parameters	**Contaminant Sub-Layer Load (CONCIN)**
Units	(µg/g)/month
SESOIL Variables	CONCIN### ### indicates the layer and sub-layer numbers
Description	The monthly contaminant load in ppm [(µg/g)/month] for each sub-layer. If an initial soil-sorbed concentration is desired, a contaminant concentration it is applied at the beginning of the first month of the first year to create the initial condition.
Source of Data	Geotechnical analysis or estimated based on site characteristics.

6.7.5 Source Size



Project Description
Plume 1A

Source Description
UST 1 (Soil Source 1)

Source Location and Dimensions
Location (Distance from the upper left corner of the base map)
East (meters): 17.2
South (meters): 85.9

Source size in meters
Parallel to groundwater flow: 15.0
Perpendicular to groundwater flow: 11.0
Plume thickness
Starting depth: 0.0
Ending depth: 0.0

Parameters	**Project Description**
Description	Title of the project displayed on the base map and output results.
Source of Data	Site designations.

Parameters	**Source Description**
Description	Title of the source description displayed on the base map and output results.
Source of Data	Site designations.

Parameters	**Distance East**
Units	Meters
Description	The distance in meters that the source is from the western (left) edge of the base map.
Source of Data	Site-specific.

Parameters	**Distance South**
Units	Meters
Description	The distance in meters that the source is from the northern (top) edge of the base map.
Source of Data	Site-specific.

Parameters	**Source Width**
Units	Meters

Description	The width of the source trending west and east (left – right) on the base map.
Source of Data	Site-specific.

Parameters	**Source Height**
Units	Meters
Description	The height of the source trending north and south (top – bottom) on the base map.
Source of Data	Site-specific.

Parameter	**Starting Coordinate of the Source in the Z-Direction**
Units	meters
AT123D Variable	RH1
Description	Starting coordinate of the source in the z-direction.
Source of Data	Set to 0.0 for both SESOIL and AT123D sources.

Parameter	**Ending Coordinate of the Source in the Z-Direction**
Units	meters
AT123D Variable	RH2
Description	Ending coordinate of the source in the z-direction.
Source of Data	Uses the depth value entered in the "Default AT123D Parameters" screen. Typically set to 0.0 for a SESOIL source. Or the thickness of the groundwater plume for a AT123D source.

☞ *The SESOIL release depth is set by the default AT123D parameter. The AT123D release depth can be entered independently for each source.*

☞ *The AT123D release depth should be set based on the depth of the groundwater plume.*

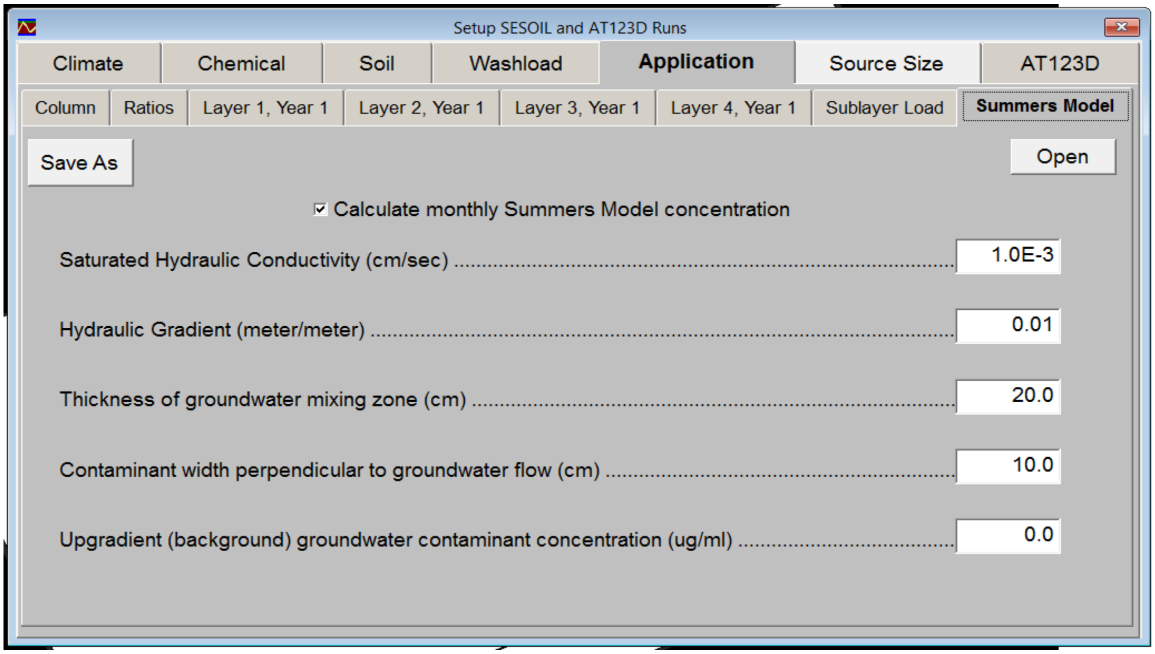
☞

- *Contaminant loads from injection wells can be simulated as a line source in the z-direction. Where the starting and ending coordinates in the z-direction (RH1 and RH2) define the top and bottom of the screened interval of the well.*
- *Contaminant loads from shallow trenches that do not penetrate below the water table may be simulated as a line source in along either the x- or y-axis.*
- *Contaminant loads that do not penetrate very far into the water table can be simulated as a plane source on the surface of the groundwater. This approach should provide a conservative estimate of contaminant concentrations, as limited dilution due to dispersion can occur. Depending*

on load dimensions the user may also establish a line source at the top of the water table, oriented perpendicular to groundwater flow.

- *Contaminant spills that occurred over a relatively short time span may be simulated using an instantaneous source. However, if the user is interested in predicted contaminant concentrations over a relatively short period of time a continuous source may provide better results.*
- *Contaminant sources that are not aligned along the x or y axis can be simulated using the width of the source perpendicular to groundwater flow. As with the other methods the user should try varying contaminant load dimensions to identify the best fit.*
- *Irregularly shaped contaminant loads can be separated into several smaller loads and solved independently. The results must then be summed to establish predicted groundwater concentrations for each time step. As this is a very time-consuming process it should be only utilized for cases where maximum accuracy is called for.*

6.8 SUMMERS Model Parameters



☑ Calculate monthly Summers Model concentration

Saturated Hydraulic Conductivity (cm/sec) 1.0E-3

Hydraulic Gradient (meter/meter) 0.01

Thickness of groundwater mixing zone (cm) 20.0

Contaminant width perpendicular to groundwater flow (cm) 10.0

Upgradient (background) groundwater contaminant concentration (ug/ml) 0.0

The SUMMERS model is not typically used.

<table>
<tr><th>Parameters</th><th colspan="2">Saturated Hydraulic Conductivity (SATCON)</th></tr>
<tr><td>Units</td><td colspan="2">cm/sec</td></tr>
<tr><td>SESOIL Variable</td><td colspan="2">SATCON</td></tr>
<tr><td>Description</td><td colspan="2">Horizontal hydraulic conductivity of the saturated porous medium.</td></tr>
<tr><td rowspan="2">Typical Values</td><td>Clay</td><td>$1\text{x}10^{-6}$ cm/sec</td></tr>
<tr><td>Silt</td><td>$1\text{x}10^{-6}$ - $1\text{x}10^{-3}$ cm/sec</td></tr>
</table>

	Silty sand	$1x10^{-5}$ - $1x10^{-1}$ cm/sec
	Clean gravel	$1x10^{-3}$ - 1 cm/sec
	Gravel	> 1 cm/sec
Source of Data	Pump tests or slug tests or estimated values based on soil type.	

Parameters	**Hydraulic Gradient (HYDRA)**
Units	ft/ft
SESOIL Variable	HYDRA
Description	The slope of the potentiometric surface. In unconfined aquifers, this is equivalent to the slope of the water table.
Typical Values	0.0001 - 0.05 ft/ft
Source of Data	Determined from potentiometric surface maps of the static water level data from monitoring wells.

Parameters	**Thickness of Groundwater Mixing Zone (THICKS)**
Units	cm
SESOIL Variable	THICKS
Description	The thickness of the groundwater mixing zone along the z-axis.
Typical Values	1 to 20, Site-specific
Source of Data	Based on site aquifer characteristics or regulatory requirements.

Parameters	**Source Width Perpendicular to Groundwater Flow (WIDTH)**
Units	cm
SESOIL Variable	WIDTH
Description	The width of the contaminant release along the y-axis (perpendicular to groundwater flow).
Typical Values	Site-specific
Source of Data	Based on geometry of the site contamination.

Parameters	**Background Concentration in Groundwater (Summers)**
Units	µg/ml
SESOIL Variable	BACKCA
Description	Background contaminant concentration in groundwater upgradient of the SESOIL load.
Typical Values	1 to 20, Site-specific
Source of Data	Geotechnical analysis or estimated based on site characteristics.

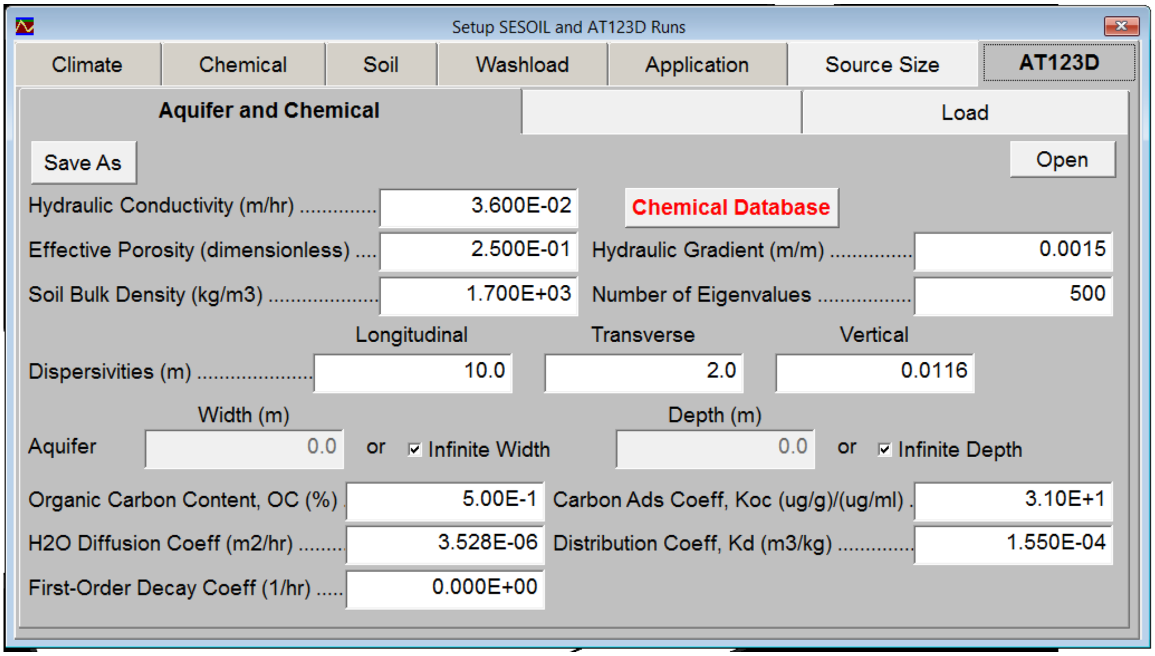
7 AT123D Parameter Specifications

7.1 Introduction

This section provides a detailed description of each AT123D input parameter. The AT123D input file parameters are divided into the **Aquifer, Input and Output** data sets. A description of the input parameters for each section is provided below.

7.2 Aquifer and Chemical Parameters

The AT123D aquifer and chemical parameters contain information describing the aquifer characteristics and geometry. This includes hydraulic conductivity, hydraulic gradient, effective porosity, bulk density longitudinal, transverse and vertical dispersivities, aquifer width and depth, and the number of eigenvalues. It also contains chemical properties of the contaminant.



Hydraulic Conductivity (m/hr) 3.600E-02
Effective Porosity (dimensionless) 2.500E-01
Soil Bulk Density (kg/m3) .... 1.700E+03
Hydraulic Gradient (m/m) 0.0015
Number of Eigenvalues 500
Dispersivities (m) .... Longitudinal 10.0 Transverse 2.0 Vertical 0.0116
Aquifer Width (m) 0.0 or ☑ Infinite Width Depth (m) 0.0 or ☑ Infinite Depth
Organic Carbon Content, OC (%) 5.00E-1
H2O Diffusion Coeff (m2/hr) 3.528E-06
First-Order Decay Coeff (1/hr) ..... 0.000E+00
Carbon Ads Coeff, Koc (ug/g)/(ug/ml) . 3.10E+1
Distribution Coeff, Kd (m3/kg) 1.550E-04

*The following descriptions also apply to the **Establish Default AT123D Input Parameters** window. The **Establish Default AT123D Input Parameters** window is opened by clicking on the **Establish Default AT123D Data** command on the SEVIEW Toolbar.*

*The **Establish Default AT123D Input Parameters** window looks very much like the input screen, except some of the parameters are followed by check boxes. If a check box is not marked, SEVIEW will use the value entered in the parameter when creating an AT123D input file. If a check box is mark, SEVIEW will use the value entered in SESOIL when creating an AT123D input file.*

Parameter	**Hydraulic Conductivity**
Units	meters/hour
AT123D Variable	HCOND
Description	Horizontal hydraulic conductivity of the saturated porous medium.
Typical Values	Clays: $<3.6\times10^{-5}$ m/hr $<1\times10^{-6}$ cm/sec Silts: 3.6×10^{-5} - 3.6×10^{-2} m/hr 1×10^{-6} - 1×10^{-3} cm/sec Silty sands: 3.6×10^{-4} - 3.6 m/hr 1×10^{-5} - 1×10^{-1} cm/sec Clean sands: 3.6×10^{-2} - 36 m/hr 1×10^{-3} - 1 cm/sec Gravels: > 36 m/hr > 1 cm/sec
Source of Data	Pump tests or slug tests or estimated values based on soil type.
SEVIEW Link	Place a ☑ in the **Permeability** check box to use the SESOIL value for permeability. SEVIEW will transfer the soil permeability from the soil input file (K1) or the lowermost permeability in the SESOIL application file if K1 is zero. If the use SESOIL permeability box is not checked the value entered will be used.

☞ *SEVIEW converts the intrinsic permeability used in SESOIL to m/hr prior to transferring the value to AT123D.*

Parameter	**Effective Porosity**
Units	dimensionless
AT123D Variable	POR
Description	Dimensionless ratio of the volume of interconnected voids to the bulk volume of the aquifer matrix. Note that "total porosity" is the ratio of all voids (included non-connected voids) to the bulk volume of the aquifer matrix. Difference between total and effective porosity reflect lithologic controls on pore structure. In unconsolidated sediments coarser than silt size, effective porosity can be less than total porosity by 2-5% (e.g. 0.28 vs., 0.30) (Smith and Wheatcraft, 1993).
Typical Values	Clay 0.01 - 0.20 Silt 0.01 - 0.30 Fine Sand 0.10 - 0.30 Medium Sand 0.15 - 0.30 Coarse Sand 0.20 - 0.35 Gravel 0.10 - 0.35 *(From Wiedemeier, Wilson, et al., 1995; originally from Domenico and Schwartz, 1990 and Walton, 1988).* Sandstone 0.005 - 0.10 Unfract. Limestone 0.001 - 0.05 Fract. Granite 0.00005 - 0.01 *(From Domenico and Schwartz, 1990)* Commonly used value for silts and sands is an effective porosity of 0.25.
Source of Data	Typically estimated based on soil type.

SEVIEW Link	The effective porosity for the SESOIL soil column (N in the SESOIL soil input file) if a ☑ is placed in the **Porosity** check box. If the **SESOIL Porosity** box is not checked the value entered will be used.

Parameter	**Hydraulic Gradient**
Units	meter/meter
AT123D Variable	HGRAD
Description	The slope of the potentiometric surface. In unconfined aquifers, this is equivalent to the slope of the water table. Assumed to be along the longitudinal direction (x-axis)
Typical Values	0.0001 - 0.05 m/m
Source of Data	Determined from potentiometric surface maps of the static water level data from monitoring wells.

Parameter	**Soil Bulk Density**
Units	kilogram/meter^3
AT123D Variable	RHOB
Description	Bulk density of the aquifer matrix.
Typical Values	Typical values for soil bulk density in kilogram/meter^3. Clay 1,400 - 2,200 Silt 1,290 - 1,800 Sand 1,180 - 1,580
Source of Data	Obtained from geotechnical laboratory analysis of soil samples or estimated values based on soil type.
SEVIEW Link	The average dry soil bulk density (g/cm^3) converted to kilogram/meter^3 for the entire soil column (RS in the SESOIL soil input file) if a ☑ is placed in the **Bulk Density** check box. User defined value if a ☐ is placed in the **Bulk Density** check box.

Parameter	**Number of Eigenvalues**
AT123D Variable	NROOT
Description	The number of eigenvalues establishes the maximum number of terms that will be calculated for a series solution before truncation occurs.
Typical Values	Start with 500 and increase it to a 1000 if a warning message is printed out with the solution. The eigenvalues value may not exceed 1000.
SEVIEW Link	The default value is 500.

Parameter	**Longitudinal Dispersivity, α_L** **Transverse Dispersivity, α_T** **Vertical Dispersivity, α_V**
Units	meters
AT123D Variables	AELONG, ATRANV and AVERTI
Description	The process whereby a plume will spread out in a longitudinal direction (along the direction of groundwater flow), transversely (perpendicular to groundwater flow), and vertically downwards due to mechanical mixing in the aquifer and chemical diffusion.
Typical Values	Selection of dispersivity values is a difficult process, given the impracticability of measuring dispersion in the field. Typically estimated based on site characteristics. Methods to establish dispersivities based on contaminant plume length (L_p) are presented below: **Longitudinal Dispersivity (α_L)** $\alpha_L = 0.83 \times \left\{\log_{10}\left(L_p\right)\right\}^{2.414}$ *(Xu & Eckstein, 1995)* Note: L_p is in meters **Transverse Dispersivity (α_T)** $(\alpha_T) = 0.10\ (\alpha_L)$ *Gelhar et al., 1992 in BIOSCREEN, 1996* **Vertical Dispersivity (α_V)** (α_V) = *very low (i.e.* 1×10^{-99} *ft) BIOSCREEN, 1996*
	Other commonly used relationships include: $\alpha_L = 0.1\ L_p$ *(Pickens and Grisak, 1981)* $\alpha_T = 0.33\ \alpha_L$ *(ASTM, 1995) (EPA, 1986)* $\alpha_V = 0.05\ \alpha_L$ *(ASTM, 1995)* $\alpha_V = 0.025\alpha_L$ *to* $0.1\ \alpha_L$ *(EPA, 1986)*
Source of Data	Typically estimated using the relationships provided above.
SEVIEW Link	User defined.

Parameter	**Aquifer Width**
Units	Meters
AT123D Variable	WIDTH
Description	Aquifer width in the y-direction. Note: This value is ignored if the **Infinite Width** ☑ check box is selected.
Source of Data	Site-specific
SEVIEW Link	Default value set by the user.

Parameter	**Infinite Width**
AT123D Variable	IWID
Description	Parameter specification indicating if the aquifer is infinitely wide (y-direction).
Options	☑ - Yes ☐ - No
SEVIEW Link	Default option of ☑ or established by the user.

Parameter	**Aquifer Depth**
Units	meters
AT123D Variable	DEPTH
Description	Aquifer depth in the z-direction from below the water table. Note: This value is ignored if the **Infinite Depth** ☑ check box is selected.
Source of Data	Site-specific
SEVIEW Link	Default value set by the user.

Parameter	**Infinite Depth**
AT123D Variable	IDEP
Description	Parameter specification indicating if the aquifer is infinitely deep (z-direction).
Values	☑ - Yes ☐ - No
SEVIEW Link	Default option of ☑ or established by the user.

☞ *Aquifer boundaries located at infinity are easier to calculate than those of finite width or depth are. Thus, if the aquifer boundaries are relatively large in relation to the size of the source area or if the distance from the source to the area of interest is large, an infinite aquifer along either or both the x- or y- directions may be best.*

Parameter	**Organic Carbon Content, OC**
Units	percent
AT123D Variable	ROC

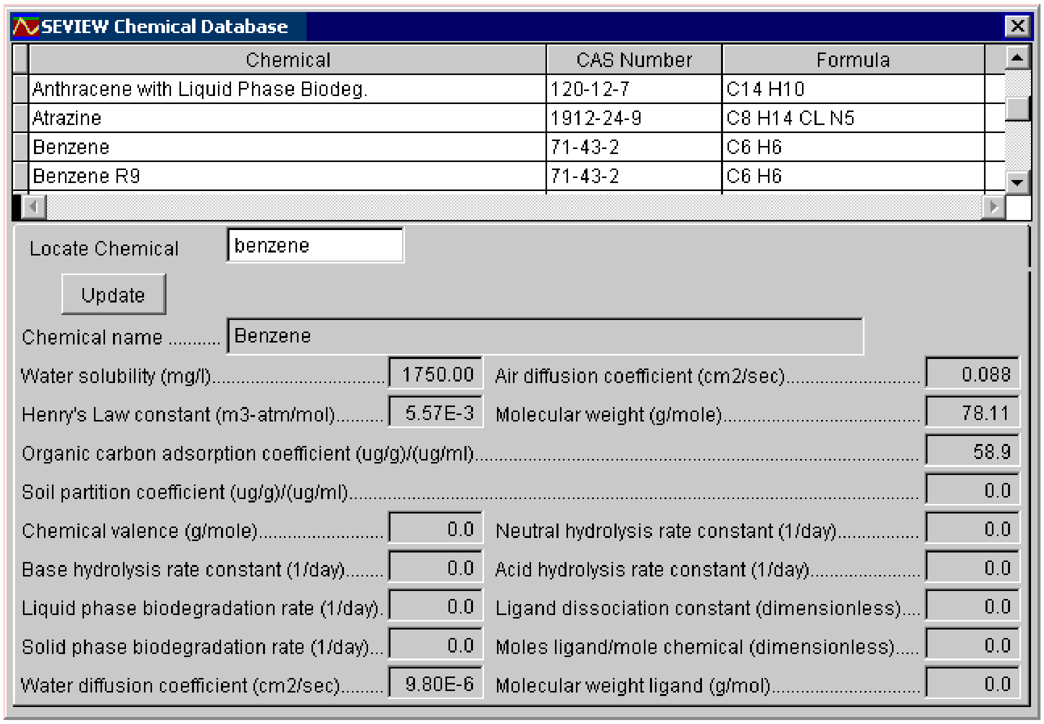
Description	The organic carbon content of the saturated soil.
Source of Data	Geotechnical laboratory analysis.
SEVIEW Link	User defined value if a ☐ is placed in the **Soil Organic Carbon** check box.

Parameter	**Water Diffusion Coefficient Multiplied by Tortuosity**
Units	meters^2/hour
AT123D Variable	AMTAU
Description	Water diffusion coefficient multiplied by tortuosity.
Source of Data	Chemical-specific.

☞ *AT123D was modified to simulate independent chemical parameters in each of the sources.*

☞ *You can select water diffusion coefficient values from the chemical database. The chemical database is opened by clicking on the* Chemical Database *command displayed next to the **Water Diffusion Coefficient** input parameter. The **Water Diffusion Coefficient** parameter is displayed at the lower left. To copy the **Water Diffusion Coefficient** data to the AT123D parameter move to the desired chemical and click on the* Save As *command and close the database window. If you do not want to update the AT123D data simply close the window. A copy of the chemical database screen is presented below.*

SEVIEW converts the water diffusion coefficient in the chemical database from cm^2/second to meters^2/hour as the value is transferred.



Chemical	CAS Number	Formula
Anthracene with Liquid Phase Biodeg.	120-12-7	C14 H10
Atrazine	1912-24-9	C8 H14 CL N5
Benzene	71-43-2	C6 H6
Benzene R9	71-43-2	C6 H6

Locate Chemical: benzene

Chemical name .... Benzene

Water solubility (mg/l)................................	1750.00	Air diffusion coefficient (cm2/sec)...........................	0.088
Henry's Law constant (m3-atm/mol)..........	5.57E-3	Molecular weight (g/mole)..	78.11
Organic carbon adsorption coefficient (ug/g)/(ug/ml)........			58.9
Soil partition coefficient (ug/g)/(ug/ml)........			0.0
Chemical valence (g/mole).........................	0.0	Neutral hydrolysis rate constant (1/day)................	0.0
Base hydrolysis rate constant (1/day)........	0.0	Acid hydrolysis rate constant (1/day)......................	0.0
Liquid phase biodegradation rate (1/day).	0.0	Ligand dissociation constant (dimensionless)....	0.0
Solid phase biodegradation rate (1/day)...	0.0	Moles ligand/mole chemical (dimensionless).....	0.0
Water diffusion coefficient (cm2/sec).........	9.80E-6	Molecular weight ligand (g/mol)............................	0.0

☞ *The water diffusion coefficient was added to the SESOIL version 6.0 chemical input file. Remember, if you use an older version of the chemical file SESOIL 6.0 cannot transfer a water diffusion value to AT123D. Versions 2.1 and 3.0 of SESOIL simply ignore the water diffusion value.*

Parameter	**First-Order Decay Coefficient, λ**
Units	1/hour
AT123D Variable	RAMADA
Description	Coefficient describing first-order decay rate for dissolved constituents.
Typical Values	Chemical-specific
Source of Data	Methods for selection of appropriate decay coefficients include: **Literature Values:** Published references are available listing decay half-life values for hydrolysis and biodegradation (e.g., see Howard *et al.*, 1991). Many references report the half-lives; these values can be converted to the first-order decay coefficients using $k = 0.693/t_{1/2}$. **Calibrate to Existing Plume Data:** If the plume is in a steady-state or diminishing condition, AT123D can be used to determine first-order decay coefficients that best match the observed site concentrations. One may adopt a trial-and-error procedure to derive a best-fit decay coefficient for each contaminant. For still-expanding plumes, this steady-state calibration method may over-estimate actual decay-rate coefficients and contribute to an under-estimation of predicted concentration levels.

SEVIEW Link	The liquid phase biodegradation rate of the compound (KDEL in the SESOIL chemical input file) if a ☑ is entered into the **First-Order Decay** check box. User defined value if a ☐ is placed in the **First-Order Decay** check box.

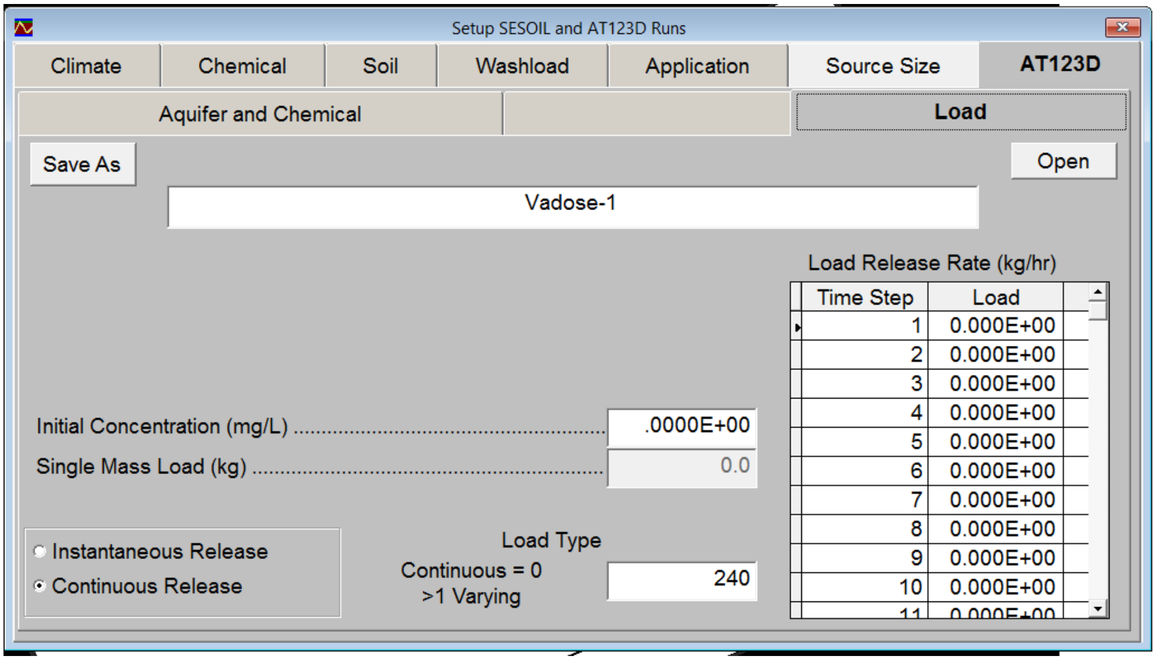
☞ *SEVIEW converts KDEL from units of 1/day to 1/hour prior to transferring the data.*

Parameter	**Organic Carbon Adsorption Coefficient, K_{oc}**
Units	(µg/g)/(µg/ml)
AT123DVariable	RKOC
Description	The adsorption coefficient for the compound on organic carbon.
Source of Data	Chemical reference literature.
SEVIEW Link	User defined value if a ☐ is placed in the **Carbon Adsorption Coeff.** check box.

Parameter	**Distribution Coefficient, K_d**
Units	meters^3/kilogram
AT123D Variable	AKD
Description	Chemical-specific partition coefficient. Calculated by SEVIEW if the percent **Organic Carbon Content** and **Organic Carbon Adsorption Coefficient** are greater than 0.
Typical Values	Chemical-specific and soil organic carbon specific.
SEVIEW Link	Established by SEVIEW as the organic carbon partition coefficient (K_{oc}) value times the fraction organic carbon (foc) in the bottom soil layer if a ☑ is entered into the **Distribution Coeff. (K_{oc} * foc)** check box. User defined value if a ☐ is placed in the **Distribution Coeff. (K_{oc} * foc)** check box.

7.3 AT123D Load Parameters

The AT123D Load Parameters contain information on contaminant load geometry and type of release.



Vadose-1

Initial Concentration (mg/L) .0000E+00

Single Mass Load (kg) 0.0

○ Instantaneous Release

● Continuous Release

Load Type
Continuous = 0
>1 Varying
240

Load Release Rate (kg/hr)

Time Step	Load
1	0.000E+00
2	0.000E+00
3	0.000E+00
4	0.000E+00
5	0.000E+00
6	0.000E+00
7	0.000E+00
8	0.000E+00
9	0.000E+00
10	0.000E+00

Parameter	**AT123D Source Description**
AT123D Variable	TITLE
Description	The title description for the AT123D source.
SEVIEW Link	The text entered in the AT123D source or the first 80 characters of the SESOIL description if a vadose zone source.

Parameter	**Initial Concentration**
Units	mg/L
AT123D Variable	CONC
Description	Used to establish an initial concentration within the contaminated groundwater plume.
Typical Values	Site-specific.

Parameter	**Single Mass Load**
Units	kg/hr
AT123D Variable	Q
Description	Single contaminant load.
Typical Values	Site-specific.

You should not use both the initial concentration and single mass load at the same time.

The single load option is only active if the continuous load option is set to 0.

Parameter	**Model Time Step**
Units	Hours
AT123D Variable	DT
Description	Time step for the model results.
Value	Is set to 730 hours (one month) in SEVIEW 7.3.

Parameter	**Instantaneous / Continuous Release**
Units	Dimensionless
AT123D Variable	INSTAN
Description	Specifies if the release is instantaneous or continuous.
Typical Values	Instantaneous when linked to SESOIL and if the Initial Concentration is used.

Parameter	**Continuous = 0 > Varying**
Units	Dimensionless
AT123D Variable	NSOURS
Description	Specifies the number of individual loads over time.
Typical Values	Length of the SESOIL scenario in months. Set to 0 for a single mass load.

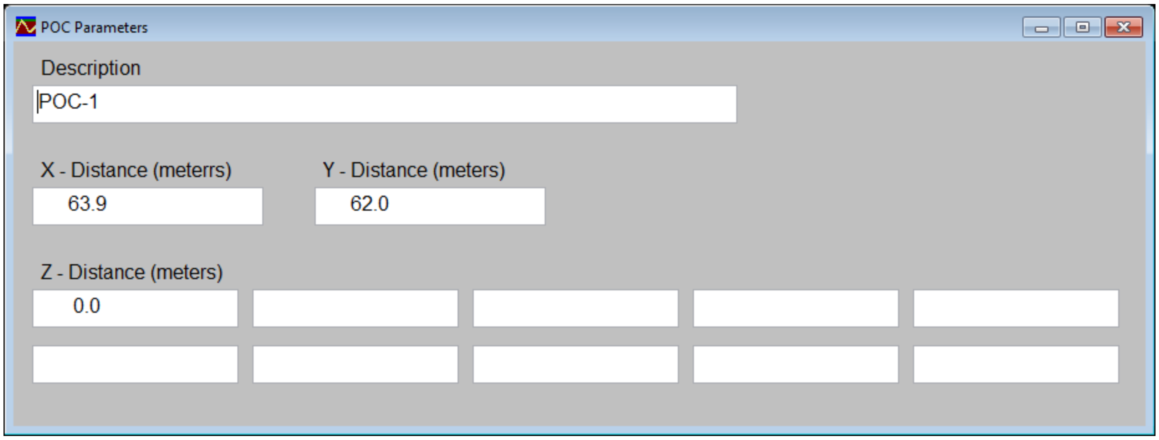
Parameter	**Varying Mass Load Releases**
Units	kg/time step
AT123D Variable	QSA(I)
Description	Varying contaminant mass load for each time step.
Typical Values	Site-specific, used when linked to SESOIL.

☞ *The varying load release rate is only active if the continuous load option is greater than 0.*

☞ *Used when AT123D is linked to SESOIL.*

7.4 AT123D Point of Compliance

The AT123D Point of Compliance parameters contain information on observation well.



Description: POC-1

X - Distance (meterrs): 63.9

Y - Distance (meters): 62.0

Z - Distance (meters): 0.0

Parameter	**POC Description**
AT123D Variable	POCT(I)
Description	The title description for the point of compliance
Source of Data	Description designation of a site monitoring well or piezometer. May also be a description of a point of compliance.

Parameter	**X-Distance**
Units	meters
AT123D Variable	POC(I,1)
Description	X-coordinate of the POC in the x-direction (direction of flow), where a concentration will be determined.
Source of Data	Based on position of the POC relative to the source.

Parameter	**Y-Distance**
Units	meters
AT123D Variable	POC(I,2)
Description	Y-coordinate of the POC in the y-direction (horizontally perpendicular to flow), where a concentration will be determined.
Source of Data	Based on position of the POC relative to the source.

Parameter	**Z-Distance**
Units	Meters
AT123D Variables	POC(I,4 - 13)
Description	Z-coordinate of the POC in the z-direction (vertically perpendicular to flow), where a concentration will be determined.
Source of Data	Based on the screen interval of the monitoring well or piezometer. May also be based on a POC.

☞ *For a POC the SEVIEW version of AT123D produces results at discreet points. SEVIEW then averages the results to produce concentration consistent with a mixing within a sampling well.*

☞ *The feature is only available in the SEVIEW version of AT123D.*

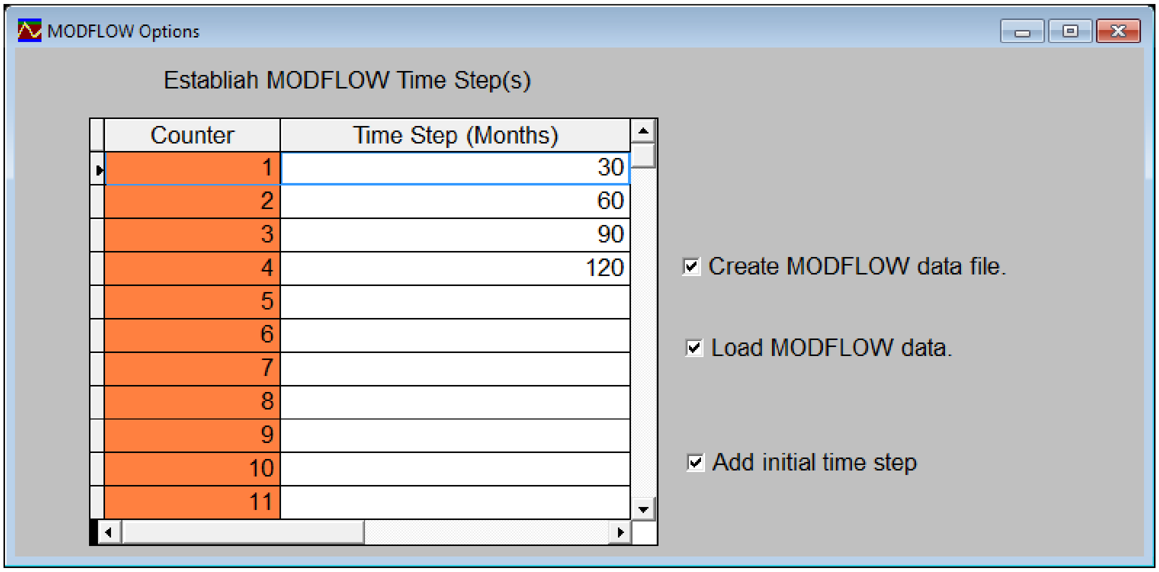
8 MODFLOW Parameter Specifications

8.1 Introduction

This section provides a detailed description of the MODFLOW link parameters. The MODFLOW data was designed to be versatile enough to be used with almost any groundwater model.

8.2 MODFLOW Parameters

These parameters are used to establish the link between SESOIL and MODFLOW.



Establiah MODFLOW Time Step(s)

Counter	Time Step (Months)
1	30
2	60
3	90
4	120
5	
6	
7	
8	
9	
10	
11	

☑ Create MODFLOW data file.

☑ Load MODFLOW data.

☑ Add initial time step

Parameter	**Time Step**
Units	Months
Description	The "Time Step (Months)" data is used to set the length of the time steps to match those in MODFLOW. The number of SESOIL monthly contaminant loads to be combined for each MODFLOW time step. Varying MODFLOW time steps are established by entering varying time step values. For instance entering values of 30, 60, 90 and 120 would produce four MODFLOW time steps. The first would be 30 months long, the second 60 months long, the third would be 90 months long and the forth would be 120 months long. The final time step of 120 months would be used for all subsequent MODFLOW time steps.
Source of Data	User defined in MODFLOW.

☞ *By default SESOIL produces monthly loads to groundwater. However, MODFLOW is not typically run with such short time steps. The "Time Step*

(Months)" values are used to establish the number of monthly SESOIL time steps to be combined for each MODFLOW time step. This means that MODFLOW need not be run using a monthly time step when linked to SESOIL.

Parameter	**Create MODFLOW Data File**
Description	Checking this box will cause SEVIEW to create a data file which can be imported in to MODFLOW. The file will have the same name as the SESOIL output file but with a .DAT extension.

Example MODFLOW *.DAT File.

```
             1        0.000E+00         0.000E+00
             2        1.203E+02         0.000E+00
             3        2.490E+02         8.263E-09
             4        3.777E+02         1.000E-10
             5        2.490E+02         1.000E-10
```

The first column contains the time step number. The second contains the groundwater recharge during the time step. The final column contains the contaminant concentration over the time step.

Parameter	**Load MODFLOW Data**
Description	Checking this box will cause SEVIEW to load MODFLOW data to the clipboard. This data can be pasted in Excel. Clipboard data includes the time step number, length of the time step in days and months, groundwater recharge, mass load to groundwater and the soil leachate concentration.

Example MODFLOW Clipboard Data

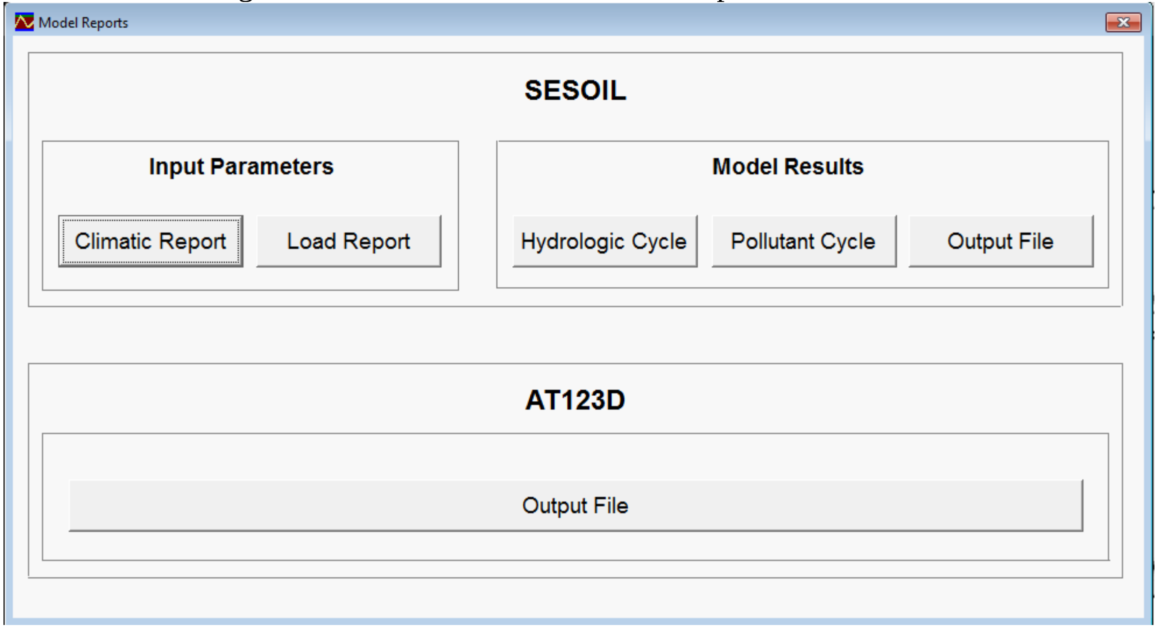
Time Step Number	**Length (months)**	**Length (days)**	**Start Time (days)**	**End Time (days)**	**Recharge (cm)**	**Mass (ug)**	**Concentration (ppm)**
1	0	0	0	0	0.00E+00	0.00E+00	0.00E+00
2	30	912	0	912	1.20E+02	0.00E+00	0.00E+00
3	60	1824	912	2736	2.49E+02	2.06E-01	8.26E-09
4	90	2736	2736	5472	3.78E+02	3.78E-03	1.00E-10
5	120	3648	5472	9120	2.49E+02	2.49E-03	1.00E-10

Parameter	**Add Initial Time Step**
Description	Checking this box will cause SEVIEW to add a short time step without any load to the beginning of the MODFLOW data.

MODFLOW data is created whenever you preview or print a ***SESOIL Pollutant Cycle Report****.*

9 SESOIL Reports

Double click on a green SESOIL source on the base map to view the model results.



In addition to the automated reports, SEVIEW provides access to all monthly SESOIL input and output parameters. This means that results are not limited to predetermined report parameters. Using SEVIEW with your spreadsheet and/or word processing software allows you to present model results that meet your specific requirements. SEVIEW provides you with almost unlimited flexibility in evaluating data contained in the SESOIL output file. As individual projects requirements vary you can use SEVIEW to extract data and create a wide combination of data plots. An overview how SEVIEW works with the SESOIL output is provided below.

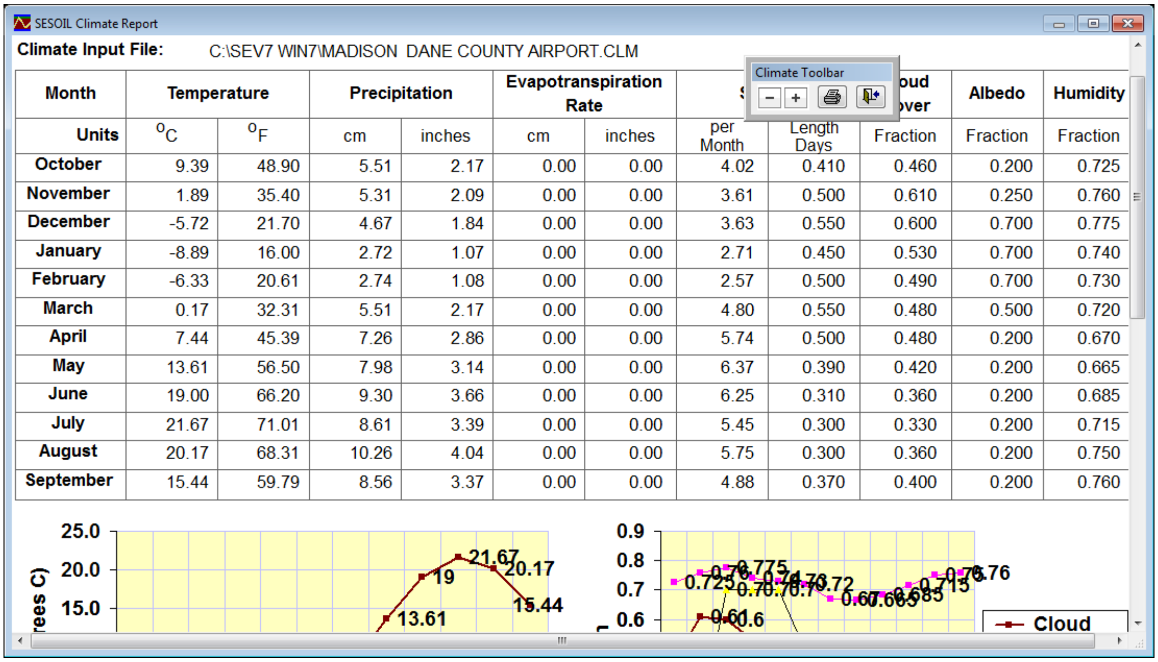
☞ *SESOIL output files can be very large containing over 815 monthly input and output data sets. A single SESOIL output file contains up to 10,000,000 monthly values for a 999 year run!*

9.1 Climate Report

The Climate Report documents the raw climatic data used by the SESOIL model. The data is presented in both a tabulated form and graphically. A description of the climate parameters is contained in Section 6.3.

☞ *These are input parameters and not results of the SESOIL hydrologic cycle.*

☞ *You can print a copy of the report by clicking the print command on the toolbar.*

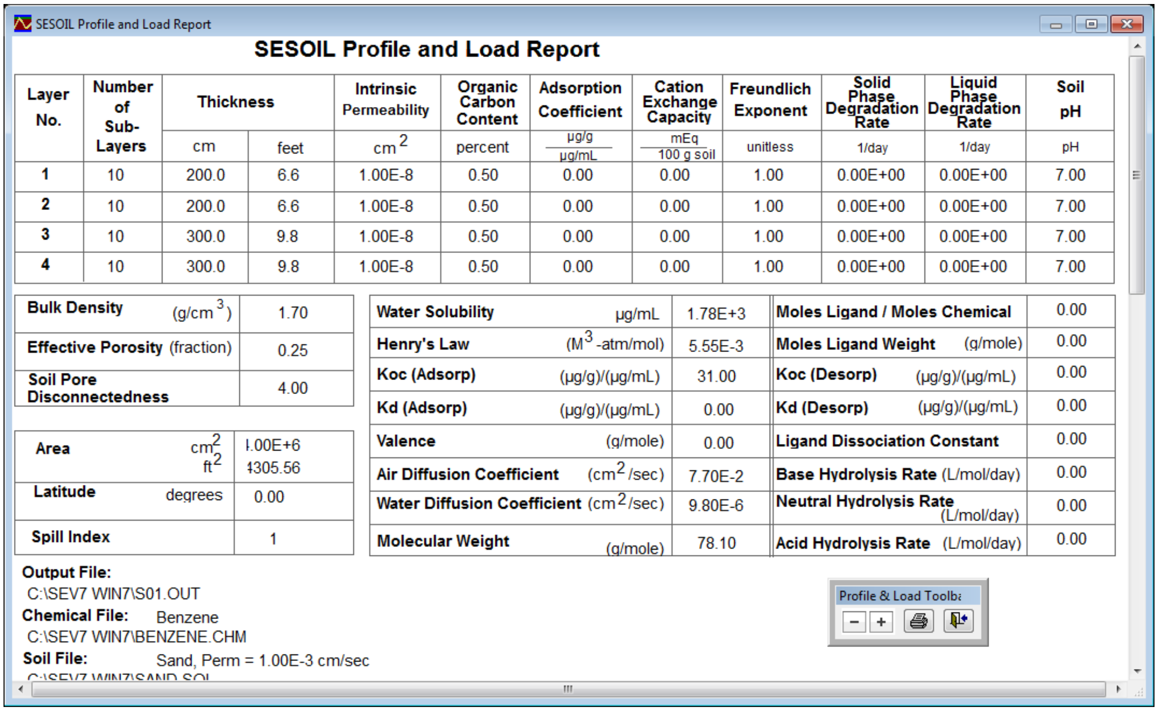


Climate Input File: C:\SEV7 WIN7\MADISON DANE COUNTY AIRPORT.CLM

Month	Temperature		Precipitation		Evapotranspiration Rate				oud over	Albedo	Humidity
Units	°C	°F	cm	inches	cm	inches	per Month	Length Days	Fraction	Fraction	Fraction
October	9.39	48.90	5.51	2.17	0.00	0.00	4.02	0.410	0.460	0.200	0.725
November	1.89	35.40	5.31	2.09	0.00	0.00	3.61	0.500	0.610	0.250	0.760
December	-5.72	21.70	4.67	1.84	0.00	0.00	3.63	0.550	0.600	0.700	0.775
January	-8.89	16.00	2.72	1.07	0.00	0.00	2.71	0.450	0.530	0.700	0.740
February	-6.33	20.61	2.74	1.08	0.00	0.00	2.57	0.500	0.490	0.700	0.730
March	0.17	32.31	5.51	2.17	0.00	0.00	4.80	0.550	0.480	0.500	0.720
April	7.44	45.39	7.26	2.86	0.00	0.00	5.74	0.500	0.480	0.200	0.670
May	13.61	56.50	7.98	3.14	0.00	0.00	6.37	0.390	0.420	0.200	0.665
June	19.00	66.20	9.30	3.66	0.00	0.00	6.25	0.310	0.360	0.200	0.685
July	21.67	71.01	8.61	3.39	0.00	0.00	5.45	0.300	0.330	0.200	0.715
August	20.17	68.31	10.26	4.04	0.00	0.00	5.75	0.300	0.360	0.200	0.750
September	15.44	59.79	8.56	3.37	0.00	0.00	4.88	0.370	0.400	0.200	0.760

9.2 Profile and Load Report

The Profile and Load Report documents the most commonly used inputs entered in the soil, chemical, and application files. As with the Climate Report this report documents the input parameters and contains no SESOIL results. A description of the model parameters is contained in Sections 0, 0, 6.6, and 6.7.



SESOIL Profile and Load Report

Layer No.	Number of Sub-Layers	Thickness		Intrinsic Permeability	Organic Carbon Content	Adsorption Coefficient	Cation Exchange Capacity	Freundlich Exponent	Solid Phase Degradation Rate	Liquid Phase Degradation Rate	Soil pH
		cm	feet	cm^2	percent	µg/g / µg/mL	mEq / 100 g soil	unitless	1/day	1/day	pH
1	10	200.0	6.6	1.00E-8	0.50	0.00	0.00	1.00	0.00E+00	0.00E+00	7.00
2	10	200.0	6.6	1.00E-8	0.50	0.00	0.00	1.00	0.00E+00	0.00E+00	7.00
3	10	300.0	9.8	1.00E-8	0.50	0.00	0.00	1.00	0.00E+00	0.00E+00	7.00
4	10	300.0	9.8	1.00E-8	0.50	0.00	0.00	1.00	0.00E+00	0.00E+00	7.00

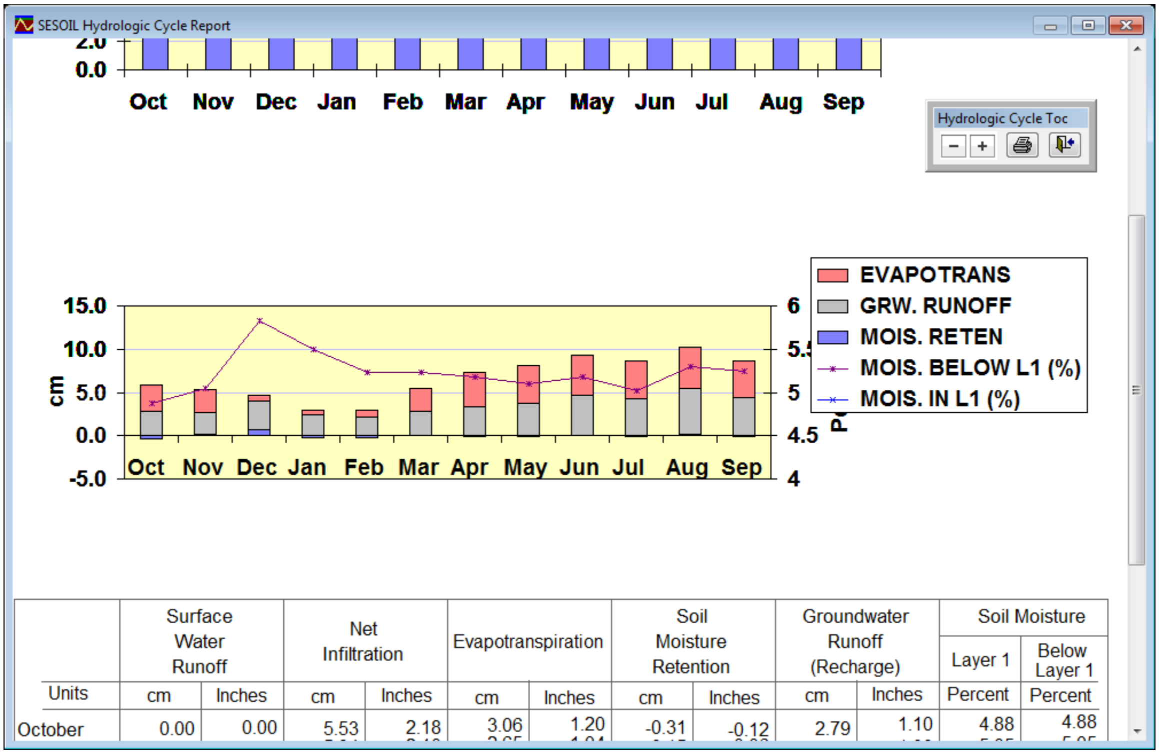
Bulk Density (g/cm^3)	1.70
Effective Porosity (fraction)	0.25
Soil Pore Disconnectedness	4.00

Area cm^2 ft^2	1.00E+6 1305.56
Latitude degrees	0.00
Spill Index	1

Water Solubility µg/mL	1.78E+3	**Moles Ligand / Moles Chemical**	0.00
Henry's Law (M^3-atm/mol)	5.55E-3	**Moles Ligand Weight** (g/mole)	0.00
Koc (Adsorp) (µg/g)/(µg/mL)	31.00	**Koc (Desorp)** (µg/g)/(µg/mL)	0.00
Kd (Adsorp) (µg/g)/(µg/mL)	0.00	**Kd (Desorp)** (µg/g)/(µg/mL)	0.00
Valence (g/mole)	0.00	**Ligand Dissociation Constant**	0.00
Air Diffusion Coefficient (cm^2/sec)	7.70E-2	**Base Hydrolysis Rate** (L/mol/day)	0.00
Water Diffusion Coefficient (cm^2/sec)	9.80E-6	**Neutral Hydrolysis Rate** (L/mol/day)	0.00
Molecular Weight (g/mole)	78.10	**Acid Hydrolysis Rate** (L/mol/day)	0.00

Output File:
C:\SEV7 WIN7\S01.OUT
Chemical File: Benzene
C:\SEV7 WIN7\BENZENE.CHM
Soil File: Sand, Perm = 1.00E-3 cm/sec

9.3 Hydrologic Cycle Report



	Surface Water Runoff		Net Infiltration		Evapotranspiration		Soil Moisture Retention		Groundwater Runoff (Recharge)		Soil Moisture	
											Layer 1	Below Layer 1
Units	cm	Inches	cm	Inches	cm	Inches	cm	Inches	cm	Inches	Percent	Percent
October	0.00	0.00	5.53	2.18	3.06	1.20	-0.31	-0.12	2.79	1.10	4.88	4.88

9.3.1 SESOIL Hydrologic Cycle Reports

Precipitation within the SESOIL hydrologic cycle is divided into two separate components. The first component is composed of monthly surface water runoff and net monthly infiltration at the top of the soil. The sum of these two data sets is equal to the monthly precipitation.

The second component is composed of evapotranspiration, soil moisture retention and groundwater recharge which are equal to the net monthly infiltration at the top of the soil column. Reviewing SESOIL water balance information can be used to calibrate the model to known site conditions (see Appendix A, Section A2.3.3).

9.3.1.1 Precipitation

Precipitation is distributed between surface water runoff and net infiltration. Surface water runoff is calculated based on the duration and distribution of rain fall events along with soil permeability (see Appendix A, Section A2.3). The difference between surface water runoff and precipitation enters the top of the SESOIL column as net infiltration.

SEVIEW extracts the “SUR. RUNOFF (CM)” and “NET INFILT. (CM)” data sets which are plotted and tabulated in the **Hydrologic Cycle Report**. A graphical presentation of the monthly surface water runoff and infiltration is presented at the top of the report. The table at the bottom of the report contains the “SUR. RUNOFF (CM)”, and “NET INFILT. (CM)” data sets.

☞ *Net infiltration entering the top of the soil column is typically not equal to the groundwater recharge due to evapotranspiration.*

☞ *Hydrologic water balance parameters are based on year 2 results, as the values are slightly different for the first year. See Appendix A, Section A2.3 Equations A1 and A2 for additional information.*

9.3.1.2 SESOIL Water Balance

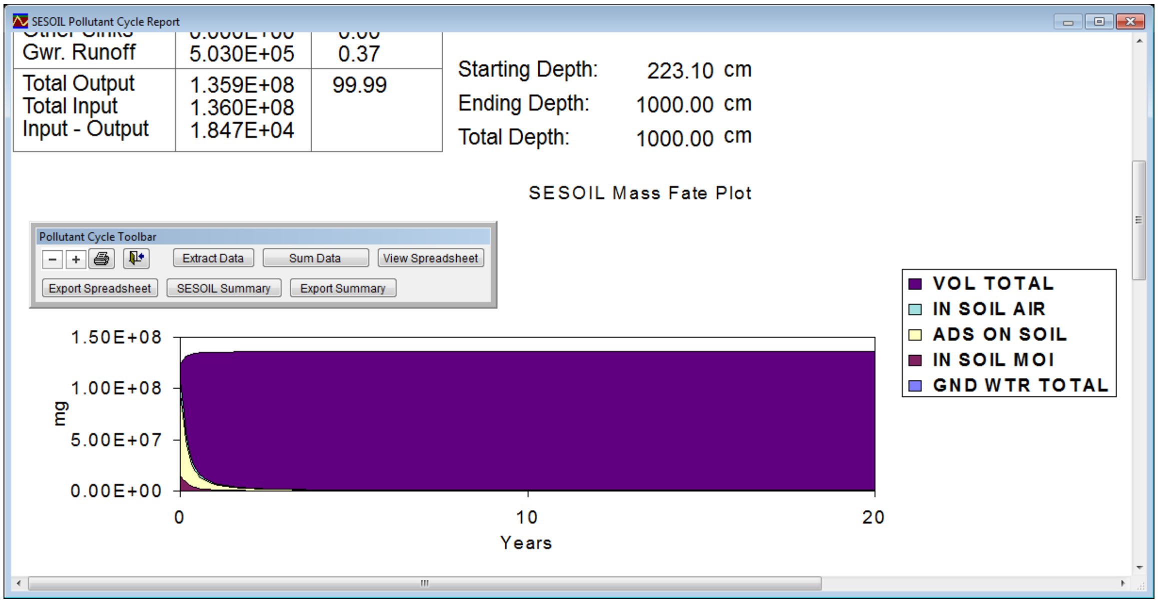
Precipitation entering the top of the soil column can evaporate to the atmosphere, remain bound as soil moisture or recharge groundwater. This means that the sum of the “EVAPOTRANS. (CM)”, “MOIS. RETEN (CM)” and “GRW. RUNOFF (CM) data sets equals the “NET INFILT. (CM) for each month. SEVIEW extracts the “EVAPOTRANS. (CM)”, “MOIS. RETEN (CM)” and “GRW. RUNOFF (CM)” data to plot and tabulate the results. The graphical presentation of the monthly water balance is presented in the Hydrologic Cycle Report. The table at the bottom of the **Hydrologic Cycle Report** contains the “EVAPOTRANS. (CM)”, “MOIS. RETEN (CM)” and “GRW. RUNOFF (CM)” data sets.

☞ *The monthly “GRW. RUNOFF (CM)” is used along with the monthly mass entering groundwater and the area of the soil column to establish the SESOIL leachate concentration in the Pollutant Cycle Report.*

9.3.1.3 Soil Moisture

The percent of soil moisture content and/or groundwater recharge can be used to calibrate SESOIL to known site conditions. The average volumetric soil moisture content percent for the soil column is contained in the “MOIS. BELOW L1 (%)” data set. The “MOIS. IN L1 (%)” data set contains the volumetric soil moisture content in the root zone (upper 100 cm of the soil column), see Section 9.5.3. SEVIEW and your spreadsheet can be used to plot or tabulate the soil moisture percentages. A plot of the “MOIS. BELOW L1 (%)” and “MOIS. IN L1 (%)” data set is presented below.

9.4 Pollutant Cycle Report



Gwr. Runoff	5.030E+05	0.37
Total Output	1.359E+08	99.99
Total Input	1.360E+08	
Input - Output	1.847E+04	

Starting Depth: 223.10 cm
Ending Depth: 1000.00 cm
Total Depth: 1000.00 cm

9.4.1 Mass Balance Table

The upper left portion of the Pollutant Cycle Report displays a mass balance table. This table presents mass distribution results for the final month of the SESOIL scenario. The table contains results for all 17 SESOIL processes presented as both mass in µg and percentage of the total mass. It also displays both the input (load) and output mass.

9.4.2 Mass Fate Plot

SEVIEW is the only SESOIL post-processor that includes a mass balance report. The mass balance report is generated as part of the **Pollutant Cycle Report**. SEVIEW also calculates the mass balance distribution for the final month of the SESOIL output file.

The mass balance report displays the monthly mass in each SESOIL process. Total input is the sum of the contaminant mass for all SESOIL processes for all months and is not the same as the "TOTAL INPUT" data set. The "TOTAL INPUT" data set contains the monthly contaminant load, while the mass balance report total load is the sum of all loads.

☞ *The SEVIEW mass balance report was used to identify a significant mass balance error in SESOIL.*

☞ *Although SEVIEW can produce a mass balance report within several seconds, creating the report is not simple. For example: Mass within a SESOIL output file with 40 sub-layers can be distributed in up to 6,761,232 individual values for a 999 year run.*

9.4.3 Leachate Concentration

A SESOIL leachate concentration plot is displayed below the mass fate plot. The leachate concentration plot displays the monthly concentration of the contaminant leaving the bottom of the soil column. The maximum SESOIL leachate concentration is also presented just below the leachate concentration plot.

☞ ***SESOIL produces a leachate concentration not a groundwater concentration. The leachate concentration must be converted to a groundwater concentration for comparison with groundwater standards. This is accomplished in SEVIEW by linking SESOIL to the AT123D groundwater model.***

☞ *SEVIEW determines the SESOIL leachate concentration by dividing the monthly mass entering groundwater by the monthly volume of groundwater recharge.*

9.4.4 Contaminant Depth Plot

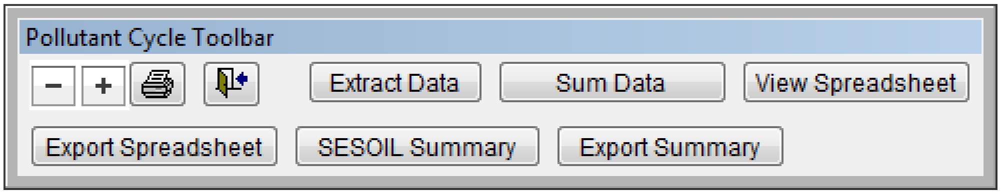
The SESOIL output file includes the "POL DEP CM" data set which contains the monthly depth below ground surface of the leading edge of the contaminant. SEVIEW extracts this data and plots the results in the **Pollutant Cycle Report**.

☞ *Once the leading edge of the contaminant reaches the water table, the depth of the contaminant equals the depth of the water table.*

☞ *SEVIEW estimates a travel time to the water table for model scenarios in which the contaminant did not reach groundwater. The estimate is based on the rate of contaminant mobility.*

9.4.5 Pollutant Cycle Toolbar

In addition to the zoom, print and close commands the Pollutant Cycle Toolbar contains commands to extract additional SESOIL results and to view a summary of the model run.

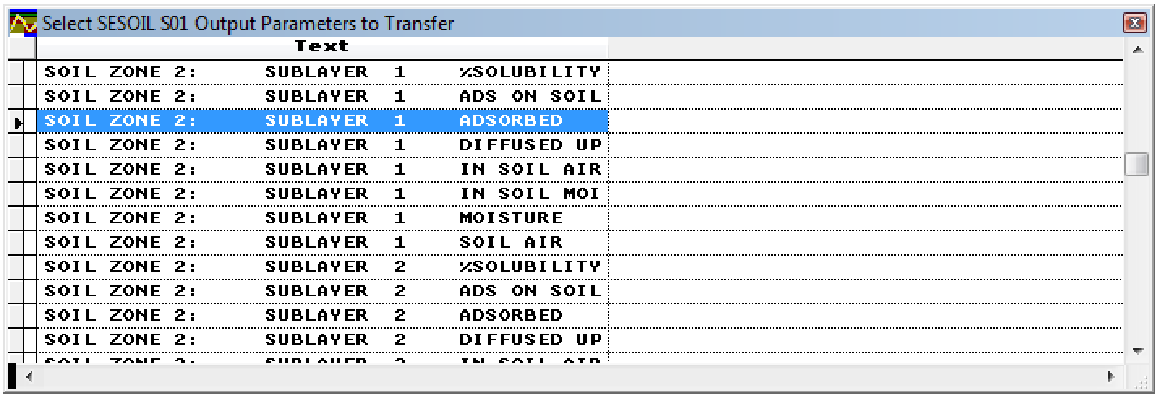


9.4.5.1 Extract Data

In addition to the Pollutant Cycle and Hydrologic Cycle reports, SEVIEW can be used to extract any monthly SESOIL results. This method can also be used to extract monthly input parameters. SEVIEW can be used to extract select results for evaluation. Click on the **Extract Data** command on the **Pollutant Cycle Toolbar**. A window displaying all the monthly input data and results will open.

A listing of contaminant mass process by the SESOIL model are presented in Table 10 Contaminant Mass (µg) Processes in the Output File*.*

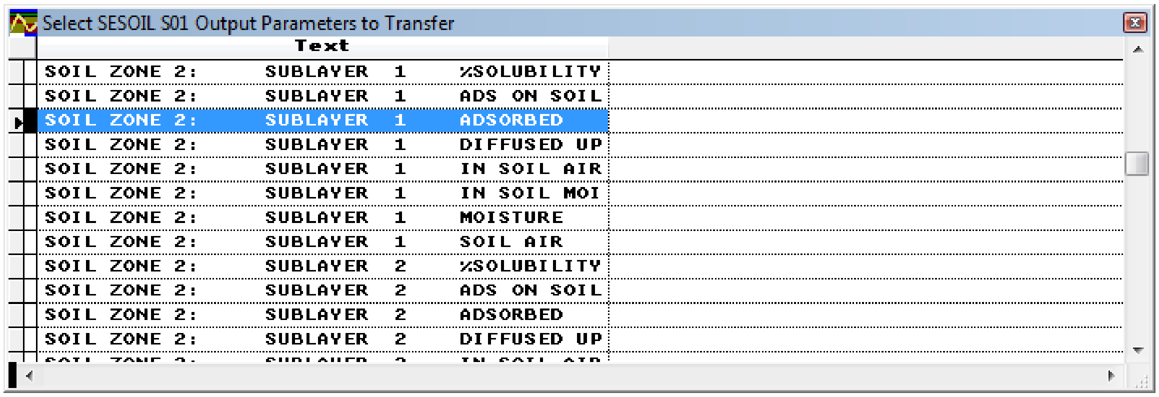
A listing of the concentrations produced by the SESOIL model are presented in Table 11.



Select SESOIL S01 Output Parameters to Transfer

Text
SOIL ZONE 2: SUBLAYER 1 %SOLUBILITY
SOIL ZONE 2: SUBLAYER 1 ADS ON SOIL
SOIL ZONE 2: SUBLAYER 1 ADSORBED
SOIL ZONE 2: SUBLAYER 1 DIFFUSED UP
SOIL ZONE 2: SUBLAYER 1 IN SOIL AIR
SOIL ZONE 2: SUBLAYER 1 IN SOIL MOI
SOIL ZONE 2: SUBLAYER 1 MOISTURE
SOIL ZONE 2: SUBLAYER 1 SOIL AIR
SOIL ZONE 2: SUBLAYER 2 %SOLUBILITY
SOIL ZONE 2: SUBLAYER 2 ADS ON SOIL
SOIL ZONE 2: SUBLAYER 2 ADSORBED
SOIL ZONE 2: SUBLAYER 2 DIFFUSED UP

To extract the concentration adsorbed on soil in the second soil layer move to the "SOIL ZONE 2: SUBLAYER 1 ADSORBED" row of the window. Click on the small rectangle located at the beginning of the row and it will turn black.

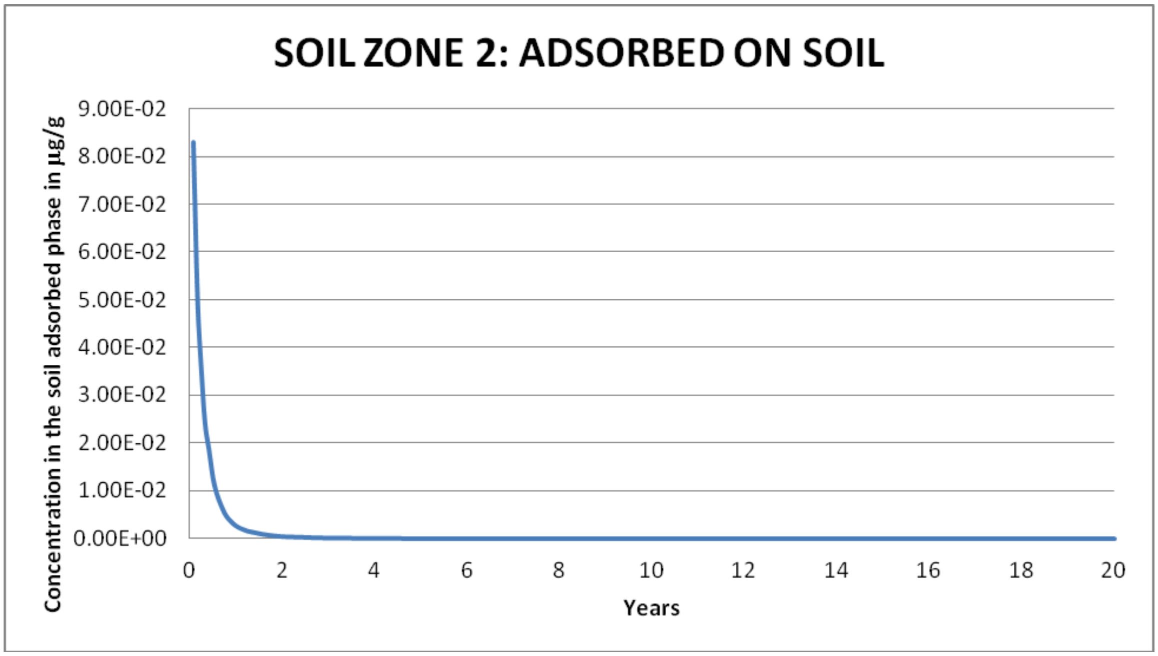


Select SESOIL S01 Output Parameters to Transfer

Text
SOIL ZONE 2: SUBLAYER 1 %SOLUBILITY
SOIL ZONE 2: SUBLAYER 1 ADS ON SOIL
SOIL ZONE 2: SUBLAYER 1 ADSORBED
SOIL ZONE 2: SUBLAYER 1 DIFFUSED UP
SOIL ZONE 2: SUBLAYER 1 IN SOIL AIR
SOIL ZONE 2: SUBLAYER 1 IN SOIL MOI
SOIL ZONE 2: SUBLAYER 1 MOISTURE
SOIL ZONE 2: SUBLAYER 1 SOIL AIR
SOIL ZONE 2: SUBLAYER 2 %SOLUBILITY
SOIL ZONE 2: SUBLAYER 2 ADS ON SOIL
SOIL ZONE 2: SUBLAYER 2 ADSORBED
SOIL ZONE 2: SUBLAYER 2 DIFFUSED UP

9.4.5.2 Export Spreadsheet

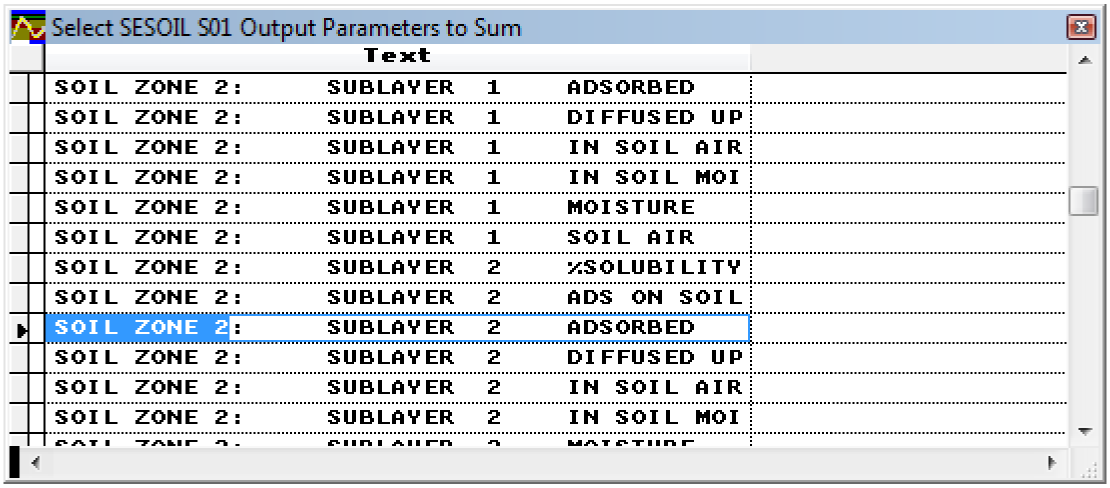
Click **Export Spreadsheet** command located on the **Pollutant Cycle Report** toolbar. Save the spreadsheet table as a tab delimited .txt file. Open the .txt file using Excel and plat the data.



9.4.5.3 Sum Data

Mass within a SESOIL output file can be distributed in up to 564 monthly data sets. SEVIEW can be used to sum multiple data sets creating new SESOIL data sets. The summation of SESOIL data is one of the most powerful commands within SEVIEW; as individual SESOIL data sets may be summed to create additional data sets. For example, you could sum the data sets for the mass volatilized, in soil air, adsorbed on soil, contained in soil moisture and in groundwater runoff for all layers and sub-layers within the SESOIL output file. Or you could restrict the summation to the mass in soil moisture contained all sub-layers of a layer.

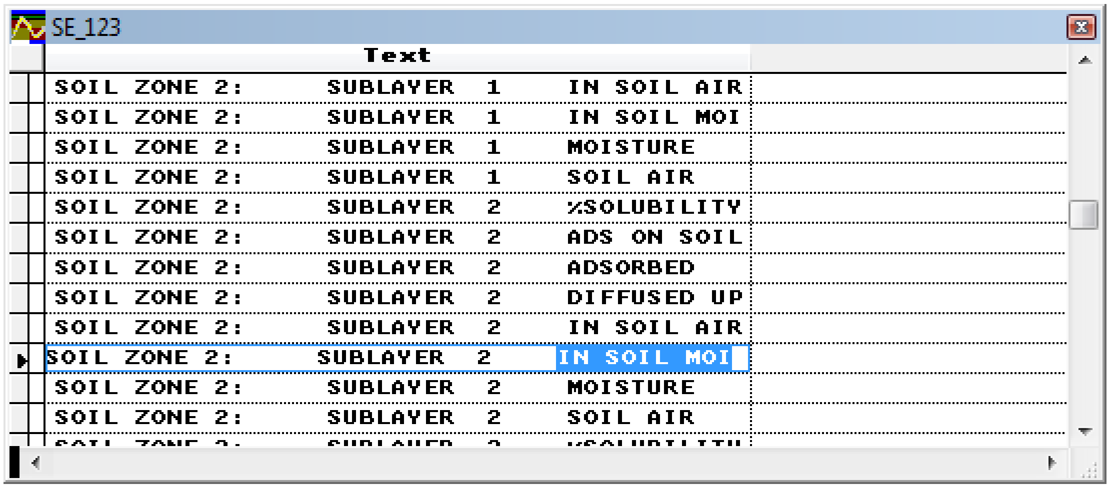
Use the sum data command to combine data sets. For example to look at the montly contaminant mass contained in soil moisture in layer 2. You will need to combine the soil moisture mass contained in all ten sub-layers. Click on the **Sum Data** command on the **Pollutant Cycle Toolbar**. Use the scrool bar to move through window until you see the "SOIL ZONE 2" data. Highlight the **SOIL ZONE 2** text and press <CTRL + C> to copy the text to the clipboard.



Select SESOIL S01 Output Parameters to Sum

Text
SOIL ZONE 2: SUBLAYER 1 ADSORBED
SOIL ZONE 2: SUBLAYER 1 DIFFUSED UP
SOIL ZONE 2: SUBLAYER 1 IN SOIL AIR
SOIL ZONE 2: SUBLAYER 1 IN SOIL MOI
SOIL ZONE 2: SUBLAYER 1 MOISTURE
SOIL ZONE 2: SUBLAYER 1 SOIL AIR
SOIL ZONE 2: SUBLAYER 2 %SOLUBILITY
SOIL ZONE 2: SUBLAYER 2 ADS ON SOIL
SOIL ZONE 2: SUBLAYER 2 ADSORBED
SOIL ZONE 2: SUBLAYER 2 DIFFUSED UP
SOIL ZONE 2: SUBLAYER 2 IN SOIL AIR
SOIL ZONE 2: SUBLAYER 2 IN SOIL MOI
SOIL ZONE 2: SUBLAYER 2 MOISTURE

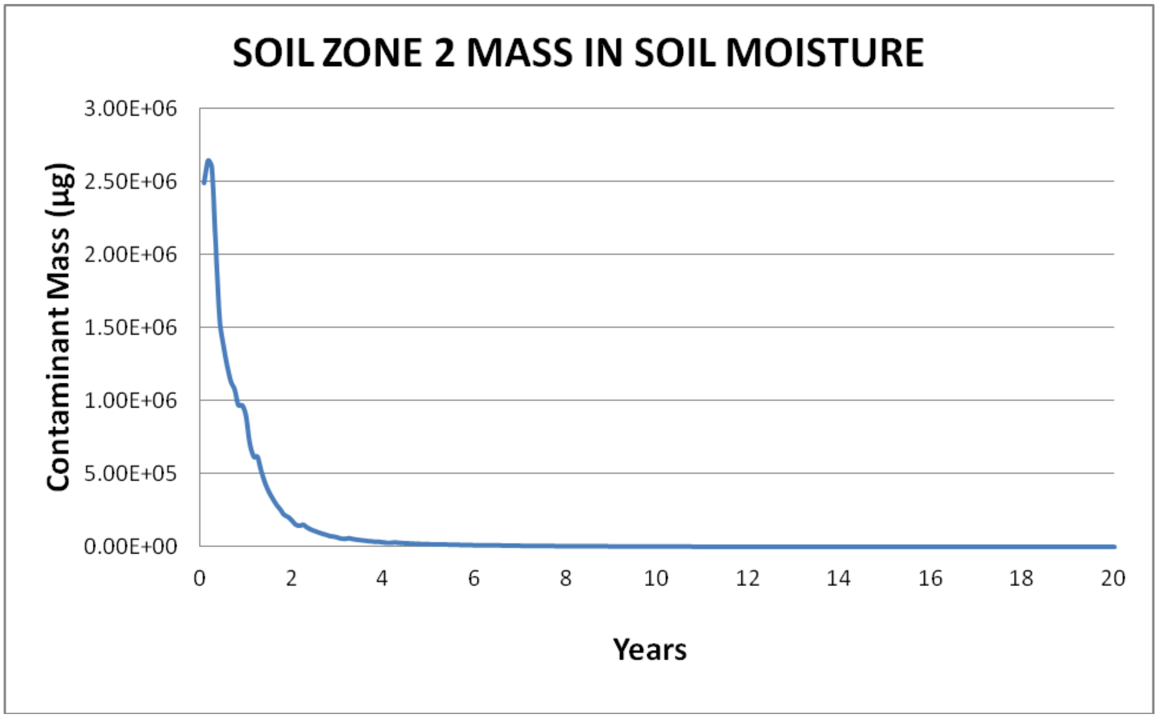
Then close the window and a second window will appear. This time highlight the "IN SOIL MOI" data. Highlight the **IN SOIL MOI** text and press <CTRL + C> to copy the text to the clipboard.



SE_123

Text
SOIL ZONE 2: SUBLAYER 1 IN SOIL AIR
SOIL ZONE 2: SUBLAYER 1 IN SOIL MOI
SOIL ZONE 2: SUBLAYER 1 MOISTURE
SOIL ZONE 2: SUBLAYER 1 SOIL AIR
SOIL ZONE 2: SUBLAYER 2 %SOLUBILITY
SOIL ZONE 2: SUBLAYER 2 ADS ON SOIL
SOIL ZONE 2: SUBLAYER 2 ADSORBED
SOIL ZONE 2: SUBLAYER 2 DIFFUSED UP
SOIL ZONE 2: SUBLAYER 2 IN SOIL AIR
SOIL ZONE 2: SUBLAYER 2 IN SOIL MOI
SOIL ZONE 2: SUBLAYER 2 MOISTURE
SOIL ZONE 2: SUBLAYER 2 SOIL AIR
SOIL ZONE 2: SUBLAYER 2 %SOLUBILITY

When you close the second window SEVIEW will create a new monthly data set "SOIL ZONE 2 IN SOIL MOI". Close the third window and click on the **Extract Data** command on the **Pollutant Cycle Toolbar**. Click on the small rectangle at the start of the "SOIL ZONE 2 IN SOIL MOI" row and close the window. Finaly save it as a tab delimited .txt file and open the file in Excel to produce the graph below.



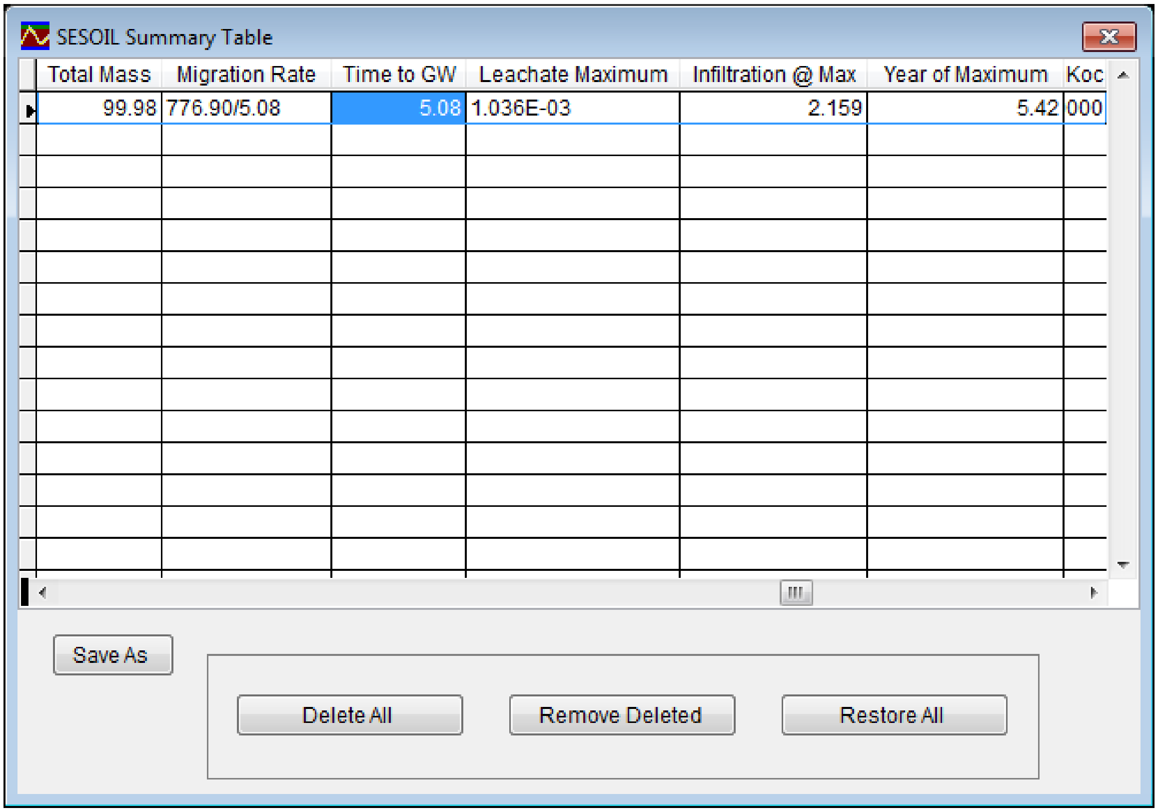
9.4.5.4 View Spreadsheet

Use this option to view the contants of the SEVIEW spreadsheet.

☞ *The spreadsheet will already contain the data use to produce the **Pollutant Cycle Report**.*

9.4.5.5 SESOIL Summary

SEVIEW produces a SESOIL summary every time you view a pollutant cycle report. This summary table looks like an Excel spreadsheet. The summary table includes the description of the SESOIL scenario, the SESOIL output file used, the percent of the mass contained or lost in each of the SESOIL process, the percent of the total mass accounted for in the last month, a contaminant migration rate, a travel time to the water table, the maximum SESOIL leachate concentration, the infiltration rate at the month of the maximum leachate concentration and the year of the maximum concentration. The summary table also includes several SESOIL parameters that are often used to determine dilution in groundwater.



Total Mass	Migration Rate	Time to GW	Leachate Maximum	Infiltration @ Max	Year of Maximum	Koc
99.98	776.90/5.08	5.08	1.036E-03	2.159	5.42	000

*You can use the **Delete All**, **Remove Deleted** and **Restore All** commands to control the data within the summary table.*

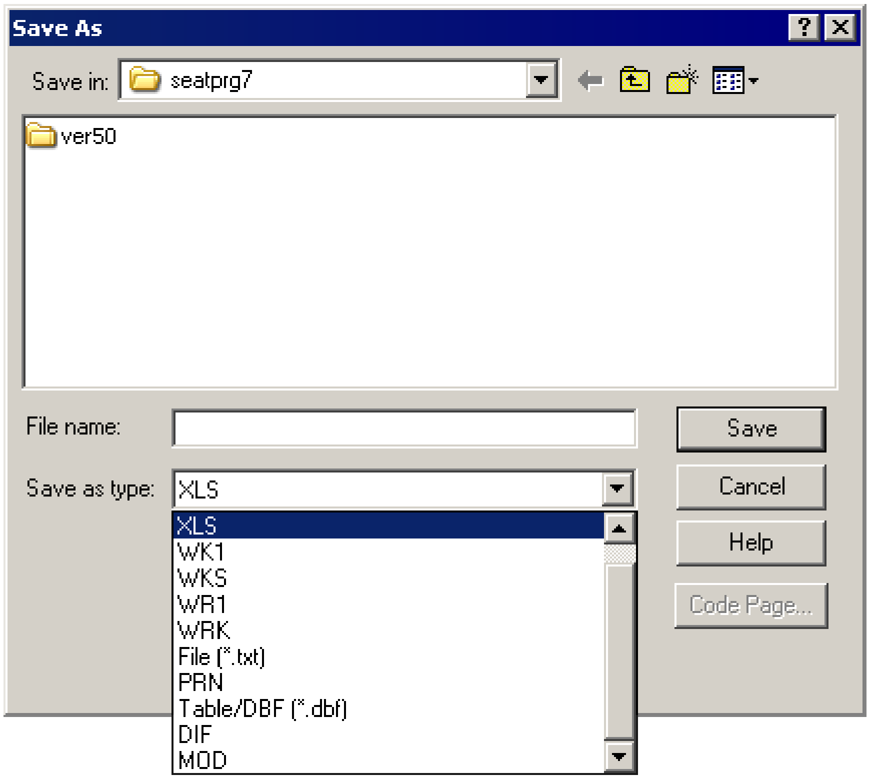
*You can export the summary table using the **Save As** command.*

9.4.5.6 Export Summary

The SEVIEW summary table of the SESOIL results can be saved in a number of different file formats. Once converted the table it can be used in spreadsheet programs to calculate groundwater dilution or in word processors programs to summarize the modeling results. The summary table can be converted to any of the following file formats presented in below.

Table 6 Export File Formats

File Type	Default Extension
Excel Version 5	.XLS
LOTUS	.WK1
LOTUS	.WKS
Symphony	.WR1
Symphony	.WRK
ASCII Tab Delimited	File (.TXT)
ASCII Comma Delimited	.PRN
FoxPro 2.x	.DBF
VisiCalc	.DIF
MultiPlan	.MOD



Save in: seatprg7

File name:

Save as type: XLS

Table 7 SESOIL Summary Table

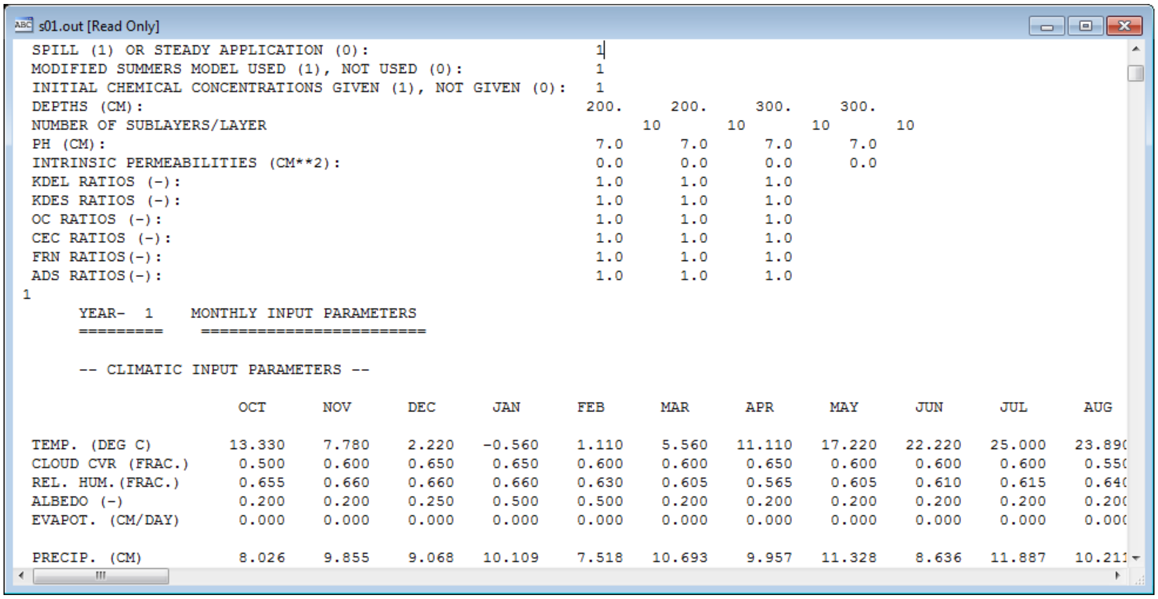
Output File	Volatilized	In Soil Air	Ads on Soil	In Soil Moisture	Total Mass	Migration Rate	Travel Time to Groundwater	Maximum Leachate Conc.	Year of Maximum Conc.
units	%	%	%	%	%	cm/year	years	mg/L	years
S01	99.61	0.00	0.00	0.00	99.98	776.90/5.08	5.08	0.001037	5.42
S03	93.05	0.00	0.03	0.01	99.98	573.90/4.08	4.08	0.047911	4.25

☞ *The File format option produces a tab delimited ASCII file with a .TXT extension.*

9.5 SESOIL Output File

The SESOIL output file contains the model input and results for the hydrologic cycle, washload cycle (if used), and pollutant cycle. The SESOIL report is divided into the heading, input and output sections. An annual summary report is also printed for each year. SESOIL output files can be quite lengthy, for example, a 100-year simulation that includes four layers can produce a 1.0 Mbyte output file. A detailed description of the SESOIL output file is presented below.

SESOIL produces ASCII output file reports which are used by SEVIEW. Each output file includes a summary of all input parameters used in the simulation and the monthly results.



```
  SPILL (1) OR STEADY APPLICATION (0):                        1
  MODIFIED SUMMERS MODEL USED (1), NOT USED (0):              1
  INITIAL CHEMICAL CONCENTRATIONS GIVEN (1), NOT GIVEN (0):   1
  DEPTHS (CM):                                               200.     200.     300.     300.
  NUMBER OF SUBLAYERS/LAYER                                        10       10       10       10
  PH (CM):                                                    7.0      7.0      7.0      7.0
  INTRINSIC PERMEABILITIES (CM**2):                           0.0      0.0      0.0      0.0
  KDEL RATIOS (-):                                            1.0      1.0      1.0
  KDES RATIOS (-):                                            1.0      1.0      1.0
  OC RATIOS (-):                                              1.0      1.0      1.0
  CEC RATIOS (-):                                             1.0      1.0      1.0
  FRN RATIOS(-):                                              1.0      1.0      1.0
  ADS RATIOS(-):                                              1.0      1.0      1.0
 1
       YEAR-  1    MONTHLY INPUT PARAMETERS
       =========    ========================

       -- CLIMATIC INPUT PARAMETERS --

                            OCT       NOV       DEC       JAN       FEB       MAR       APR       MAY       JUN       JUL       AUG

  TEMP. (DEG C)          13.330     7.780     2.220    -0.560     1.110     5.560    11.110    17.220    22.220    25.000    23.89
  CLOUD CVR (FRAC.)       0.500     0.600     0.650     0.650     0.600     0.600     0.650     0.600     0.600     0.600     0.55
  REL. HUM.(FRAC.)        0.655     0.660     0.660     0.660     0.630     0.605     0.565     0.605     0.610     0.615     0.64
  ALBEDO (-)              0.200     0.200     0.250     0.500     0.500     0.200     0.200     0.200     0.200     0.200     0.20
  EVAPOT. (CM/DAY)        0.000     0.000     0.000     0.000     0.000     0.000     0.000     0.000     0.000     0.000     0.00

  PRECIP. (CM)            8.026     9.855     9.068    10.109     7.518    10.693     9.957    11.328     8.636    11.887    10.211
```

A SESOIL output file can be opened by clicking on the Open following the **SESOIL Output File** in the **Setup SESOIL & AT123D Runs** window. When an output file is opened SEVIEW will display the file in a read only format.

☞ *You can also open a SESOIL output file, by selecting the **View SESOIL Output File** option of the **File** menu. A window displaying all SESOIL output files in the current working directory will be displayed. If a SESOIL output file is not selected (Cancel is selected, <ESCAPE> is pressed or the window is closed) and no file will be selected and the main menu will be displayed.*

☞ *SEVIEW includes its own text editor that can be used to examine the contents of any SESOIL (.OUT) or AT123D (.ATO) output file. The basic features of the SEVIEW edit command are similar to other Windows text editors and word processors, except it is much faster when working with the very large output files created by SESOIL and AT123D! See Appendix C for additional information on the SEVIEW text editor.*

☞ *Although, the SESOIL output file cannot be modified, the file may be saved as a new file. In addition, the output file may be searched using the **Find** and **Find Again** commands. Selected data may be copied from the output file using the Windows **Copy** command.*

9.5.1 SESOIL Heading

The heading portion of the SESOIL output file contains a description of the version of SESOIL being used. It also contains notes regarding the modifications to the program and who made them.

9.5.2 SESOIL Input

The input section is presented below the heading, it contains a summary of the input file descriptions followed by a list of the input parameters used by the model. The input parameters are subdivided into tables containing soil, chemical, washload (if used), and application data. The table (labeled "YEAR - 1 MONTHLY INPUT PARAMETERS") reports the monthly climatic data, the contaminant input parameters for each month, and the monthly washload factors (if used) for the first year. A description of the input parameters is presented in Section 6. Additional input information concerning SESOIL input parameters is presented in Appendix A "Introduction and Overview of the SESOIL Model".

Following the data for the first year, the monthly input parameters for the climate, contaminant, and washload are given for each year. If the data for any of these categories (i.e., climatic, pollutant, or washload) are the same as the previous year, they will not be printed, instead a message is presented stating, for example, "CLIMATIC INPUT PARAMETERS ARE SAME AS LAST YEAR.". This is common when long-term monthly averaged data are used.

☞ *The output file should be checked carefully to verify that the input parameters are correct and to review any warning or error messages that may have been generated.*

SESOIL can identify some obvious errors in the input data and insert the error or warning messages into the output file. The messages will be printed immediately preceding the section entitled "GENERAL INPUT PARAMETERS". For example, the fraction of cloud cover must be between 0.0 and 1.0 and an error message is printed if it is not. Warnings or errors associated with the hydrologic cycle will be printed following the input data. A list of all SESOIL error and warning messages including a description is presented in Appendix A.

9.5.3 SESOIL Results

The next section of the output file contains the model results, which are divided into annual subsections. These data tables are grouped by the year simulated, with the results reported for each month. The monthly results are organized in the following sequence:

- Hydrologic cycle components
- Washload cycle components (if used)
- Contaminant mass input
- Contaminant concentration distribution for each layer or sub-layer
- Contaminant depth

The monthly output results are followed by an annual summary. The following sections discuss each portion of the output file in detail.

9.5.3.1 Hydrologic Cycle

Reports for each year begin with the monthly results for the hydrologic cycle. The first parameter printed, labeled “MOIS. IN L1 (%)”, is the volumetric soil moisture content in the root zone, defined in SESOIL as the first 100 cm of the unsaturated soil zone. The next parameter, labeled “MOIS. BELOW L1 (%)”, is the average volumetric soil moisture content for the entire soil column (from the surface to the groundwater table). For most applications the values for these parameters will be identical for each month. The hydrologic cycle of SESOIL needs further refinement to produce any significant difference between these two parameters since an average permeability is used for the entire soil column in the hydrologic cycle. At present, only very dry climatic conditions are likely to produce a difference in the values.

The calculated precipitation “PRECIPITATION (CM)” in centimeters per month is presented next. The precipitation data is followed the by monthly infiltration, evapotranspiration, soil moisture retention, surface water runoff, and groundwater runoff (recharge) parameters, in centimeters per month.

☞ *The results for the first year of the hydrologic cycle are slightly different than all subsequent years, as SESOIL iterates on soil moisture content until the calculated precipitation is within one percent of the precipitation entered. See Section A2.3 for additional information on the hydrologic cycle.*

Infiltration into the soil column is established as the difference between the precipitation and the surface runoff. The infiltration rate is equal to the moisture retention plus the evapotranspiration plus the groundwater runoff (see Section 9.3.1). The yield is simply the surface runoff plus the groundwater runoff (recharge). The next two lines, “PAU/MPA (GZU)” and “PA/MPA (GZ)”, are the calculated precipitation for each month for the root zone and the entire soil column, respectively, divided by the measured precipitation. (See Appendix A, Section A2.3 for more information concerning the hydrologic cycle components.) A list of all SESOIL hydrological output parameters is presented in Table 8.

Table 8 SESOIL Hydrological Output Parameters

Hydrological Parameters	Process Definition
EVAPOT. (CM/DAY)	Daily calculated evapotranspiration in cm.
EVAPOTRANS. (CM)	Monthly calculated evapotranspiration in cm.
GRW. RUNOFF (CM)	Monthly calculated groundwater runoff (groundwater recharge) in cm.
MOIS. BELOW L1 (%)	The average volumetric soil moisture content of the entire soil column (from ground surface to the groundwater table).
MOIS. IN L1 (%)	The volumetric soil moisture content of the root zone (the upper 100 cm of the soil column).
MOIS. RETEN (CM)	Calculated monthly soil moisture retention (cm).

NET INFILT. (CM)	Calculated monthly infiltration (precipitation entering the top of the soil column in cm).
PA/MPA (GZ)	The calculated monthly precipitation of the entire soil column (from ground surface to the groundwater table) divided by the measured precipitation.
PAU/MPA (GZU)	The calculated monthly precipitation of the root zone (the upper 100 cm of the soil column) divided by the measured precipitation.
PRECIP. (CM)	User specified input precipitation data in cm.
PRECIPATION (CM)	Calculated precipitation in cm. SESOIL does not directly utilize the user supplied precipitation data. It iterates on soil moisture until the calculated precipitation is within one percent of the measured input data (See Appendix A Section A2.3 for more information).
SUR. RUNOFF (CM)	Calculated monthly surface water runoff in cm.
YIELD (CM)	Monthly sum of surface runoff plus the groundwater runoff (recharge).

9.5.3.2 Washload Cycle

If used the monthly washload cycle information is presented following the hydrologic cycle results. The sediment yield is given on the first two lines in kg/km^2 and g/cm^2, respectively (labeled as "WASHLD (KG/SQ KM)" and "(G/SQ CM)"). The next line, labeled "ENRICHMT RATIO (-)", is defined as the ratio of the total specific surface area for the sediment and organic matter to that of the original soil (Knisel et. al., 1983). The index of specific surface in m^2/g of total sediment and is labeled "SURF. IDX (M**2/G)" (see Knisel et. al., 1983). Next, the relative amounts of clay, silt, and sand in the eroded topsoil particles are given, labeled as "SED. FRAC CLAY", "SED. FRAC SILT", and "SED. FRAC SAND". These three numbers should add to 1.0 for each month. The last line of the washload results labeled "SED. FRAC OC", is the fraction of organic matter in the eroded sediment. Refer to Appendix A, Section A2.4 for a detailed description of the washload cycle. A description of all SESOIL washload output parameters is presented on Table 9.

Table 9 Sediment Washload Output File Parameters

Washload Parameters	Process Definition
WASHLD (KG/SQ KM)	Sediment yield in kg/km^2.
(G/SQ CM)	Sediment yield in g/cm^2.
ENRICHMT RATIO (-)	The ratio of the total specific surface area for the sediment and organic matter to that of the original soil.
SURF. IDX (M**2/G	The index of specific surface in m^2/g of the total sediment.
SED. FRAC CLAY	Relative amount of clay in the eroded particles.
SED. FRAC SILT	Relative amount silt in the eroded particles.

SED. FRAC SAND	Relative amount of sand in the eroded particles.
SED. FRAC OC	The fraction of organic matter in the eroded sediment.

9.5.3.3 Contaminant Mass Load

The monthly contaminant mass load, in units of μg, is the next table in the output file. These values include the amount of chemical load in precipitation (labeled “PRECIP.”) and the load in each of the layers (or sub-layers) specified in the simulation, labeled “LOAD UPPER”, “LOAD ZONE 2”, “LOAD ZONE 3”, and “LOAD LOWER” in μg. PRECIP is computed by multiplying the contaminant load in precipitation (ASL), by the water solubility (SL), by the infiltration rate computed by the hydrologic cycle (NET. INFILT.), and the area of the application (AR from the application file). Values displayed in the load for each layer are simply the area of application (AR) multiplied by the contaminant application (POLIN for each layer defined in the application file). Note that if there are sub-layers within a major layer, then the load for the major layer is added to the first sub-layer of that layer, not evenly for each of the sub-layers.

If an instantaneous load was specified (see the line labeled “SPILL (1) OR STEADY APPLICATION (0):” under “-- APPLICATION INPUT PARAMETERS -”) the input listed for the month for the surface layer is loaded into the layer in the first time step of the month. If steady loading was specified, the input for the month is spread out evenly during each time step of the month. Note that spill loading applies only to the first layer. (Refer to Appendix A, Sections A2.5.2 and Section 6.7 for more details.) The total input to the soil column is given next (labeled “TOTAL INPUT”) and is simply the sum of all mass loads for a given month.

9.5.3.4 Contaminant Mass

The next table in the output file displays the distribution of contaminant mass in μg for each process for each sub-layer of the soil column and for each month of the year. Table 10 lists of all of the SESOIL mass components in the order in which they are displayed in the output file. The contaminant mass is printed for each layer and sub-layer from the surface to the bottom of the soil column.

☞ *If a monthly SESOIL output process in a particular layer or sub-layer is zero for each month of the year, it will not be printed in the output file to conserve disk space.*

If there is more than one sub-layer in the first layer (upper soil zone), then the output for the second sub-layer follows and the order of the parameters and their definitions are the same as given in Table 10. However, the first three components listed in Table 10 (i.e., “SUR. RUNOFF”, “IN WASHLOAD”, and “VOLATILIZED”) apply only to the uppermost sub-layer of the first layer (upper soil zone). The fourth component listed in Table 10 (i.e., “DIFFUSED UP”) applies to all layers and sub-layers except the uppermost sub-layer of the first layer (upper soil zone). Likewise, this table continues for each layer (and sub-layer) down through the soil column.

If all results for all components of a layer or sub-layer are zero for the year, then the only label printed is the number of the sub-layer. When the contaminant reaches the bottom of the soil column (the lowest sub-layer of the "LOWER SOIL ZONE"), the last component printed in the mass distribution table is the mass of contaminant that leaves the unsaturated zone and enters the groundwater in μg (labeled "GWR. RUNOFF").

Table 10 Contaminant Mass (μg) Processes in the Output File

Process Label	Process Definition
SUR. RUNOFF	Mass lost via surface runoff (upper most sub-layer only).
IN WASHLD	Mass lost via soil erosion (upper most sub-layer only).
VOLATILIZED	Mass volatilized to air (upper most sub-layer only).
DIFFUSED UP	Mass diffused upward from the layer (sub-layer) to the layer (sub-layer) above it.
DEGRAD MOIS	Mass degraded in the soil moisture phase.
DEGRAD SOIL	Mass degraded in the soil adsorbed phase.
HYDROL MOIS	Mass degraded due to hydrolysis in the soil moisture phase.
HYDROL SOIL	Mass degraded due to hydrolysis in the adsorbed soil phase.
HYDROL CEC	Mass degraded due to hydrolysis of the mass of the contaminant immobilized by cation exchange.
OTHER SINKS	Mass removed by a user defined process.
OTHER TRANS	Mass transformed by a user defined process.
IN SOIL MOI	Mass in the soil moisture phase.
ADS ON SOIL	Mass adsorbed on the soil.
IN SOIL AIR	Mass in the soil air phase.
PURE PHASE	Mass in pure phase.
COMPLEXED	Mass that is complexed.
IMMOBIL CEC	Mass immobilized by cation exchange.
GWR. RUNOFF	Mass that leaves the unsaturated zone and enters the groundwater (lower most sub-layer only).
TOTAL INPUT	Total contaminant mass load (monthly sum of all input loads)

Following the contaminant mass distribution results is a table of the monthly contaminant concentrations for each chemical phase for each sub-layer in μg/ml. Table 11 presents a list of all chemical phases. If all concentrations for a particular phase are zero for each month of the entire year, the results are not printed. The pure phase concentration will be zero unless the simulated contaminant concentration in the soil moisture exceeds the solubility of the chemical. When this happens, the model sets the soil moisture concentration to the solubility (the %SOLUBILITY defined in Table 11 will be 100.0), and the excess chemical is assumed to be in the pure phase.

☞ *Transport of the chemical in the pure phase is not simulated; the pure phase is treated as an immobile storage term and the mass of the chemical in this phase is used as input to the same layer in the next time step.*

Table 11 Contaminant Concentration in the Output File

Concentration Label	Process Definition
MOISTURE	Contaminant concentration in the soil moisture phase in µg/ml (ppm).
ADSORBED	Contaminant concentration in the soil adsorbed phase in µg/g (ppm).
SOIL AIR	Contaminant concentration in the soil air phase in µg/ml (ppm).
FREE LIGAND	Free ligand concentration in µg/ml (ppm).
PURE PHASE	Contaminant concentration in the pure phase in µg/ml (ppm).
%SOLUBILITY	Not a concentration, it is the predicted soil moisture contaminant concentration divided by the solubility for the chemical, multiplied by 100 to give percent.

9.5.3.5 Contaminant Depth

Contaminant depth in cm is presented next (labeled “POL DEP CM”). This depth is calculated from Equation A11 in Appendix A, Section A2.5.2 and is simply the depth of the leading edge of the contaminant. Once the contaminant reaches groundwater, the depth will always be equal to the depth to the groundwater table.

9.5.4 Output of Annual Summary

SESOIL prints an annual summary report following the table of the concentration data. Parameters in this report are the same as listed above for monthly results, but either a “TOTAL” or an “AVERAGE” is given for each parameter. “TOTAL” is simply the sum of values given for the 12 months for the parameter listed and “AVERAGE” is the sum for the year divided by 12. The annual summary is organized in the following order:

- Total contaminant mass inputs
- Hydrologic cycle components (average or total)
- Total contaminant mass removed from each layer or sub-layer
- Average contaminant concentration distributions for each layer or sub-layer
- Maximum contaminant depth

The final end-of-the-year contaminant mass in the soil moisture, adsorbed on soil, in soil air, immobilized by cation exchange, complexed, and in the pure phase would be found under the last month of the year (September) in the monthly mass distribution (Table 8).

The final portion of the annual report, contains the maximum depth below ground surface that the contaminant has migrated to in meters is given (labeled “MAX. POLL. DEPTH (M)”). This depth will always be the same as the last month of the year (September) presented above in the SESOIL output file (see line labeled “POL DEP CM”).

10 AT123D Results

There are two way of viewing the results of the AT123D groundwater model.

10.1 Point of Compliance (Base Map)

After you run AT123D you can double click on a point of compliance to open the POC report. The POC report will display the concentration at the selected point. The "AT123D POC Controls" and the "Select Sources" toolbars will be displayed as part of the report.
The SEVIEW POC report can display results for any combination of up to 15 SESOIL and / or AT123D sources. Results from each source are averaged over the depth interval established for designated for each POC.

10.1.1 AT123D POC Toolbar

The -/+ commands are used to zoom in / out on the report. The **graph** symbol is used to update the POC report based on the selected sources. The **print** symbol is used to produce a printed output. The **Close** symbol is used to close the report. Please note that you can also the POC report by clicking on the X on the upper right corner of the window.

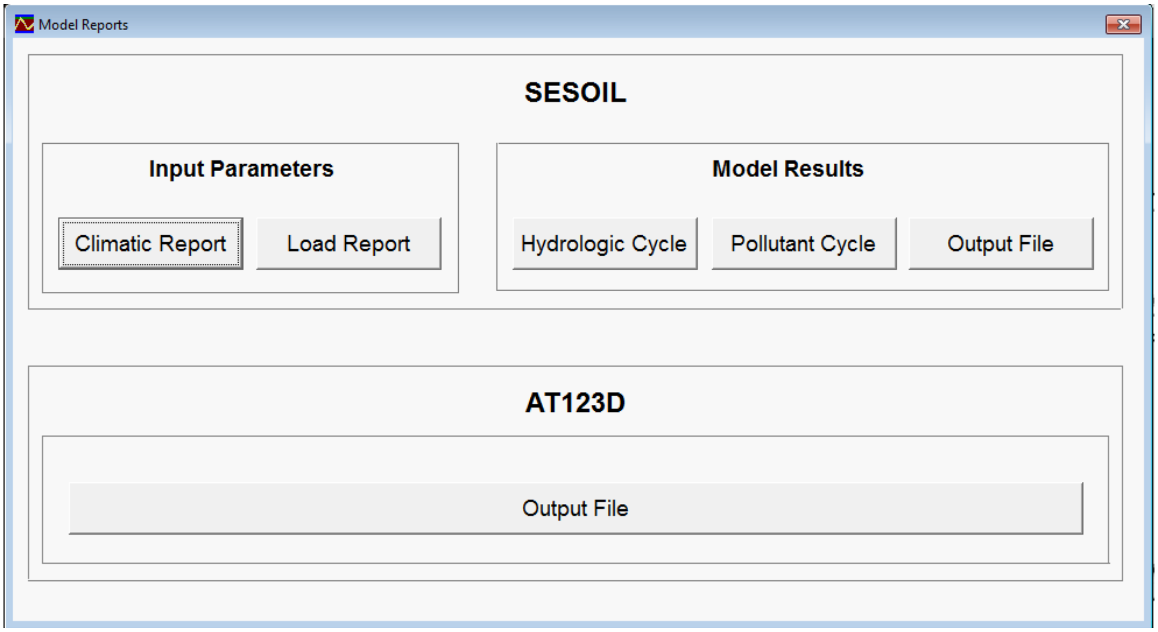
10.1.2 Select Sources Toolbar

Use the mouse to select which sources to include in the report. Then **Click** on the **Graph Symbol** to update the report. The description and number of options is dependent upon the number of sources established on the base map.

The AT123D model produces ASCII output files which are used by SEVIEW. Each output file contains a summary of all model input parameters and the results of the model scenario.

10.2 Output File

Double Click on a red AT123D source to open the **Model Reports** window. Then click on the **Output File** command.



The AT123D output file contains input parameters and output results for the model scenario. The AT123D output file is divided into the heading, input and output sections. A detailed description of the AT123D output file is presented below. Results from all sources are contained in a single AT123D output file.

10.2.1 AT123D Heading

The heading portion at the top of the output file contains a description of the version of AT123D used. It also contains a description of modifications to the code and who made them.

10.2.2 AT123D Input Parameters

The first portion of the output file contains a summary of the input parameters used by the model. A description of the AT123D input parameters used by SEVIEW is presented in Section 7. A complete description of all AT123D input parameters is presented in Appendix B "AT123D Data Input Guide".

The user should check this section of the output file carefully and verify that the input data is correct and to review any warning or error messages that may have been generated.

The AT123D output file contains a report of all input parameters. The following is an example of an AT123D input parameter report.

```
Benzene in Sand
     NO. OF POINTS IN X-DIRECTION ......................    7
     NO. OF POINTS IN Y-DIRECTION ......................    5
     NO. OF POINTS IN Z-DIRECTION ......................    2
```

```
     NO. OF ROOTS & NO. OF SERIES TERMS ...............  500
     NO. OF BEGINNING TIME STEPS .......................   25
     NO. OF ENDING TIME STEP ...........................  241
     NO. OF TIME INTERVALS FOR PRINTED OUT SOLUTION ....    1
     INSTANTANEOUS SOURCE CONTROL = 0 FOR INSTANT SOURCE    1
     SOURCE CONDITION CONTROL = 0 FOR STEADY SOURCE ....  240
     INTERMITTENT OUTPUT CONTROL = 0 NO SUCH OUTPUT ....    1
     CASE CONTROL =1 THERMAL, = 2 FOR CHEMICAL, = 3 RAD     2

     SOIL ORGANIC CARBON CONTENT (OC) ..................   0.50000
     ORGANIC CARBON ADSORPTION COEFFICIENT (KOC) .......  0.3100E+02
     INITIAL CONTAMINANT LOAD (MG/KG) ..................  0.0000E+00
     INITIAL CONTAMINANT LOAD (KG) .....................  0.7300E+03

     AQUIFER DEPTH, = 0.0 FOR INFINITE DEEP (METERS) ...   0.00000
     AQUIFER WIDTH, = 0.0 FOR INFINITE WIDE (METERS) ...   0.00000
     BEGIN POINT OF X-SOURCE LOCATION (METERS) .........  -1.58100
     END POINT OF X-SOURCE LOCATION (METERS) ...........   1.58100
     BEGIN POINT OF Y-SOURCE LOCATION (METERS) .........  -1.58100
     END POINT OF Y-SOURCE LOCATION (METERS) ...........   1.58100
     BEGIN POINT OF Z-SOURCE LOCATION (METERS) .........   0.00000
     END POINT OF Z-SOURCE LOCATION (METERS) ...........   0.00000

     POROSITY ..........................................   0.25000
     HYDRAULIC CONDUCTIVITY (METER/HOUR) ...............   0.03600
     HYDRAULIC GRADIENT ................................   0.00300
     LONGITUDINAL DISPERSIVITY (METER) .................   2.16000
     LATERAL DISPERSIVITY (METER) ......................   0.20000
     VERTICAL DISPERSIVITY (METER) .....................   0.02000
     DISTRIBUTION COEFFICIENT, KD (M**3/KG) ............   0.00016
     SOURCE CONCENTRATION (mg/L) .......................   0.00000

     MOLECULAR DIFFUSION MULTIPLY BY TORTUOSITY(M**2/HR)  0.3528E-05
     DECAY CONSTANT (PER HOUR) .........................  0.0000E+00
     BULK DENSITY OF THE SOIL (KG/M**3) ................  0.1700E+04
     DENSITY OF WATER (KG/M**3) ........................  0.1000E+04
     ACCURACY TOLERANCE FOR REACHING STEADY STATE ......  0.1000E-01
     TIME INTERVAL SIZE FOR THE DESIRED SOLUTION (HR) ..  0.7300E+03
     DISCHARGE TIME (HR) ...............................  0.1752E+06
     WASTE RELEASE RATE (KCAL/HR), (KG/HR), OR (CI/HR) .  0.7300E+03
```

The next section of the AT123D output file contains the coordinates (in meters) where contaminant concentrations were determined. The number of points for each direction are dependent on values entered for x, y and z axis displayed above.

```
X COORDINATES ...
        .00      5.00     10.00     15.00     20.00     25.00     30.00     35.00

              Y COORDINATES ...
      20.00     10.00       .00    -10.00    -20.00

              Z COORDINATES ...
        .00      5.00     10.00
```

The next portion of the output report contains a list of transient source release rates in kilograms per month. The number of transient source release rates is dependent on the length of the SESOIL model scenario.

☞ *The transient source release data is the monthly contaminant load from the soil column as determined by SESOIL.*

```
LIST OF TRANSIENT SOURCE RELEASE RATE
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .2011E-03   .6709E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .1362E-02   .1639E-02   .1394E-02   .9408E-03   .6251E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .1272E-02   .1533E-02   .1304E-02   .8794E-03   .5842E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .1187E-02   .1428E-02   .1214E-02   .8180E-03   .5431E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .1102E-02   .1324E-02   .1125E-02   .7576E-03   .5029E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .1020E-02   .1224E-02   .1039E-02   .6995E-03   .4642E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .9404E-03   .1128E-02   .9569E-03   .6442E-03   .4275E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .8655E-03   .1038E-02   .8798E-03   .5922E-03   .3930E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .7952E-03   .9531E-03   .8078E-03   .5437E-03   .3607E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00   .7296E-03   .8743E-03   .7408E-03   .4985E-03   .3307E-03
   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00   .0000E+00
   .0000E+00
```

10.2.3 AT123D Results

The next section of the AT123D output file presents the model results. This section is divided into the initial results and predicted contaminant groundwater concentrations.

10.2.3.1 Initial Results

The initial model results include the retardation factor, retarded Darcy velocity, retarded longitudinal dispersion coefficient, retarded lateral dispersion coefficient and retarded vertical dispersion coefficient. A portion of the AT123D output is presented below.

```
RETARDATION FACTOR ...............................   .3822E+01
RETARDED DARCY VELOCITY (M/HR) ...................   .3768E-06
RETARDED LONGITUDINAL DISPERSION COEF. (M**2/HR) ..  .2901E-01
RETARDED LATERAL DISPERSION COEFFICIENT (M**2/HR) .  .2901E-01
RETARDED VERTICAL DISPERSION COEFFICIENT (M**2/HR)   .2901E-01
```

10.2.3.1.1 Retardation Factor

The retardation factor is the unitless ratio of the groundwater seepage velocity to the rate of organic contaminant migration. The retardation factor is used to estimate the slower rate of contaminant migration due to sorption to the solid aquifer matrix. The retardation factor is determined based on aquifer and contaminant properties using the following expression:

$$R_d = 1 + \frac{\rho_b K_d}{n_e}$$

Where:

Parameter	Description
K_d	Distribution coefficient
n_e	Effective porosity
ρ_b	Bulk density of the soil
R_d	Retardation factor

10.2.3.1.2 Retarded Darcy Velocity

The retarded Darcy velocity in meters/hour is determined using the following equation.

$$\vec{U} = \frac{K_h \nabla}{n_e R_d}$$

Parameter	Description
∇	Hydraulic gradient (Del operator with respect to *x*, *y*, and *z*)
K_h	Hydraulic conductivity
n_e	Effective porosity
R_d	Retardation factor
$\vec{U}$	The retarded Darcy velocity vector

10.2.3.1.3 Retarded Dispersion Coefficients

The next three lines of the output file contain the retarded longitudinal, lateral and vertical dispersion coefficient in meters^2/hour. The retarded dispersion coefficients are calculated using the following equations.

$$K_{xx} = \alpha_L U + \frac{D}{n_e R_d}$$

$$K_{yy} = \alpha_T U + \frac{D}{n_e R_d}$$

$$K_{zz} = \alpha_V U + \frac{D}{n_e R_d}$$

Where:

Parameter	Description
α_L	Longitudinal dispersivity
α_T	Transverse dispersivity
α_V	Vertical dispersivity
D	Molecular diffusion coefficient multiply by tortuosity
K_{xx}	Longitudinal component of the retarded dispersion tensor (x-axis)
K_{yy}	Transverse component of the retarded dispersion tensor (y-axis)
K_{zz}	Vertical component of the retarded dispersion tensor (z-axis)
n_e	Effective porosity
R_d	Retardation factor
U	The magnitude of the retarded seepage velocity vector ($\vec{U}$)

10.2.4 Contaminant Concentration Results

The next section of the output file displays the distribution of contaminant mass in ppm for each time step and coordinate simulated. The results of the AT123D program are presented as concentration data tables grouped by time steps in days. A portion of an AT123D output file is presented below:

```
DISTRIBUTION OF CHEMICALS IN PPM AT   3650.00 DAY

                    Z =        .00
                                                             X
   Y          .00        5.00       10.00       15.00       20.00       25.00       30.00       35.00

 20.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
 10.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
   .00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
-10.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
-20.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00

                    Z =       5.00
                                                             X
   Y          .00        5.00       10.00       15.00       20.00       25.00       30.00       35.00
```

```
 20.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
 10.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
   .00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
-10.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
-20.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00

                    Z =      10.00
                                                        X
   Y         .00        5.00       10.00       15.00       20.00       25.00       30.00       35.00

 20.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
 10.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
   .00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
-10.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
-20.00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00    .000E+00
```

☞ *SEVIEW includes its own text editor that can be used to examine the contents of any SESOIL (.OUT) or AT123D (.ATO) output file. The basic features of the SEVIEW edit command are similar to other Windows text editors and word processors, except it is much faster when working with the very large output files created by SESOIL! See Appendix C for additional information on the SEVIEW text editor.*

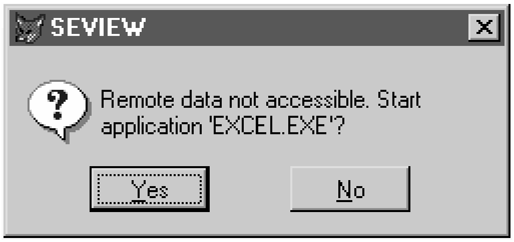
☞ *Although, the AT123D output file cannot be modified, the file may be saved as a new file. In addition, the output file may be searched using the* ***Find*** *and* ***Find Again*** *commands. Selected data may be copied from the output file using the Windows* ***Copy*** *command.*

11 Trouble Shooting

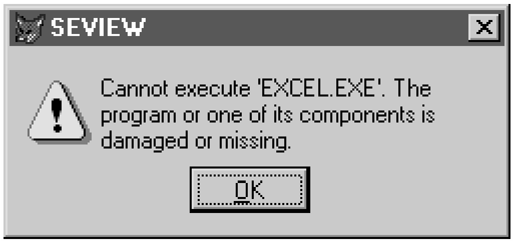
11.1 Solutions to Common Problems

This section provides solutions to common problems users have encountered using SEVIEW.

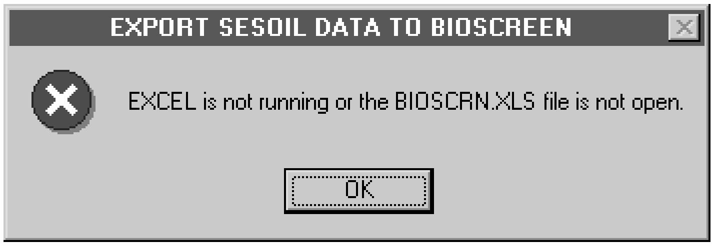
Problem: SEVIEW displays the following set of error messages when you copy the SESOIL data to BIOSCREEN.



Remote data not accessible. Start application 'EXCEL.EXE'?



Cannot execute 'EXCEL.EXE'. The program or one of its components is damaged or missing.



EXCEL is not running or the BIOSCRN.XLS file is not open.

Solution: Start Microsoft EXCEL and/or open the BIOSCRN4.XLS spreadsheet file.

12 References

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Appendix A

Introduction and Overview of the SESOIL Model

Portions of this Appendix were originally presented
as part of
"The New SESOIL User's Guide"
prepared for the
Wisconsin Department of Natural Resources

[redacted]

A1.0 Introduction to SESOIL

SESOIL is an acronym for **Seasonal Soil** compartment model and is a one-dimensional vertical transport model for the unsaturated soil zone. It is an integrated screening-level soil compartment model designed to simultaneously model water transport, sediment transport, and contaminant fate. It was developed for EPA's Office of Water and the Office of Toxic Substances (OTS) in 1981 by Arthur D. Little, Inc. SESOIL was updated in 1984 to include a fourth soil compartment (the original model included up to three layers) and the soil erosion algorithms (Bonazountas and Wagner, 1984). SESOIL is based on mass balance and partitioning of the contaminant between the dissolved, sorbed, vapor, and pure phases. A comprehensive evaluation of SESOIL performed by Watson and Brown (1985) uncovered numerous deficiencies in the model, and subsequently, SESOIL was modified extensively by Hetrick et al., at Oak Ridge National Laboratory (ORNL) to enhance its capabilities (see Hetrick et al., 1986, 1988, 1989). The version of SESOIL included with SEVIEW was modified in 1997 by M. J. Barden then of the Wisconsin Department of Natural Resources to correct a mass balance error and by R. A. Schneiker to run to 999 years. SESOIL is a public model and is written in FORTRAN.

☞ *The version of SESOIL included with SEVIEW includes an improved mass balance routine.*

SESOIL was developed as a screening-level model, utilizing less soil, chemical, and climatological data than most other similar models. Output from the SESOIL model includes time-varying contaminant concentrations at various soil depths and contaminant loss from the unsaturated zone in terms of surface runoff, leaching to groundwater, volatilization, and biodegradation.

The SESOIL model accepts time-varying contaminant loading. For example, it is able to simulate chemical releases to soil from a variety of sources such as landfill disposal, spills, agricultural applications, leaking underground storage tanks, or deposition from the atmosphere. Other potential applications of SESOIL include long term leaching studies from waste disposal sites, pesticide and sediment transport on watersheds, studies of hydrologic cycles and water balances of soil compartments, and pre-calibration runs for other simulation models. One may also run the model to estimate the effect of various site management or design strategies on contaminant distribution in the environment.

SESOIL can be used as a screening tool in performing exposure assessments. OTS used the model to predict the behavior of contaminants in soil compartments for analyzing and prioritizing chemical exposures. A number of studies have been conducted on the SESOIL model including sensitivity analysis, comparison with other models, and comparisons with field data (Bonazountas et al., 1982; Wagner et al., 1983; Hetrick, 1984; Kincaid et al., 1984; Watson and Brown, 1985; Hetrick et al., 1986; Melancon et al., 1986; Hetrick et al., 1988; Hetrick et al., 1989). SESOIL has been applied to: risk assessments concerning direct coal liquefaction (Walsh et al., 1984), incineration of hazardous waste (Holton et al., 1985; Travis et al., 1986), transport of benzene to groundwater (Tucker et al., 1986), soil cleanup levels in California (Odencrantz et al., 1991, 1992), and site sensitivity ranking for Wisconsin soils for the Wisconsin Department of Natural Resources (Ladwig et al., 1993)

The soil compartment in SESOIL extends from the surface through the unsaturated zone to the groundwater table. Typically, SESOIL is used to estimate the rate of migration of chemicals through soil and the concentration of the chemicals in soil layers following chemical release to the soil environment. SESOIL simulation of chemical persistence considers mobility, volatility, and degradation. The model performs calculations on an annual or monthly basis, and can simulate up to 999 years of chemical transport.

The model requires several types of chemical- and site-specific data to estimate the concentration of the chemical in the soil, its rate of leaching toward groundwater, and the impact of other environmental pathways. The user is required to provide chemical properties and release rates, and soil and climate data. This Appendix along with the SEVIEW User's Guide are designed to provide users of SESOIL with the information needed to efficiently and appropriately run the model and interpret the results.

A2.0 SESOIL Model Description

SESOIL is a one-dimensional vertical transport model for the unsaturated soil zone. SESOIL can consider only one chemical at a time and the model is based on mass balance and equilibrium partitioning of the chemical between different phases (dissolved, sorbed, vapor, and pure). The SESOIL model was designed to perform long-term simulations of chemical transport and transformations in the soil. The model uses theoretically derived equations to represent water transport, sediment transport on the land surface, contaminant transformation, and migration of the contaminant to the atmosphere and groundwater. Climatic data, compartment geometry, and soil and chemical property data are the major components used in the equations.

The expression "long term" applies to both annual and monthly simulations in SESOIL, and is used in contrast to "short-term" models which employ a storm-by-storm resolution. Some soil models are designed to estimate contaminant distribution in the soil after each major storm event, and determine chemical concentrations in the soil on a daily basis (e.g., see Patterson et al., 1984). These models are data intensive, requiring, for example, hourly rainfall input and daily maximum and minimum temperatures. SESOIL, on the other hand, estimates contaminant distribution in the soil column and on the watershed after a "season", which can be defined by the user as a year or a month. This is accomplished using a statistical water balance analysis and a washload routine statistically driven within the season. This approach saves time for the user by reducing the amount of data that must be provided, and also reduces computer time and resource requirements since fewer computations are required.

Two operation options are available for running SESOIL: annual estimates (Option A) requiring annual climatic data, and monthly estimates (Option M) requiring monthly data. It is recommended that the monthly option always be selected as it will provide a better estimate of chemical movement through the soil. Option A will not be discussed further in this report with the exception of the hydrologic cycle, which implements the annual algorithm as described below. The annual option has not been changed from the original model, and those users interested in the annual option are referred to the report by Bonazountas and Wagner (1984).

☞ *When used within SEVIEW, all SESOIL runs are performed using the monthly option.*

The processes modeled by SESOIL are categorized into three cycles: hydrology, sediment, and contaminant transport. Each cycle is a separate sub-model within the SESOIL code. Most mathematical environmental simulation models may be categorized as stochastic or deterministic models. Both the stochastic and deterministic models are theoretically derived. Stochastic models incorporate the concept of probability or some other measure of uncertainty, while deterministic models describe the system in terms of cause/effect relationships. SESOIL employs a stochastic approach for the hydrologic and washload cycles, and a deterministic approach for the pollutant transport cycle.

A2.1 The Soil Compartment

In SESOIL, the soil compartment (or column) is a cell extending from the surface through the unsaturated zone to the upper level of the saturated soil zone, also referred to as the aquifer or groundwater table. While SESOIL estimates the contaminant mass entering groundwater, the saturated zone is not modeled. The output from SESOIL can be used for generating input values for groundwater transport models to simulate chemical movement in the saturated zone.

> *SEVIEW provides a link to the AT123D and BIOSCREEN saturated zone transport and fate models.*

The soil compartment is treated differently by the hydrologic cycle and the pollutant cycle in SESOIL. In the hydrologic cycle, the whole soil column is treated as a single homogeneous compartment extending from the land surface to the water table. The pollutant cycle breaks the soil column into several compartments, also called layers. The layers in the pollutant cycle can be further broken up into sub-layers. Each soil layer (sub-layer) is considered as a compartment with a set volume and the total soil column is treated as a series of interconnected layers (sub-layers). Each layer (sub-layer) can receive and release contaminants to and from adjacent layers (sub-layers).

The dimensions of the soil compartment are defined by the user. The width and length of the column are defined as the area of application of contaminant released to the soil, and the depth to the groundwater is determined from the total thickness of user-defined soil layers that are used in the pollutant cycle. The soil column can be represented in 2, 3, or 4 distinct layers. Up to 10 sub-layers can be specified for each layer, each having the same soil properties as the layer in which they reside.

There is no optimal areal size for the soil layers (sub-layers); the dimensions of the soil column can be specified to cover any area from one square centimeter to several square kilometers. The area of the compartments is important for mass balance, but in terms of contaminant concentrations the area of the soil column is irrelevant since it is constant for all layers (sub-layers). Note that the equations in SESOIL have been normalized to an area of one square centimeter.

Depending on the application, layer thicknesses can range from a shallow root zone of 5-25 centimeters, to a deep layer of more than 10 meters. It is suggested that the minimum thickness of a layer is one centimeter. When a contaminant enters a layer or sub-layer, the model assumes instantaneous and uniform distribution of the chemical throughout that layer or sub-layer. The model performs mass balance calculations over each entire soil layer (sub-layer); there is no concentration gradient within a layer (sub-layer). For a given amount of chemical released, the larger the layer (sub-layer), the lower the calculated chemical concentration. For this reason, SESOIL was discretized to allow as many as ten sub-layers in each of the four possible major layers. Thus, the user may define as many as 40 smaller compartments using these sub-layers. The result is an increase in the resolution of the model.

A2.2 SESOIL Cycles

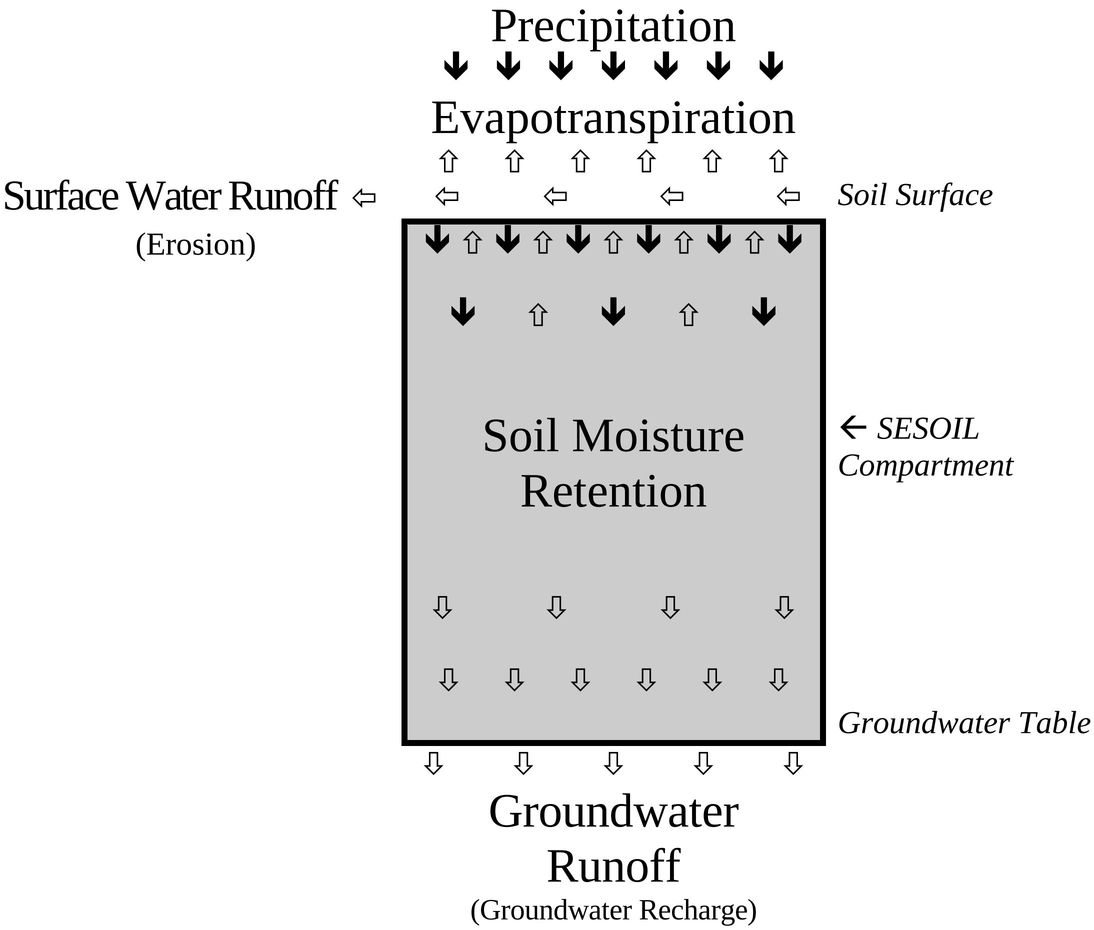
Contaminant transport and fate in the unsaturated soil zone is controlled by complex processes affected by chemical, soil, and hydrogeological properties. In SESOIL, these processes are included in one of three cycles: the hydrologic cycle (moisture movement or flow through the compartment), the sediment or washload cycle (soil erosion), and the pollutant fate cycle (contaminant transport and fate). SESOIL integrates the three sub-models, in to one. The specific processes associated with each cycle are accounted for in the sub-models. The cycles and their associated processes are summarized in Table 12. Figure A2.1 shows a schematic of the soil column.

Table 12 SESOIL Cycles

Hydrologic Cycle
• Rainfall • Groundwater runoff (recharge) • Capillary rise • Soil moisture retention (storage) • Infiltration • Surface runoff • Evapotranspiration
Sediment Cycle
• Sediment washload (erosion due to storms)
Pollutant Fate Cycle
• Advection • Diffusion (air phase) • Sorption • Washload • Leaching to groundwater • Chemical degradation/decay • Cation exchange • Volatilization • Hydrolysis • Surface runoff • Metal complexation

The hydrologic cycle is completed first in SESOIL, followed by the sediment cycle, and these results are used in the pollutant fate cycle. The hydrologic cycle is based on a statistical, dynamic formulation of a vertical water budget. It has been adapted to account for either yearly or monthly simulations and for moisture variations in the soil. The hydrologic cycle controls the sediment cycle, which is a theoretical monthly washload routine. The pollutant cycle simulates transport and transformation processes in three phases present in the soil compartment: soil-air or gaseous phase, soil-moisture phase, and adsorbed or soil-solids phase. The three major cycles are summarized in the sections that follow.

Figure A2.1
Schematic of the Monthly Hydrologic Cycle



A2.3 Hydrologic Cycle

The hydrologic cycle is one-dimensional (considers vertical movement only) and focuses on the role of soil moisture (or interstitial pore water) in the soil compartment. The hydrologic cycle sub-model calculates results for the hydrology of a site and passes these results to both the sediment washload cycle and the pollutant fate cycle. The hydrologic cycle used in SESOIL is an adaptation of the water balance dynamics theory of Eagleson (1978). The theory can be described as a dimensionless analytical representation of an annual water balance. It is itself a model based on simplified models of interacting hydraulic processes, including terms for the climate, soil, and vegetation. These processes are coupled through statistically based modeling. A schematic of the hydrologic cycle is presented in Figure A2.1.

It is beyond the scope of this guide to present the detailed physics and mathematical expressions of the model. The hydrologic cycle is thoroughly described by Eagleson (1978) and summarized by Bonazountas and Wagner (1984), and is based on the water balance equations shown below. All of these parameters are expected or mean annual values, and in SESOIL they are expressed in centimeters.

$$P - E - MR = S + G = Y \qquad \text{(A1)}$$

$$I = P - S \qquad \text{(A2)}$$

Where:

Parameter	Description
P	Precipitation
E	Evapotranspiration
MR	Moisture retention
S	Surface runoff
I	Infiltration
Y	Yield
G	Groundwater runoff or recharge (includes term for capillary rise)

Precipitation is represented by Poisson arrivals of rectangular gamma-distributed intensity pulses that have random depth and duration. Infiltration is described by the Philip equation (Philip, 1969), which assumes the medium to be effectively semi-infinite, and the internal soil moisture content at the beginning of each storm and inter-storm period to be uniform at its long-term average. Percolation to the groundwater is assumed to be steady throughout each time step of the simulation, at a rate determined by the long-term average soil moisture content. Capillary rise from the water table is assumed to be steady throughout the time period and to take place to a dry surface. The work of Penman (1963), Van den Honert (1948), and Cowan (1965) is employed in calculating evapotranspiration (Eagleson, 1978). Surface runoff is derived from the distribution of rainfall intensity and duration, and by use of the Philip infiltration equation. The effects of moisture storage are included in the monthly option in SESOIL, based on the work of Metzger and Eagleson (1980).

Eagleson's theory assumes a one-dimensional vertical analysis in which all processes are stationary in the long-term average. The expression "long term" applies to both annual and monthly simulations in SESOIL, and is used in contrast to "short-term" models which employ a storm-by-storm resolution. Also, Eagleson's approach assumes that the soil is homogeneous and that the soil column is semi-infinite in relation to the surface processes. Thus, in the hydrologic cycle of SESOIL, the entire unsaturated soil zone is conceptualized as a single layer (or compartment) and the prediction for soil water content is an average value for the entire unsaturated zone.

While the user can provide varying permeability values as input for each of the four major soil layers for the pollutant cycle in SESOIL, the hydrologic cycle will compute and use the depth-weighted average permeability according to the formula:

$$K_z = \frac{d}{\sum_{i-1}^{n} \frac{d_i}{K_i}} \qquad \text{(A2)}$$

Where:

Parameter	Description
K_z	Vertical averaged permeability (cm^2),
K_i	Permeability of layer *i* (cm^2),
d	Depth from surface to groundwater (cm),
d_i	Thickness of layer *i* (cm)

Thus, the user should exercise care when applying SESOIL to sites with large vertical variations in soil properties. The average permeability calculated by Equation A2 in the hydrologic cycle may not be what the user intended and the resulting computed average soil moisture content may not be valid.

There is no explicit consideration of snow and ice, which are entered as precipitation. The model assumes that the water table elevation is constant with no change in groundwater storage from year to year. Bonazountas et al. (1984) adopted this theory for both annual and monthly simulations.

The process in Equations A1 and A2 are written in terms of the soil moisture content, and solution of the equations is accomplished by iterating on soil moisture until the calculated value for precipitation is within 1.0% of the input value. When this iteration is complete, the components such as infiltration, evapotranspiration, etc., in Equations A1 and A2 are also established. SESOIL uses this procedure in both the annual and monthly routines. The monthly routine is an extension of the annual routine; both are discussed further below.

A2.3.1 Annual Cycle

The annual water balance routine is based on Eagleson's (1978) theory. It encompasses one year, so multiple years have to be simulated as separate cycles. This routine simply determines the soil moisture content based on solution to Equations A1 and A2 using annual climatic parameters. When the value for soil moisture content is arrived at through the iteration technique, the various processes described in Equations A1 and A2 are established. The theoretical basis for the annual dynamic hydrologic cycle used in SESOIL has been validated by Eagleson (1978). Annual model predictions were compared with empirical observations for five years of precipitation data at both a subhumid and arid climate location, with close agreement.

☞ *The storage effects in the soil are not considered in the annual option.*

A2.3.2 Monthly Cycle

The monthly water balance routine is based on the same theory as the annual routine, with modifications made to the details of moisture transfer from month-to-month (handling of moisture storage), and the radiation effects. The initial value for soil moisture content is calculated in SESOIL by summing the appropriate monthly climatic input data (for the first year) to obtain annual values and using the annual cycle algorithm. For each month the values for precipitation, mean storm number, and mean length of the rain season are multiplied by 12 in order to obtain "annual" values. Equations A1 and A2 are solved to compute the soil moisture content. Results for the components (infiltration, evapotranspiration, etc.) are divided by 12 to attain average monthly values.

Note that if long-term average climatic data are used as input for each year (input for each month is the same from year to year), one would expect that the results for the hydrology for each month would be identical from year to year. However, since the initial soil moisture content is computed as stated above for the first month (of the first year), this value will be different than the soil moisture calculated for the twelfth month that is used for the first month of the following year. Thus, hydrology results will not be identical for the first two years, however, they will be identical thereafter.

The monthly cycle in SESOIL does account for the change in moisture storage from month to month, incorporating the work of Metzger and Eagleson (1980). Also, the SESOIL evapotranspiration algorithm has been modified from the original work of Eagleson (1978) to include seasonal changes in average monthly radiation (radiation was a constant function of latitude before). Hetrick (1984) observed that hydrology predictions of the original SESOIL were insensitive to seasonal changes in meteorological data. To model the hydrology more realistically, an algorithm from the AGTEHM model (Hetrick et al., 1982) which computes daily potential radiation (incoming radiation for cloudless skies) for a given latitude and Julian date (December 31 = 365) is now used. The middle day of the month is used in the algorithm and the effect of cloud cover is calculated with the expression (Hetrick et al., 1982):

$$\overline{S} = S\left[\left(1 - C\right) + kC\right] \qquad \text{(A4)}$$

Where:

Parameter	Description
$\overline{S}$	Average monthly radiation,
S	Potential radiation,
C	Fraction of sky covered by clouds, and
K	Transmission factor of cloud cover.

The value for k used in the models 0.32, suggested by Hetrick et al. (1982). Since latitude and monthly cloud cover are required input for SESOIL, no new input data are needed to support this modification. There are now more pronounced monthly changes in evapotranspiration predictions (see Hetrick et al., 1986).

Although SESOIL does produce monthly results for soil moisture content of the root zone, defined in the model as the first 100 cm depth from the surface, this option has not been fully developed. Thus, values for soil moisture for the root zone will usually be identical to those for the entire soil column, and only very dry climates may cause a difference (M. Bonazountas, personal communication, 1986).

SESOIL model predictions (using the monthly option) of watershed hydrologic components have been compared with those of the more data intensive terrestrial ecosystem hydrology model AGTEHM (Hetrick et. al., 1982) as well as to empirical measurements at a deciduous forest watershed and a grassland watershed (see Hetrick et al., 1986). Although there were some differences in monthly results between the two models, good agreement was obtained between model predictions for annual values of infiltration, evapotranspiration, surface runoff, and groundwater runoff (recharge). Also, SESOIL model predictions compared well with the empirical measurements at the forest stand and the grassland watersheds.

A2.3.3 Hydrologic Model Calibration

Calibration of unsaturated soil zone models can be uncertain and difficult because climate, soil moisture, soil infiltration and percolation are strongly interrelated parameters that are difficult and expensive to measure in the field. However, if at all possible, input parameters for any unsaturated soil zone model should be calibrated so that hydrologic predictions agree with observations. In SESOIL, all input parameters required for the hydrologic cycle can be estimated from field studies with the exception of the soil pore disconnectedness index. This parameter is defined as the exponent relating the "wetting" or "drying" time-dependent permeability of a soil to its saturated permeability (Eagleson, 1978; Eagleson and Tellers, 1982). Brooks and Corey (1966) presented the following relationship:

$$K(S) = K(1)S^c \qquad \text{(A5)}$$

Where:

Parameter	Description
K(1)	Saturated hydraulic conductivity (cm/s),
K(S)	Hydraulic conductivity at S (cm/s),
S	Percent saturation,
c	Soil pore disconnectedness index.

This parameter is not commonly found in the literature. Default values for soil pore disconnectedness index suggested by Eagleson (1978) and Bonazountas and Wagner (1981, 1984) are: clay 12; silty clay loam 10; clay loam 7.5; silt loam 5.5; sandy loam 6; sandy clay loam 4; and sand 3.7 (see Section 0). However, when data are available, this parameter should be varied first to optimize agreement between SESOIL results and hydrologic measurements. It should be noted that most unsaturated soil zone models require detailed data (which are difficult to obtain), such as soil moisture characteristic curves. The "one variable" approach of Eagleson (1978) simplifies the data estimation process and reduces computational time.

Other sensitive parameters for the hydrologic cycle are the effective porosity and the intrinsic permeability (e.g., see Hetrick et al., 1986, 1989). While other parameters can be varied when calibrating the model to measured hydrologic data, it is recommended that the user vary the soil pore disconnectedness index first, followed by the permeability and/or porosity. See Section 0 for additional information on required soil property parameters.

A2.4 Sediment Washload Cycle

☞ *The SESOIL sediment cycle is optional.*

In contaminant transport models, estimates of erosion and sediment yield on watersheds may be needed in order to compute the removal of sorbed chemicals on eroded sediments. A major factor in this process is the surface runoff, rainwater which does not infiltrate the soil and may carry dissolved contaminant. Surface runoff is computed as part of the hydrologic cycle. Erosion is a function of the rate of surface runoff and several other factors. These factors include the impact of raindrops which detaches soil particles and keeps them in motion as overland flow, surface features such as vegetation and roughness, and infiltration capacity. Because of the difficulty in directly measuring washload using water quality monitoring techniques, estimation techniques and models are widely employed.

If contaminant erosion (surface runoff) is considered negligible, the washload cycle can be neglected. If the option is used, SESOIL employs EROS, a theoretical sediment yield model (Foster et al., 1980), which is part of CREAMS model (Knisel, 1980; Foster et al., 1980). The erosion component considers the basic processes of soil detachment, transport, and deposition. The EROS model uses separate theoretically derived equations for soil detachment and sediment transport. Separate equations are needed for these two processes because the relationship of the detachment process to erosion is different than the relationship between erosion and transport.

For the detachment process, the model employs the Universal Soil Loss Equation (USLE) (Wischmeier and Smith, 1978), modified by Foster et al. (1980) for single storm events. The USLE is applicable for predictions of annual sediment erosion originating mainly from small watersheds which are subject to sheet and rill erosion. Detachment of soil particles occurs when the sediment load already in the overland flow is less than the sediment capacity of this flow. The equation takes into account soil erodibility (the rate of soil loss per storm), which varies for different soil types and texture classes. The USLE considers topography, since both the length and the steepness of the land slope affect the rate of rain-induced soil erosion. Also, the land cover (e.g. vegetation) and the roughness of the soil surface affect the rate of erosion and the rate of overland transport. The USLE includes a parameter called “Manning's n”, or roughness coefficient, to model these influences.

To model the sediment transport capacity for overland flow, EROS incorporates the Yalin Transport Equation (Yalin, 1963), modified for non-uniform sediment with a mixture of particle sizes and densities. The model estimates the distribution of sediment particles transported as sand, silt, and clay, and the fraction of organic matter in the eroded sediment. SESOIL computations of sediment transport are performed for each particle size type, beginning at the upper end of a slope and routing sediment down slope.

The EROS model in SESOIL accounts for several surface features which may divert and slow the overland flow, allowing settling and deposition of the washload. These include vegetation, which slows the flow and filters out particles, and topography, which includes surface characteristics such as roughness and the existence of small depressions. Change in slope and loss of water through infiltration into the soil will reduce the flow rate and encourage settling of soil particles. Organic matter is distributed among the particle types based on the proportion of primary clay in each type (Foster et al., 1980). Soil receiving the deposited sediment is referred to as enriched. EROS computes sediment enrichment based on the ratio of the surface area of the sediment and organic matter to that of the surface area of the residual soil (Knisel et al., 1983).

A2.4.1 Implementation in SESOIL

The EROS model uses characteristic rainfall and runoff factors for a storm to compute erosion and sediment transport for that storm (Foster et al., 1980). Hydrologic input to the erosion component consists of rainfall volume, rainfall erosivity, runoff volume, and the peak rate of runoff for each storm event. These terms drive soil detachment and subsequent transport by overland flow. Note that input data for the hydrologic cycle of SESOIL includes total monthly precipitation, the number of storms per month, and the mean duration of each rainfall event. Since SESOIL provides only monthly estimates of hydrologic parameters and in order to couple the SESOIL and EROS models, a statistical method is used to generate the amount of rainfall and duration of each storm for every rainfall event during the month. This algorithm employs a model featuring probability distributions in order to estimate the individual storm parameters (Eagleson, 1978; Grayman and Eagleson, 1969).

The washload cycle has been implemented with two subroutines in addition to the EROS; model PARAM and STORM, which take the input data for and results generated by the hydrologic cycle and adapt them for use. The PARAM subroutine supports EROS by first retrieving the hydrologic input data (e.g. the number of storm events per month and the depth of rainfall) read by SESOIL and then setting specific parameters applicable to the STORM and EROS subroutines. The STORM subroutine then uses the PARAM results and statistically generates information about each storm using the algorithm mentioned above. Thus, the coupled SESOIL EROS model does not require any additional hydrologic input parameters for individual storms. However, it should be recognized that estimates of rainfall for each storm may be quite different than the actual values.

Additional data needed for the sediment cycle include the washload area, the fraction of sand, silt and clay in the soil, the average slope, slope length of the representative overland flow profile, the soil erodibility factor, the soil loss ratio, the contouring factor, and Manning's n coefficient for soil cover and surface roughness. Example values for these parameters can be found in the CREAMS documentation (Knisel, 1980; Foster et al., 1980). Note that the washload area should be less than or equal to the pollutant application area.

EROS takes the information generated by both the PARAM and STORM subroutines and computes estimates of the sediment yield for each month. Information from the sediment cycle, along with information from the hydrologic cycle, is then provided to the pollutant fate cycle, which will be discussed in the next subsection.

The coupled SESOIL EROS model was evaluated by comparing predictions to published measured data (Hetrick and Travis, 1988). Two cornfield watersheds and one grassland watershed were included in the study. The sites differed in their management practices, soil type, ground cover, and meteorology. The model predictions were in fair to good agreement with observed data from the three watersheds, except for months where surface runoff came from one or two high intensity storms (Hetrick and Travis, 1988).

A2.5 Pollutant Fate Cycle

The pollutant fate cycle focuses on the various contaminant transport and transformation processes which may occur in the soil. These processes are summarized in Table 12, and are discussed in more detail in the subsections that follow. The pollutant fate cycle uses calculated results from the hydrologic cycle and the sediment washload cycle. Information from these cycles is automatically provided to the pollutant fate cycle.

In SESOIL, the ultimate fate and distribution of the contaminant is controlled by the processes interrelated by the mass balance Equation A6 below. The processes are selectively employed and combined by the pollutant fate cycle based on the chemical properties and the simulation scenario specified by the user. The actual quantity or mass of contaminant taking part any one process depends on the competition among all the processes for available contaminant mass. Contaminant availability for participation in these processes, and the contaminant rate of migration to the groundwater, depends on its partitioning in the soil between the gas (soil air), dissolved (soil moisture), and solid (adsorbed to soil) phases.

A2.5.1 Foundation

In SESOIL, any layer or sub-layer can receive contamination, store it, and export it to other sub-compartments. Downward movement of a contaminant occurs only with the soil moisture, while upward movement can occur only by vapor phase diffusion. Like the hydrologic cycle, the pollutant fate cycle is based on a mass balance equation (Equation A6) that tracks the contaminant as it moves in the soil moisture between sub-compartments. Upon reaching and entering a layer or sub-layer, the model assumes instantaneous uniform distribution of the contaminant throughout that layer or sub-layer. The mass balance equation is:

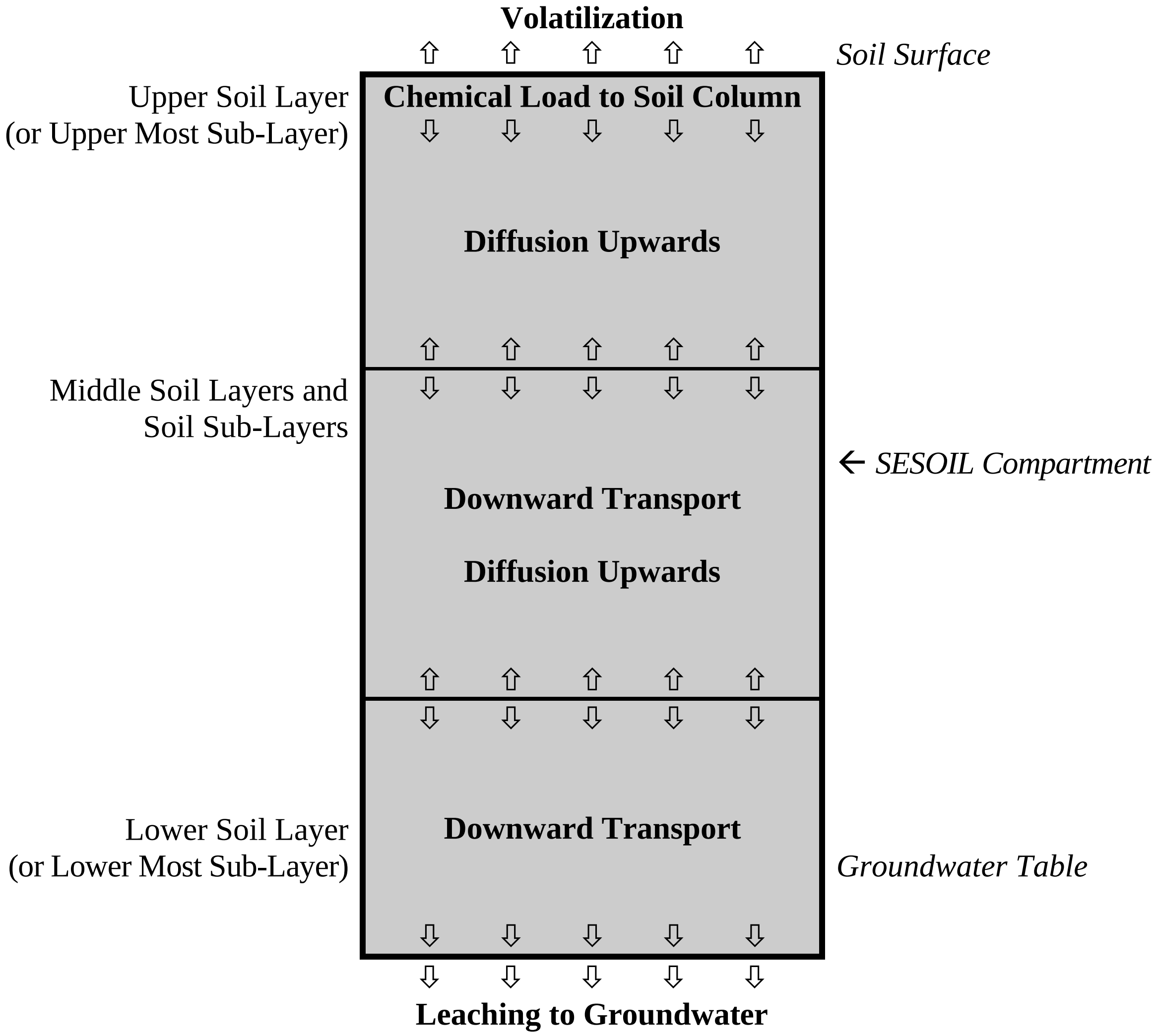
$$O(t-1) + l(t) = T(t) + R(t) + M(t) \qquad \text{(A6)}$$

Where:

Parameter	Description
$O(t-1)$	Amount of contaminant originally in the soil compartment at the time t-1 (µg/cm^2),
$l(t)$	Amount of contaminant entering the soil compartment during a time step (µg/cm^2),
$T(t)$	Amount of contaminant transformed within the soil compartment during the time step (µg/cm^2),
$R(t)$	Amount of contaminant remaining in the soil compartment at time t (µg/cm^2),
$M(t)$	Amount of contaminant migrating out of the soil compartment during the time step (µg/cm^2).

The fate of the contaminant in the soil column includes both transport and transformation processes, which depend on the chemical's partitioning among the three phases: soil air, soil moisture, and soil solids. The three phases are assumed to be in equilibrium with each other at all times (see Figure A2.2), and the partitioning is a function of user-supplied chemical-specific partition coefficients and rate constants. Once the concentration in one phase is known, the concentrations in the other phases can be calculated. The pollutant cycle of SESOIL is based on the chemical concentration in the soil water. That is, all the processes are written in terms of the contaminant concentration in soil water and the model iterates on the soil moisture concentration until the system defined by Equation A6 balances.

Figure A2.2
Schematic of Chemical Phases in the Soil Matrix



The contaminant concentration in soil air is calculated via the modified Henry's law:

$$C_{sa} = \frac{cH}{R(T + 273)} \qquad \text{(A7)}$$

Where:

Parameter	Description
C_{sa}	Contaminant concentration in soil air (µg/ml),
c	Contaminant concentration in soil water (µg/ml),
H	Henry's law constant (m^3 atm/mol),
R	Gas constant [8.2 E 10^{-5} m^3 atm/(mol ^{o} K)], and
T	Soil temperature (^{o} C).

The concentration adsorbed to the soil is calculated using the Freundlich isotherm (note that a cation exchange option, discussed later, is available in SESOIL),

$$s = K_d c^{\frac{1}{n}} \qquad \text{(A8)}$$

Where:

Parameter	Description
s	Contaminant adsorbed concentration (µg/g),
K_d	Contaminant distribution coefficient (µg/g)/ (µg/ml),
c	Contaminant concentration in soil water (µg/ml),
n	Freundlich exponent.

The total concentration of the contaminant in the soil is computed as:

$$c_o = f_a c_{sa} + \theta c + \rho_b s \qquad \text{(A9)}$$

Where:

Parameter	Description
C_o	Overall (total) contaminant concentration (µg/cm^3),
f_a	$f - \theta$ = the air-filled porosity (ml/ml),
C_{sa}	Contaminant concentration in soil air (µg/ml),
f	Soil porosity (ml/ml),
θ	Soil water content (ml/ml),
c	Contaminant concentration in soil water (µg/ml),
ρ_b	Soil bulk density (g/cm^3), and
s	Adsorbed contaminant concentration (µg/g).

In SESOIL, each soil layer (sub-layer) has a set volume and the total soil column is treated as a series of interconnected layers. Each layer (sub-layer) has its own mass balance equation (Equation A6) and can receive and release contamination to and from adjacent layers (sub-layers). Again, the individual fate processes that compose the SESOIL mass balance equations (e.g., volatilization, degradation) are functions of the contaminant concentration in the soil water of each zone and a variety of first-order rate constants, partitioning coefficients, and other constants. An iterative solution procedure is used to solve the system (the iteration parameter is the soil pore disconnectedness index). See Bonazountas and Wagner (1984) for the numerical solution procedure.

The pollutant cycle equations are formulated on a monthly basis and results are given for each month simulated. However, to account for the dynamic processes in the model more accurately, an explicit time step of 1 day is used in the equations. The monthly output represents the summation of results from each day.

In the event that the dissolved concentration exceeds the aqueous solubility of the contaminant, the dissolved concentration is assumed to equal the aqueous solubility. That is, if during solution of the mass balance equation for any one layer, the dissolved concentration exceeds the solubility of the chemical, the iteration is stopped for that time step and the solubility is used as the dissolved concentration. The adsorbed and soil-air concentrations are calculated using the chemical partitioning equations as before (Equations A7 and A8). To maintain the mass balance, the remaining contamination is assumed to remain in a pure phase (undissolved). Transport of the pure phase is not considered, but the mass of the chemical in the pure phase is used as input to that same layer in the next time step. Simulation continues until the pure phase eventually disappears. The pure phase capability was not part of the original model and was added to SESOIL by Hetrick et al. (1989).

The discussion in the subsections that follow introduces the user to major algorithms and processes simulated in the pollutant cycle of SESOIL.

A2.5.2 The Contaminant Depth Algorithm

The pollutant cycle in SESOIL is based on the contaminant concentration in soil moisture. In theory, a non-reactive dissolved contaminant originating in any unsaturated soil layer will travel to another soil layer or to the groundwater at the same speed as the moisture mass originating in the same soil layer. The movement of a reactive contaminant however, will be retarded in relation to the movement of the bulk moisture mass due to vapor phase partitioning and the adsorption of the contaminant on the soil particles. If it is assumed that no adsorption occurs, and the vapor phase is negligible, the contaminant will move at the same rate as water through the soil.

Originally, only the advective velocity was used in SESOIL to determine the depth the contaminant reached during a time step. The depth (D) was calculated as:

$$D = \frac{J_w t_c}{\theta} \tag{A10}$$

Where:

Parameter	Description
D	Contaminant depth,
J_w	Water velocity (cm/s),
t_c	Advection time (s), and
θ	Soil water content (cm^3/cm^3)

This approach allows all chemicals to reach the groundwater at the same time; irrespective of their chemical sorption characteristics. To account for retardation, SESOIL now uses the following equation to calculate the depth reached by a chemical with a linear equilibrium partitioning between its vapor, liquid, and adsorbed phases (Jury et al., 1984):

$$D = \frac{J_w t_c}{\theta + \rho_b K_d + \dfrac{f_a H}{R\left(T + 273\right)}} \tag{A11}$$

Where:

Parameter	Description
D	contaminant depth,
J_w	Water velocity (cm/s),
t_c	Advection time (s), and
θ	Soil water content (cm^3/cm^3)
ρ_b	Soil bulk density (g/cm^3)
K_d	Chemical distribution coefficient (µg/g)/ (µg/ml),
f_a	$f - \theta$ = the air-filled porosity (ml/ml),
H	Henry's law constant (m^3 atm/mol),
R	Gas constant [8.2 X 10^{-5} m^3 atm/(mol º K)], and
T	Soil temperature (º C).

SESOIL calculates the flux J_w for each layer using the infiltration rate and groundwater runoff (recharge) rate computed by the hydrologic cycle, and the depths and permeabilities input by the user. Note that a different permeability can be input for each of the four major soil layers. While the hydrologic cycle will use the depth weighted mean average of layer permeabilities according to Equation A2, the pollutant cycle does take into account the separate permeability for each layer in computing J_w at the layer boundaries according to the following equation:

$$J_{w,z} = \left[G + \left(I - G \right) \left(\frac{d_j}{d} \right) \right] \left(\frac{k_i}{K_z} \right) \qquad \text{(A12)}$$

Where:

Parameter	Description
$J_{w,z}$	Infiltration rate at depth z, which will be the boundary between two major layers (cm/s),
G	Groundwater runoff (recharge) (cm/s)
I	Infiltration at surface (cm/s)
d_j	Depth of soil column below depth z (cm),
d	Depth of soil column from surface to groundwater table (cm),
K_z	Intrinsic permeability (cm^2), defined by Equation A2, and
k_i	The vertical-averaged permeability for layer 1 (cm^2); is computed using Equation A2 except d in the numerator of Equation A2 is the sum of the layer depths above depth *z* and the summation in the denominator is from layer 1 to layer *i*.

The user is allowed two options for loading of a contaminant:

1. A spill loading where all the contamination is entered at the soil surface in the first time step of the month when the loading takes place, or
2. A steady application where the contaminant load is distributed evenly for each time step during the month at which the loading is specified.

Option 1 allows loading at the soil surface only (layer 1, sub-layer 1), whereas option 2 will allow loading in one or more of the four major layers. If sub-layers are specified, the loading will always be entered into the first (top) sub-layer of the major layer. While a contaminant can be loaded in each of the four major layers, the contamination cannot be loaded into each sub-layer of a major layer to get a specific initial concentration distribution for the major layer.

If there is a spill loading or if the contaminant is entered as a steady application in layer 1 (sub-layer 1), then the depth of the contaminant front is calculated using Equation A11 starting from the surface. If a steady loading is specified in layers 2, 3, and/or 4, then the depth of the contaminant front is assumed to begin at the middle of the lowest layer at which contaminant is loaded (sub-layer 1 of that layer if sub-layers are included) and Equation A11 is used to compute the depth of the contaminant front from that point. Subsequently, the contaminant is not allowed to enter a layer/sub-layer until the depth of the contaminant front has reached the top of that layer/sub-layer. When the contaminant depth reaches the groundwater table, contamination leaves the unsaturated zone by simply multiplying the groundwater runoff (recharge) rate by the concentration in the soil moisture.

Although a spill loading cannot be used in SESOIL for layers 2, 3, or 4, an initial soil-sorbed concentration can still be approximated for these layers. See Section 6.7.3 for more information.

A2.5.3 Volatilization/Diffusion

In SESOIL, volatilization/diffusion includes movement of the contaminant from the soil surface to the atmosphere and from lower soil layers to upper ones. Note that vapor phase diffusion in SESOIL operates in the upward direction only. The rate of diffusion for a chemical is determined by the properties of the chemical, the soil properties, and environmental conditions. The volatilization/diffusion model in SESOIL is based on the model of Farmer et al. (1980) and Millington and Quirk (1961) and is a discretized version of Fick's first law over space, assuming vapor phase diffusion as the rate controlling process. That is, the same equation is used for volatilization to the atmosphere as is used for diffusion from lower layers to upper ones. The vapor phase diffusion flux through the soil J_a (µg/cm^{2}s) is described as:

$$J_a = -D_a \left(\frac{f_a^{\frac{10}{3}}}{f^2} \right) \frac{dC_{sa}}{dz} \qquad \text{(A13)}$$

Where:

Parameter	Description
J_a	Vapor phase diffusion flux through the soil (µg/cm^{2}s),
D_a	Vapor diffusion coefficient of the compound in air (cm^2/s),
f_a	$f - \theta$ = the air-filled porosity (ml/ml),
f	Soil porosity (ml/ml),
d	Depth of soil column from surface to groundwater table (cm),
C_{sa}	Contaminant concentration in soil air (µg/ml) (from Equation A7), and
dz	Contaminant depth from the ground surface.

The volatilization algorithm in the original version of SESOIL allowed contaminant in the second (or lower) layer to volatilize directly to the atmosphere. This algorithm was modified by Hetrick et al. (1989). The contaminant can volatilize directly to the atmosphere from the surface layer, but if the chemical is in the second or lower layer, and the concentration in that layer is greater than the layer above it, then the chemical will diffuse into the upper layer rather than volatilize directly into the atmosphere.

An option the user has in the volatilization algorithm is to "turn off" the calculation by use of an input index parameter (for each layer). For example, if the index is set to 0.0 for each layer, the contaminant would not be allowed to diffuse upward or volatilize to the atmosphere; only downward movement of the contaminant with the soil moisture would occur. Also, if data are available, this index parameter can be varied to calibrate calculations to the measurements.

A2.5.4 Sorption Adsorption/Desorption And Cation Exchange

SESOIL includes two partitioning processes for movement of a contaminant from soil moisture to soil air or soil solids. These are the sorption process and the cation exchange mechanism.

The sorption process may be defined as the adhesion of contaminant molecules or ions to the surface of soil solids. Most sorption processes are reversible; adsorption describing the movement of contaminant onto soil solids and desorption being the partitioning of the chemical from solid into the liquid or gas phase (Lyman et al., 1982). Adsorption and desorption are usually assumed to be occurring in equilibrium and are therefore modeled as a single process (Bonazountas et al., 1984). Adsorption is assumed to occur rapidly relative to the migration of the contamination in soil moisture; it can drastically retard contaminant migration through the soil column.

SESOIL employs the general Freundlich equation (see Equation A8 above) to model soil sorption processes. The equation correlates adsorbed concentration with the dissolved concentration of the contaminant, by means of an adsorption coefficient and the Freundlich parameter. This equation has been found to most nearly approximate the adsorption of many contaminants, especially organic chemicals, and a large amount of data have been generated and are available in the literature (see Bonazountas and Wagner, 1984; Fairbridge and Finke, 1979; Lyman et al., 1982).

For most organic chemicals, adsorption occurs mainly on the organic carbon particles within the soil (Lyman et al., 1982). The organic carbon partition coefficient (K_{oc}) for organic chemicals can be measured or estimated (Lyman et al., 1982). K_{oc} is converted to the distribution coefficient (K_d) by multiplying by the fraction of organic carbon in the soil.

Values for the Freundlich exponent can be found in the literature. They generally range between 0.9 and 1.4, although values can be found as low as 0.3 and as high as 1.7. In the absence of data, a value of 1.0 is recommended since no estimation techniques for this parameter have yet been developed. Note that using 1.0 for the Freundlich exponent assumes a linear model for sorption (see Equation A8).

The user is cautioned regarding indiscriminately using literature values for the distribution coefficient K_d or the Freundlich exponent, or estimation methods for K_d. There can be much variability in the values that are estimated or found in the literature compared to actual measurements for a site. For examples, refer to the study of Melancon et al. (1986).

Another option for modeling adsorption in SESOIL uses the cation exchange capacity (CEC). Cation exchange occurs when positively charged atoms or molecules (cations such as heavy metals) are exchanged with the cations of minerals and other soil constituents. CEC is a measure amount of cations per unit of soil that are available for exchange with the contaminant.

The cation exchange algorithm in SESOIL is very simple and estimates the maximum amount of contaminant that can be adsorbed. The calculation of the contaminant immobilized by cation exchange is given by (from Bonazountas and Wagner, 1984):

$$MCEC = a \times CEC \times \frac{MWT}{VAL} \qquad \text{(A14)}$$

Where:

Parameter	Description
$MCEC$	Maximum contaminant cation exchanged by the soil (μg/g soil),
a	Units coefficient = 10,
CEC	Cation exchange capacity of the soil (meg/100g of dry weight soil),
MWT	Molecular weight of the contaminant cation (g/mol),
VAL	Valence of the cation (-)

☞ *The cation exchange algorithm has been verified to be computationally correct in SESOIL, but it has not been validated with measured data.*

With clay soil, the exchanged ion is often calcium, and clay soils tend to have the highest cation exchange capacity. Note that the CEC value of a soil increases with increase in pH, but pH is not included in the CEC algorithm in SESOIL. The CEC value must be adjusted manually to include effects due to pH.

In SESOIL, cation exchange computed by Equation A14 is assumed to occur instantaneously, and irreversibly. Once maximum adsorption via exchange has been reached, no additional adsorption will be calculated. The process is also assumed to take precedence over all other soil processes in competition for the contaminant cation.

The use of the cation exchange subroutines is optional. If it is used, Equation A8 should not be used [i.e., model inputs for the organic carbon adsorption coefficient (K_{oc}) and soil distribution coefficient (K_d), should be 0.0] unless the user has selected the model inputs in such a way as to avoid double accounting. It is up to the user to be sure that cation exchange is the predominant adsorption mechanism at the modeled site. This determination includes considerations of leachate characteristics such as pH, ionic strength, and the presence and concentration of other cations. The other cations, often found in landfill leachate and aqueous industrial wastes, may have higher affinity for exchange with soil cations, and may effectively block exchange between the contaminant and the soil cations. In addition, the speciation of the contaminant should be considered (Bonazountas and Wagner, 1984).

A2.5.5 Degradation: Biodegradation and Hydrolysis

The pollutant cycle of SESOIL contains two transformation routines which can be used to estimate contaminant degradation in the soil. Biodegradation is the biologic breakdown of organic chemicals, most often by microorganisms. Hydrolysis is a chemical reaction of the pollutant with water. Both processes result in the loss of the original contaminant and the creation of new chemicals. The SESOIL model accounts for the mass of contaminant lost via degradation but does not keep track of any degradation products. The user is responsible for knowing what the degradation products will be and their potential significance.

The biodegradation process is usually a significant loss mechanism in soil systems since soil environments have a diverse microbial population and a large variety of food sources and habitats (Hamaker, 1972). Many environmental factors affect the rate of biodegradation in soil, including pH, moisture content of the soil, temperature, redox potential, availability of nutrients, oxygen content of the soil air, concentration of the chemical, presence of appropriate microorganisms, and presence of other compounds that may be preferred substrates. However, SESOIL does not consider these factors.

Biodegradation in SESOIL is handled as primary degradation, which is defined as any structural transformation in the parent compound which results in a change in the chemical's identity. It is estimated using the chemical's rate of decay in both the dissolved and adsorbed phases according to the first-order rate equation:

$$P_d = \left(C\theta k_{dl} + S\rho_b k_{ds}\right) A d_s \Delta t \qquad \text{(A15)}$$

Where:

Parameter	Description
P_d	Decayed contaminant mass during time step Δt (μg),
k_{dl}	Biodegradation rate of the compound in the liquid phase (day^{-1}),
k_{ds}	Biodegradation rate of the compound in the solid phase (day^{-1}),
A	Area of the contaminant application (cm^3),
d_s	Depth of the soil sub-layer (cm),
Δt	Time step (day),
c	Contaminant concentration in soil water (μg/ml),
θ	Soil water content (ml/ml), and
s	Adsorbed contaminant concentration (μg/g).

Note that c, θ, and s are functions of time in the SESOIL model.

The use of a first-order rate equation is typical for fate and transport models and generally is an adequate representation of biodegradation for many chemicals. However, due to the many factors affecting biodegradation, in some cases a first-order rate may not be applicable to the site field conditions and a zero-order or a second- or higher-order rate might be more appropriate. The biodegradation algorithm in SESOIL that is described by Equation A15 cannot handle these cases.

The user is cautioned regarding the use of literature values for the biodegradation rates since these values are quite variable and in many cases are not applicable to site field conditions. In most cases, biodegradation rates are very site-specific and uncertainty in these rates must be recognized. The user-supplied first-order decay rate constants (for moisture and solids) should be values measured for the contaminant in a soil culture test under conditions similar to the site being modeled.

The SESOIL hydrolysis algorithm allows the simulation of neutral, acid- or base-catalyzed reactions and assumes that both dissolved and adsorbed contaminants are susceptible to hydrolysis (Lyman et al., 1982). Since hydrolysis is the reaction of the contaminant with water, this reaction may occur at any depth as the contaminant moves through the soil column. The hydrolysis subroutine requires user-supplied rate constants for the neutral, acid and base hydrolysis reactions of the contaminant, and the pH for each soil layer. The model does not correct for the temperature of the modeled soil.

The hydrolysis algorithm has been verified but has not been validated.

As for the biodegradation process, the algorithm for hydrolysis uses Equation A15 except the rates k_{dl} and k_{ds} are both replaced by the rate constant k_h defined as (from Bonazountas and Wagner, 1984):

$$k_h = k_o + k_H\left[H^+\right] + k_{OH}\left[OH^-\right] \qquad \text{(A16)}$$

Where:

Parameter	Description
k_h	Hydrolysis rate constant (day^{-1}),
k_o	Rate constant for neutral hydrolysis (day^{-1}),
k_H	Rate constant for acid-catalyzed hydrolysis (days^{-1} mol^{-1} liter),
$[H^+]$	10^{-pH}, the hydrogen ion concentration (mol/l),
k_{OH}	Rate constant for base-catalyzed hydrolysis (days^{-1} mol^{-1} liter), and
$[OH^-]$	10^{pH-14}, the hydroxyl ion concentration (mol/l).

If cation exchange is considered, the following formula is used:

$$P_d = MCECk_h\rho_b A d_s \Delta t \qquad \text{(A17)}$$

Where:

Parameter	Description
$MCEC$	Maximum contaminant cation exchanged by the soil (μg/g soil),
k_h	Hydrolysis rate constant (day^{-1}),
ρ_b	Soil bulk density (g/cm^3),
A	Area of the contaminant application (cm^3),
d_s	Depth of the soil sub-layer (cm), and
Δt	Time step (day).

Extrapolating hydrolysis rates measured in a laboratory to the environment increases the uncertainty of model results if the hydrolysis rate is not corrected for the influences of temperature, adsorption, the soil ionic strength, and the possible catalytic effect of dissolved material or solid surfaces. Since there are usually large uncertainties in hydrolysis rates, the SESOIL model results for hydrolysis should be considered only as approximations. The rate of hydrolysis for various organic chemicals may vary over more than 14 orders of magnitude. In addition, the hydrolysis routine does not consider the influence of ionic strength or the presence of other dissolved organics on the hydrolysis rate of the contaminant.

A2.5.6 Metal Complexation

Complexation, also called chelation, is defined here as a transformation process. In SESOIL, complexation incorporates the contaminant as part of a larger molecule and results in the binding of the contaminant to the soil. For example, metal cations (e.g. copper, lead, iron, zinc, cadmium) combine with organic or other nonmetallic molecules (ligands) to form stable complexes. The complex that is formed will generally prevent the metal from undergoing other reactions or interactions of the free ion.

☞ *The complexation routine has been verified but has not been validated.*

The pollutant fate cycle incorporates a simplified representation of the complexation process as a removal process. It is only available for scenarios in which the contaminant is a heavy metal. The model assumes a reversible process in which a metal ion is complexed by a specified soluble organic ligand to form a complex which is soluble, non-absorbable, and non-migrating. Possible ligands are humic acid, fulvic acid, and low molecular weight carboxylic acids, which are commonly found in landfill leachate (Bonazountas and Wagner, 1984). It is the responsibility of the user to determine whether this process is likely to occur in the scenario being modeled, and to supply the appropriate information.

The complexation subroutine employs a nonlinear equation which must be solved numerically. It uses the same iterative procedure as the general pollutant cycle for monthly simulations. Required data include the stability (or dissociation) constant for the specific complex, and the mole ratio of ligand to metal. Also required are the molecular weights of the metallic contaminant and the organic ligand. Equations used by this subroutine are based on the work of Giesy and Alberts (1984), Brinkman and Bellama (1978), and Sposito (1981). The model does not consider competition with metal ions in the soil which may have higher affinity for the ligand. Note that if the user chooses to model both cation exchange and metal complexation, the cation exchange process is assumed to occur first; ions involved in cation exchange are then unavailable for complexation. The general adsorption processes are modeled as being competitive with the complexation process (Bonazountas and Wagner. 1984).

A2.5.7 Contamination in Surface Runoff and Washload

Contaminant mass can be removed from the soil area being simulated by SESOIL via surface runoff and washload. The contamination in surface runoff is simply the surface runoff computed in the hydrologic cycle (for each month) multiplied by the contaminant concentration in the soil moisture of the surface layer (for each time step). The result of this calculation is multiplied by the index of contaminant transport in surface runoff (ISRM), which controls the amount of chemical partitioned into runoff. There is no basis for estimating the index of contaminant transport in surface runoff; it can be set to 0.0 to "turn off" the contaminant participation in runoff, or it can be used essentially as a fitting parameter if data are available. In a calibration/validation exercise used to predict atrazine runoff at a site in Watkinsville, Georgia, the index of contaminant transport in surface runoff was found to be 0.06 (see Hetrick et al., 1989).

See Section 6.7.3 for additional information on the index of contaminant transport in surface runoff (ISRM).

Contaminant loss via washload is computed by taking the sediment yield from the washload cycle multiplied by the adsorbed contaminant concentration in the surface layer. While studies have been conducted comparing results of sediment yield with field data (Hetrick and Travis, 1988), contaminant loss via washload has not been validated in SESOIL.

A2.5.8 Soil Temperature

The original SESOIL model assumed that soil temperature was equal to the user-supplied air temperature. The model was modified by Hetrick et al. (1989) to predict soil temperature from air temperature according to the following (Toy et al., 1978):

Summer: $Y = 16.115 + 0.856X,$
Fall: $Y = 1.578 + 1.023X,$
Winter: $Y = 15.322 + 0.656X,$
Spring: $Y = 0.179 + 1.052X,$

Where:

Parameter	Description
Y	Mean monthly soil temperature (°F).
X	Mean monthly air temperature (°F).

These regression equations are very crude and not depth dependent. However, further complexity is not warranted since soil temperature is used only in Equation A7 and does not significantly affect results. It should be noted that some chemical parameters and processes are dependent on temperature (for example, solubility, Henry's law constant, and rate constants for biodegradation and hydrolysis). No explicit consideration of these effects is included in SESOIL, and the user should adjust the input values for such parameters if temperature effects are judged to be important.

A2.5.9 Pollutant Cycle Evaluation

There are several approaches used to evaluate the reliability and usefulness of an environmental model, such as verification, calibration, sensitivity analysis, uncertainty analysis, and validation. Verification establishes that results from each of the algorithms of the model are correct. Calibration is the process of adjusting selected model parameters within an accepted range until the differences between model predictions and field observations are within selected criteria of performance (Donnigan and Dean, 1985).

Sensitivity analysis focuses on the relative impact each parameter or term has on the model output, in order to determine the effect of data quality on output reliability. Uncertainty analysis seeks to quantify the uncertainty in the model output as a function of uncertainty in both model input and model operations. Validation also compares measured with predicted results, but includes analysis of the theoretical foundations of the model, focusing on the model's performance in simulating actual behavior of the chemical in the environment under study. (Note that the term validation has often been broadly used to mean a variety of things, including all five of the techniques mentioned above.)

A number of calibration, validation, and sensitivity studies have been performed on the SESOIL model. The model has been verified by extensive testing using extreme ranges of input data. Studies of the hydrologic and washload cycles have already been discussed above (see Sections A2.3 and A2.4). The following discusses the kinds of evaluations that have been performed on the pollutant cycle of the SESOIL model. Note that model validation is a continuing process; no model is ever completely validated.

To assess SESOIL's predictive capabilities for contaminant movement, a contaminant transport and validation study was performed by Arthur D, Little, Inc. under contract to EPA (Bonazountas et al., 1982). The application/validation study was conducted on two field sites, one in Kansas and one in Montana. SESOIL results were compared to data for the metals chromium, copper, nickel, and sodium at the Kansas site and the organics naphthalene and anthracene at the Montana site. Results showed reasonable agreement between predictions and measurements, although the concentrations of the metals were consistently underestimated, and the rate of metal movement at the Kansas site was consistently overestimated. At the Montana site, the concentrations of the organics were overestimated by SESOIL. Bonazountas et al. (1982) state that the over estimations for the organics were probably due to the fact that biodegradation was not considered in the simulations. Note that this study was done with the original SESOIL model, not the modified model that is described herein.

Hetrick et al. (1989) compared predictions of the improved version of SESOIL with empirical data from a laboratory study involving six organic chemicals (Melancon et al., 1986) and from three different field studies invoking the application of aldicarb to two field plots (Homsby et al., 1983; R. L. Jones, 1986; Jones et al., 1983, 1985) and atrazine to a single-field watershed (Smith et al., 1978). Results for several measures of contaminant transport were compared including the location of chemical peak vs. time, the time-dependent amount of contaminant leached to groundwater, the depth distribution of the contaminant at various times, the mass of the chemical degraded, and the amount of contaminant in surface runoff. This study showed that SESOIL predictions were in good agreement with observed data for both the laboratory study and the field studies.

SESOIL does a good job of predicting the leading edge of the chemical profile (Hetrick et. al., 1989), due mainly to the improvement of the contaminant depth algorithm to include the chemical sorption characteristics (see Section A2.5.2 above). Also, when a split-sample calibration/validation procedure was used on 3 years of data from the single-field watershed, SESOIL did a good job of predicting the amount of chemical in the runoff. The model was less effective in predicting actual concentration profiles; the simulated concentrations near the soil surface under estimated the measurements in most cases. One explanation is that SESOIL does not consider the potential upward movement of the chemical with the upward movement of water due to soil evaporation losses.

SESOIL is a useful screening-level chemical migration and fate model. The model is relatively easy to use, the input data are straight forward to compile, and most of the model parameters can be readily estimated or obtained. Sensitivity analysis studies with SESOIL can be done efficiently. SESOIL can be applied to generic environmental scenarios for purposes of evaluating the general behavior of chemicals. Care should be taken when applying SESOIL to sites with large vertical variations in soil properties since the hydrologic cycle assumes a homogeneous soil profile. Only one value for the soil moisture content is computed for the entire soil column. If different permeabilities are input for each soil layer, the soil moisture content calculated in the hydrologic cycle using the vertically-averaged permeability (Equation A2) may not be valid for the entire soil column. Thus, the user is warned that even though the model can accept different permeabilities for each layer, the effects of variable permeability are not fully accounted for by the model.

It is recommended that predictions for the hydrology at a given site be calibrated to agree with known measurements. Caution should be used when making conclusions based on modeling results when little hydrologic data exist against which to calibrate predictions. In these cases, it is recommended that the user employ sensitivity analysis or evaluate results obtained by assigning distributions to the input parameters (e.g., see Gardner, 1984; O'Neill et al., 1982; Hetrick et al., 1991). However, when properly used, SESOIL is an effective screening-level tool in assessing chemical movement in soils.

[redacted]

A3.0 SESOIL Data Input Guide

This section provides a description of the SESOIL input parameters. SESOIL uses ASCII text files to store the information used in the model scenarios. These files must be formatted so that the SESOIL program correctly read the data. A description of the FORTRAN read format is also provided.

SESOIL Climate Data Parameters

Line 1

NRE		Climate Data Set Title	IYRS	
5	6	54	59	

Parameter	Format	Description
NRE	I5	Index number for the climate data set
TITLE	A48	Climate data set title
IYRS	I5	Number of years of climate data in the data set

Skip Line 2

Lines 3 to 11

	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
8	14	20	26	32	38	44	50	56	62	68	74	80

Line	Parameter	Format	Description
3	TA	F6.2	Monthly mean air temperature (Celsius)
4	NN	F6.2	Monthly mean cloud cover
5	S	F6.2	Monthly mean relative humidity
6	A	F6.2	Monthly short wave albedo fraction
7	REP	F6.2	Monthly mean evapotranspiration rate (cm/day)
8	MPM	F6.2	Monthly precipitation (cm)
9	MTR	F6.2	Monthly mean duration of individual storms (days)
10	MN	F6.2	Monthly number of storm events
11	MT	F6.2	Monthly length of rainy season (days)

Line 12

NRE	
5	

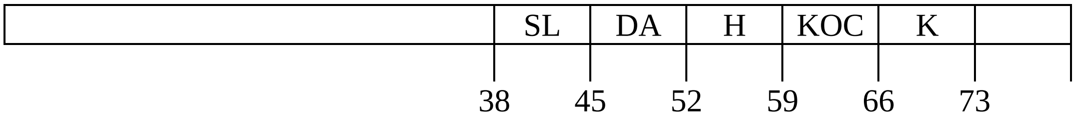
Parameter	Format	Description
NRE	I5	End of climate data file when NRE = 999

SESOIL Chemical Data Parameters

Line 1

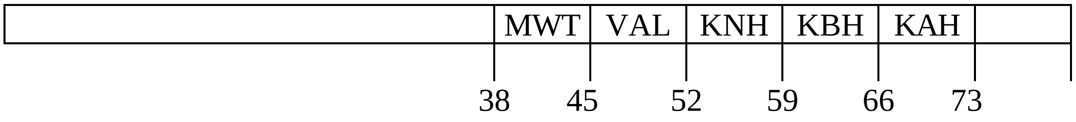
Parameter	Format	Description
NCH	I5	Index number for the chemical data set
TITLE	A48	Chemical data set title

Line 2



Parameter	Format	Description
SL	F7.2	Solubility in water (μg/ml)
DA	F7.2	Air diffusion coefficient (cm^2/sec)
H	F7.2	Henry's Law constant (m^3-atm/mol)
KOC	F7.2	Organic carbon adsorption coefficient (μg/g)/(μg/ml)
K	F7.2	Soil partition coefficient (μg/g)/(μg/ml)

Line 3



Parameter	Format	Description
MWT	F7.2	Molecular weight (g/mole)
VAL	F7.2	Valence of the compound
KNH	F7.2	Neutral hydrolysis rate constant (1/day)
KBH	F7.2	Base hydrolysis rate constant (l/mol/day)
KAH	F7.2	Acid hydrolysis rate constant (l/mol/day)

Line 4

	KDEL	KDES	SK	B	MWTLIG	DW
38	45	52	59	66	73	80

Parameter	Format	Description
KDEL	F7.2	Liquid phase biodegradation rate (1/day)
KDES	F7.2	Solid phase biodegradation rate (1/day)
SK	F7.2	Ligand stability (dissociation) constant
B	F7.2	Moles Ligand per mole compound
MWTLIG	F7.2	Molecular weight of ligand (g/mol)
DW	F7.2	Water diffusion coefficient (cm^2/sec)

Line 5

NCH	
5	

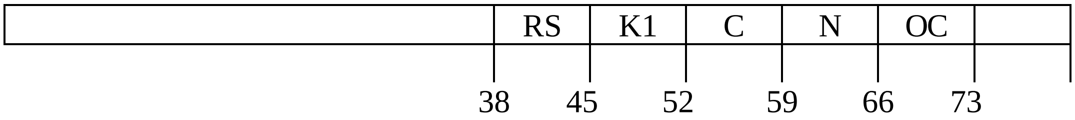
Parameter	Format	Description
NCH	I5	End of chemical data file when NCH = 999

SESOIL Soil Data Parameters

Line 1

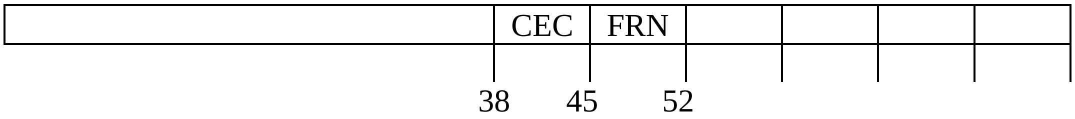
Parameter	Format	Description
NSO	I5	Index number for the soil data set
TITLE	A48	Soil data set title

Line 2



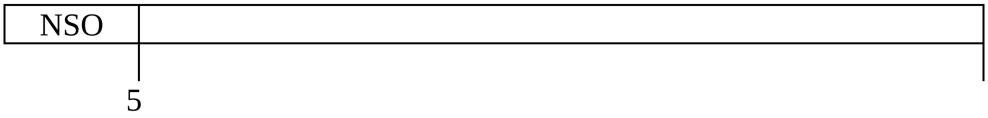
Parameter	Format	Description
RS	F7.2	Bulk density (g/cm^3)
K1	F7.2	Intrinsic permeability (cm^2)
C	F7.2	Soil pore disconnectedness index
N	F7.2	Effective porosity
OC	F7.2	Organic carbon content (percent)

Line 3



Parameter	Format	Description
CEC	F7.2	Cation exchange capacity (meg/100g)
FRN	F7.2	Freundlich exponent

Line 4



Parameter	Format	Description
NSO	I5	End of climate data file when NSO = 999

SESOIL Washload Data Parameters

Line 1

NWS		Washload Data Set Title	IYRS	
5	6	54	59	

Parameter	Format	Description
NWS	I5	Index number for the washload data set
TITLE	A48	Washload data set title
IYRS	I5	Number of years of washload in the data set

Line 2

	AWR	SLT	SND	CLY	SLEN	SLP
38	45	52	59	66	73	80

Parameter	Format	Description
ARW	F7.2	Washload area (cm^2)
SLT	F7.2	Silt fraction
SND	F7.2	Sand fraction
CLY	F7.2	Clay fraction
SLEN	F7.2	Slope length (cm)
SLP	F7.2	Average land slope (cm/cm)

Skip line 3

Lines 4 to 7

	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep
8	14	20	26	32	38	44	50	56	62	68	74	80

Line	Parameter	Format	Description
4	KSOIL	F6.2	Soil erodibility factor (tons/acre/english EI)
5	CFACT	F6.2	Soil loss ratio
6	PFACT	F6.2	Contouring factor (unitless)
7	NFACT	F6.2	Manning’s coefficient (unitless)

Line 8

NWS	
5	

Parameter	Format	Description
NWS	I5	End of washload data file when NWS = 999

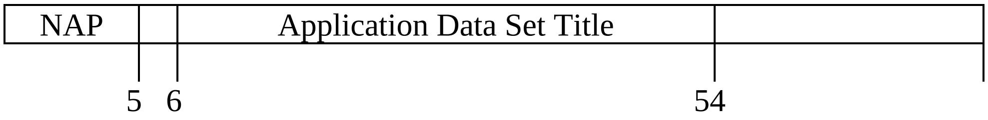
SESOIL Execution Data File Parameters

RUN		OPTN	CLIM	SOIL	CHEM	WASH	APPL	YRS
5	6	10	15	20	25	30	35	40

Parameter	Format	Description
RUN	I5	Incremental number for the model run
OPTN	A4	Simulation option (the monthly option, "M", is used for all cases)
CLIM	I5	The index number for the climate data file for the model run
SOIL	I5	The index number for the soil data file for the model run
CHEM	I5	The index number for the chemical data file for the model run
WASH	I5	The index number for the washload data file for the model run
APPL	I5	The index number for the application data file for the model run
YRS	I5	The number of years to be simulated by the model run

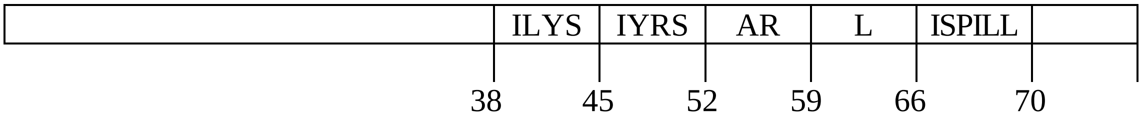
SESOIL Application Data Parameters

Line 1



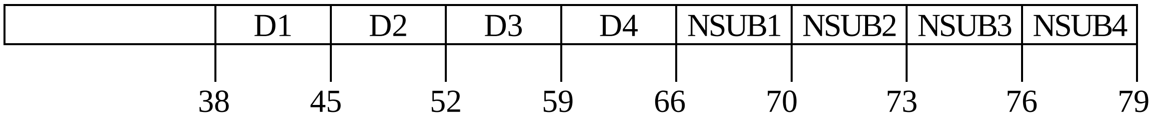
Parameter	Format	Description
NAP	I5	Index number for the application data set
TITLE	A48	Application data set title

Line 2



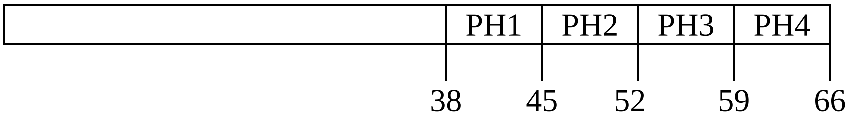
Parameter	Format	Description
ILYS	F7.2	Number of soil layers
IYRS	F7.2	Number of years of annual data in the application file
AR	F7.2	Application area (cm^2)
L	F7.2	Latitude of site (degrees)
ISPILL	I3	Spill index

Line 3



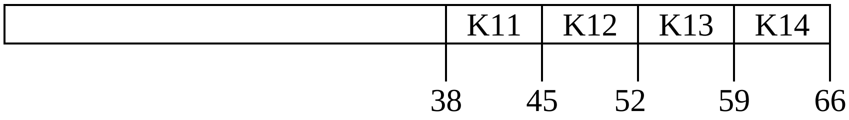
Parameter	Format	Description
D1	F7.2	Upper soil layer thickness (cm)
D2	F7.2	Second soil layer thickness (cm)
D3	F7.2	Third soil layer thickness (cm)
D4	F7.2	Lower soil layer thickness (cm)
NSUB1	I3	Number of sub-layers in upper soil layer
NSUB2	I3	Number of sub-layers in second soil layer
NSUB3	I3	Number of sub-layers in third soil layer
NSUB4	I3	Number of sub-layers in lower soil layer

Line 4



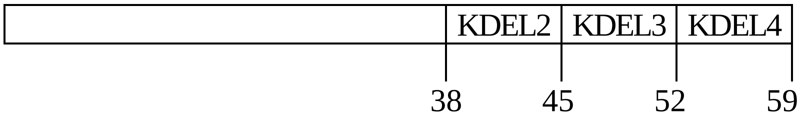
Parameter	Format	Description
PH1	F7.2	pH of upper soil layer
PH2	F7.2	pH of second soil layer
PH3	F7.2	pH of third soil layer
PH4	F7.2	pH of lower soil layer

Line 5



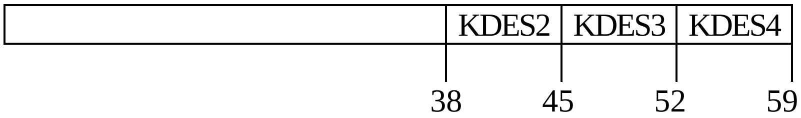
Parameter	Format	Description
K11	F7.2	Permeability of the upper soil layer (cm^2)
K12	F7.2	Permeability of second soil layer (cm^2)
K13	F7.2	Permeability of third soil layer (cm^2)
K14	F7.2	Permeability of lower soil layer (cm^2)

Line 6



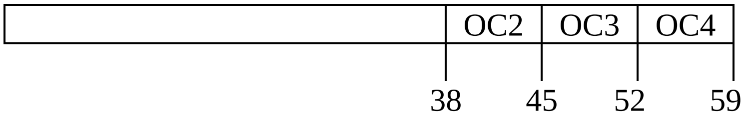
Parameter	Format	Description
KDEL2	F7.2	Ratio of KDEL (liquid phase biodegradation) layer 2 to 1
KDEL3	F7.2	Ratio of KDEL (liquid phase biodegradation) layer 3 to 1
KDEL4	F7.2	Ratio of KDEL (liquid phase biodegradation) layer 4 to 1

Line 7



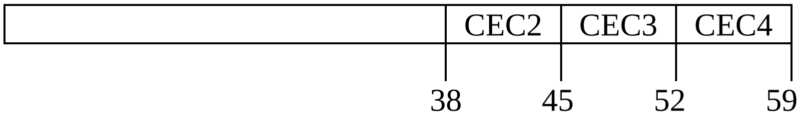
Parameter	Format	Description
KDES2	F7.2	Ratio of KDES (solid phase biodegradation) layer 2 to 1
KDES3	F7.2	Ratio of KDES (solid phase biodegradation) layer 3 to 1
KDES4	F7.2	Ratio of KDES (solid phase biodegradation) layer 4 to 1

Line 8



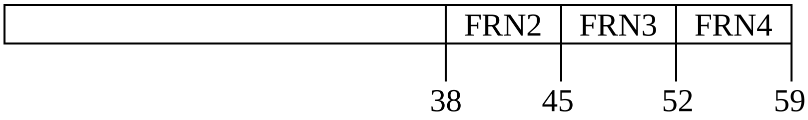
Parameter	Format	Description
OC2	F7.2	Ratio of OC (organic carbon content) layer 2 to 1
OC3	F7.2	Ratio of OC (organic carbon content) layer 3 to 1
OC4	F7.2	Ratio of OC (organic carbon content) layer 4 to 1

Line 9



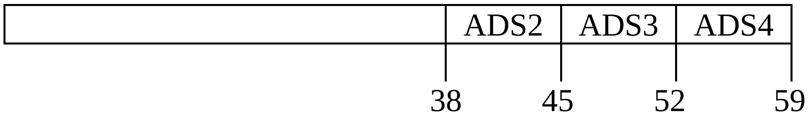
Parameter	Format	Description
CEC2	F7.2	Ratio of CEC (cation exchange capacity) layer 2 to 1
CEC3	F7.2	Ratio of CEC (cation exchange capacity) layer 3 to 1
CEC4	F7.2	Ratio of CEC (cation exchange capacity) layer 4 to 1

Line 10



Parameter	Format	Description
FRN2	F7.2	Ratio of FRN (Freundlich exponent) layer 2 to 1
FRN3	F7.2	Ratio of FRN (Freundlich exponent) layer 3 to 1
FRN4	F7.2	Ratio of FRN (Freundlich exponent) layer 4 to 1

Line 11



Parameter	Format	Description
ADS2	F7.2	Ratio of ADS (layer 2, organic carbon adsorption coefficient) to K (organic carbon adsorption coefficient from the chemical file, layer 1)
ADS3	F7.2	Ratio of ADS (layer 3, organic carbon adsorption coefficient) to K (organic carbon adsorption coefficient from the chemical file, layer 1)
ADS4	F7.2	Ratio of ADS (layer 4, organic carbon adsorption coefficient) to K (organic carbon adsorption coefficient from the chemical file, layer 1)

Lines 13 to 63

	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep

8 14 20 26 32 38 44 50 56 62 68 74 80

Parameter	Format	Description
POLIN#	F6.2	Monthly contaminant load (μg/cm^2), for layer number #
TRANS#	F6.2	Monthly mass transformed by other process (μg/cm^2), for layer number #
SINK#	F6.2	Monthly mass removed by some other processes (μg/cm^2), for layer number #
LIG#	F6.2	Monthly input ligand mass (μg/cm^2) , for layer number #
VOLF#	F6.2	Index of volatilization, for layer number #
ISMR	F6.2	Index of contaminant transport in surface runoff
ASL	F6.2	Ratio of the contaminant concentration in precipitation to the maximum water solubility

Lines 65

	SATCON	HYDRA	THICKS	WIDTH	BACKCA

8 14 20 26 32 38

Parameter	Format	Description
SATCON	F6.2	Saturated horizontal hydraulic conductivity (cm/sec).
HYDRA	F6.2	The slope of the potentiometric surface (ft/ft).
THICKS	F6.2	The thickness of the groundwater mixing zone (cm).
WIDTH	F6.2	The width of the contaminant release (cm).
BACKCA	F6.2	Upgradient background groundwater contaminant concentration (μg/ml).

Lines 67 to 70

	Sub-Layer 1	Sub-Layer 2	Sub-Layer 3	Sub-Layer 4	Sub-Layer 5	Sub-Layer 6	Sub-Layer 7	Sub-Layer 8	Sub-Layer 9	Sub-Layer 10

8 14 20 26 32 38 44 50 56 62 68

Parameter	Format	Description
CONCIN1#	F6.2	Initial layer 1 sub-layer contaminant load concentrations in ppm.
CONCIN2#	F6.2	Initial layer 2 sub-layer contaminant load concentrations in ppm.

CONCIN3#	F6.2	Initial layer 3 sub-layer contaminant load concentrations in ppm.
CONCIN4#	F6.2	Initial layer 4 sub-layer contaminant load concentrations in ppm.

Line 71

NAP	
5	

Parameter	Format	Description
NAP	I5	End of the application data file when NAP = 999

A4.0 SESOIL Example Input Data Files

MILW_WI.CLM

```
    1 MILWAUKEE WSO AP                                    1
        ****  YEAR 1  ****
 TA      10.50  2.94 -3.83 -7.39 -5.00  0.85  7.00 12.67 18.28 21.39 20.72 16.61
 NN       0.46  0.60  0.62  0.55  0.53  0.50  0.47  0.41  0.36  0.30  0.34  0.41
 S        0.73  0.75  0.76  0.72  0.72  0.72  0.69  0.69  0.70  0.72  0.76  0.76
 A        0.17  0.21  0.30  0.33  0.30  0.29  0.19  0.17  0.17  0.17  0.17  0.17
 REP       0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
 MPM      5.72  5.03  5.16  4.16  3.38  6.55  8.55  6.76  9.12  8.99  7.85  7.31
 MTR      0.29  0.37  0.43  0.47  0.44  0.46  0.47  0.38  0.36  0.31  0.30  0.29
 MN       4.02  4.50  4.38  3.48  3.00  5.05  6.31  5.88  6.05  5.40  5.62  4.55
 MT      30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40 30.40
  999 END OF FILE
```

BENZENE.CHM

```
    1 Benzene
        - SL,DA,H,KOC,K               1780.00  0.0770.00555  31.00    0.0
        - MWT,VAL,KNH,KBH,KAH           78.11    0.0    0.0    0.0    0.0
        - KDEL,KDES,SK,B,MWTLIG,DW        0.0    0.0    0.0    0.0    0.09.80E-6
  999 END OF FILE
```

SAND.SOI

```
    1 Sand, Perm = 1.00E-3 cm/sec
        -  RS,K1,C,N,OC                    1.70 1.0E-8   4.00   0.25   0.50
        -  CEC,FRN                          0.0   1.00
  999 END OF FILE
```

SITEWASH.WSH

```
1 Site Sand Washload Data                             1
    ARW,SLT,SND,CLY,SLEN,SLP          100000.   0.15   0.75   0.101000.00 0.0100
                  **MONTHLY DATA**  YR 1
 KSOIL    0.10  0.19  0.19  0.19  0.19  0.19  0.19  0.19  0.19  0.19  0.19  0.19
 CFACT    0.01  0.01  0.01  0.01  0.01  0.01  0.01  0.01  0.01  0.01  0.01  0.01
 PFACT    1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00  1.00
 NFACT   0.015 0.015 0.015 0.015 0.015 0.015 0.015 0.015 0.015 0.015 0.015 0.015
  999 END OF FILE
```

DEFAULT.APL

```
   1 SEVIEW Default Application Parameters
 -ILYS,IYRS,AR,L,ISPILL,ISUMRS,ICONC    4.00   2.001.00E+5  42.95  1  1  1
 -D1,D2,D3,D4,NSUBL1 to NSUBL4         200.0  200.0  300.0  300.010 10 10 10
 -PH1,PH2,PH3,PH4                       7.00   7.00   7.00   7.00
 -K11,K12,K13,K14                        0.0    0.0    0.0    0.0
 -KDEL MULTIPLIERS                      1.00   1.00   1.00
 -KDES MULTIPLIERS                      1.00   1.00   1.00
 -OC MULTIPLIERS                        1.00   1.00   1.00
 -CEC MULTIPLIERS                       1.00   1.00   1.00
 -FRN MULTIPLIERS                       1.00   1.00   1.00
 -ADS MULTIPLIERS                       1.00   1.00   1.00
               **** LAYER 1 **  YEAR 1 ****
POLIN1    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
TRANS1    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
SINK1     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
LIG1      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
VOLF1     1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
ISRM      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
ASL       0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
               **** LAYER 2 **  YEAR 1 ****
POLIN2    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
TRANS2    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
SINK2     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
LIG2      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
VOLF2     1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
               **** LAYER 3 **  YEAR 1 ****
POLIN3    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
TRANS3    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
SINK3     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
LIG3      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
VOLF3     1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
               **** LAYER 4 **  YEAR 1 ****
POLIN4    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
TRANS4    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
SINK4     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
LIG4      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
VOLF4     1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
               **** LAYER 1 **  YEAR 2 ****
POLIN1    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
TRANS1    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
SINK1     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
LIG1      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
VOLF1     1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
ISRM      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
ASL       0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
               **** LAYER 2 **  YEAR 2 ****
POLIN2    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
TRANS2    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
SINK2     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
LIG2      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
VOLF2     1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
               **** LAYER 3 **  YEAR 2 ****
POLIN3    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
TRANS3    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
SINK3     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
LIG3      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
VOLF3     1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
               **** LAYER 4 **  YEAR 2 ****
POLIN4    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
TRANS4    0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
SINK4     0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
LIG4      0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
VOLF4     1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0   1.0
SUMMERS MODEL PARAMETERS FOLLOW (SATCON,HYDRA,THICKS,WIDTH,BACKCA)
       1.0E-3  0.01  20.0  10.0   0.0
INITIAL CONTAMINANT CONCENTRATIONS FOLLOW
CONCIN1   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
CONCIN20.9999   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
CONCIN3   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
CONCIN4   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0   0.0
 999 END OF FILE
```

A5.0 SESOIL SERUN.BAT File

SERUN.BAT

```
set fort22=C:\SEVIEW63\SITEWASH.WSH
set fort2=C:\SEVIEW63\MILW_WI.CLM
set fort3=C:\SEVIEW63\SAND.SOI
set fort4=C:\SEVIEW63\BENZENE.CHM
set fort20=C:\SEVIEW63\DEFAULT.APL
sesoil<C:\SEVIEW63\EXEC020.EXC
copy fort21 C:\SEVIEW63\RUN01.OUT
del fort21
del serun.bat
```

A6.0 SESOIL Error and Warning Messages

This section presents error or warning messages that are detected by the SESOIL code during operation. The messages are listed in alphabetical order and include a description of the message.

☞ *The "?????" indicate a number printed by SESOIL.*

SESOIL Error Or Warning Message	Description	SESOIL Input File
ERROR, ILYS = ????? WHICH IS INCORRECT	The number of layers given must be set to either 2, 3, or 4.	Application
ERROR, NSUBL1 = ????? WHICH IS INCORRECT	The number of sub-layers in layer 1 must be at least 0 and less than or equal to 10.	Application
ERROR, NSUBL2 = ????? WHICH IS INCORRECT	The number of sub-layers in layer 2 must be at least 0 and less than or equal to 10.	Application
ERROR, NSUBL3 = ????? WHICH IS INCORRECT	The number of sub-layers in layer 3 must be at least 0 and less than or equal to 10.	Application
ERROR, NSUBLL = ????? WHICH IS INCORRECT	The number of sub-layers in lowest layer must be at least 0 and less than or equal to 10.	Application
FATAL ERROR - AREA FOR WASHLOAD (ARW) MUST BE ON THE ORDER OF 10**4 OR MORE IS: ?????	The washload area is in error.	Washload
FATAL ERROR - CLAY CONTENT (CLY) MUST BE BETWEEN 0 AND 1. IS: ?????	The clay fraction is in error.	Washload
FATAL ERROR - CLOUD COVER (NN) MUST BE BETWEEN 0. AND 1.	The cloud cover must be a fraction.	Climate
FATAL ERROR - CLOUD COVER (NN) MUST BE BETWEEN 0. AND 1. IS: ?????	Cloud cover must be a fraction.	Annual
FATAL ERROR - LATITUDE (L) MUST BE LESS THAN 90 IS: ?????	Input for latitude of the site is incorrect.	Application
FATAL ERROR - LENGTH OF SEASON (MT) MUST BE LESS THAN 31	For monthly season simulation, length of season must be less than 31.	Climate
FATAL ERROR - SAND CONTENT (SND) MUST BE BETWEEN 0. AND 1. IS: ?????	Input for the sand fraction is in error.	Washload

SESOIL Error Or Warning Message	Description	SESOIL Input File
FATAL ERROR - SILT CONTENT (SLT) MUST BE BETWEEN 0. AND 1. IS: ?????	Input for the silt fraction is in error.	Washload
FATAL ERROR - SOIL MOISTURE (SO) MUST BE BETWEEN 0. AND 100. IS: ?????	Input for soil moisture is incorrect.	Annual
FATAL ERROR - SOIL MOISTURE CALCULATED AS .LE. 0, CHECK FOR EVAPOTRANSPIRATION CLOSE TO OR EXCEEDING ANNUAL PRECIPITATION.	Check input data carefully.	Climate, Soil, and Application
FATAL ERROR - SOIL ORGANIC CARBON CONTENT (OC) MUST BE LESS THAN 100, IS: ?????	Input for organic carbon content is in error.	Soil
FATAL ERROR - SOIL POROSITY (N) MUST BE LESS THAN 1. IS: ????	Input for soil porosity is in error.	Soil
FATAL ERROR- HUMIDITY (S) MUST BE BETWEEN 0. AND 1. IS: ?????	Humidity must be a fraction.	Annual
FATAL ERROR- HUMIDITY (S) MUST BE BETWEEN 0. AND 1. IS: ?????	Humidity must be a fraction.	Climate
FATAL ERROR- LENGTH OF SEASON (MT) MUST BE LESS THAN 365 IS: ?????	The length of season must be 365 days or less.	Annual
SO OUT OF BOUNDS ***** CANNOT CONTINUE WITH THIS RUN	The SESOIL hydrologic cycle cannot converge on soil moisture - check your input data carefully.	Climate, Soil, and Application
WARNING - PROBLEM IN HYDRO CYCLE W EQUALS OR EXCEEDS EP, W SET TO EP	The velocity of the capillary rise (W), exceeds the evapotranspiration rate (EP). When this happens SESOIL sets W to 0.99 * EP. You should check the hydrologic results for reasonableness.	Climate, Soil, and Application
WARNING - PROBLEM IN HYDRO CYCLE MN, MN LESS THAN 1., RAINFALL MAY NOT FOLLOW POISSON DISTRIBUTION (SEE WRR, P. 757, EQUATION (27)	The mean number of storm events for the month, is less than 1; check input (see Eagleson (1978), page 757 for details).	Climate
WARNING - PROBLEM IN HYDRO CYCLE: BETA GREATER THAN 0.5, RAINFALL MAY NOT FOLLOW POISSON DISTRIBUTION	Check input data cycle carefully for errors. Start with the duration of individual storms (MTR), the number of storm events per month (MN) and the length of the rainy season (MT) parameters first.	Climate

SESOIL Error Or Warning Message	Description	SESOIL Input File
WARNING - PROBLEM IN HYDRO CYCLE: BETA/DELTA GREATER THAN 1., RAINFALL MAY NOT FOLLOW POISSON DISTRIBUTION (SEE WRR, P. 716, EQUATION (47))	Check the hydrologic cycle results for reasonableness. See Eagleson (1978), page 716, for details.	Climate
WARNING - PROBLEM IN HYDRO CYCLE: TIME BETWEEN STORMS LESS THAN 2 HRS. RAINFALL MAY NOT FOLLOW POISSON DISTRIBUTION (SEE WRR, P. 715, EQUATION (39))	Check input data carefully (see Eagleson (1978), page 715, for details)	Climate
WARNING - RAINFALL INPUT FLAG (ASL) IS USUALLY LESS THAN 1.	Check the values for the ratio of the contaminant concentration in precipitation to the maximum water solubility.	Application
WARNING - RAINFALL INPUT FLAG (ASL) IS USUALLY LESS THAN 1. IS: ?????	Check the values for the ratio of the contaminant concentration in precipitation to the maximum water solubility.	Annual
WARNING - RUNOFF FLAG (ISRA) IS USUALLY LESS THAN 1. IS: ?????	Input for surface runoff should be checked.	Annual
WARNING - RUNOFF FLAG (ISRM) IS USUALLY LESS THAN 1.	Input for surface runoff should be checked.	Application
WARNING - SOIL PERMEABILITY VARYS CONSIDERABLY AMONG LAYERS, SESOIL MAY NOT BE ACCURATE FOR SUCH AN INHOMOGENEOUS COLUMN	The SESOIL hydrologic cycle uses a single depth weighted average permeability value for the entire soil column. This message is printed whenever the average permeability is significantly different from the individual layer permeabilities.	Application
WARNING - SOLUBILITY ENTERED AS ZERO, SATURATION CHECKS MAY NOT WORK CORRECTLY	Check water solubility.	Chemical
WARNING - VOLATILIZATION FLAG (VOLU) IS USUALLY LESS THAN 1. IS: ?????	The input for volatilization index should be checked.	Annual
WARNING - VOLATILIZATION FLAGS (VOL1, VOL2, VOL3, VOL4) ARE USUALLY LESS THAN OR EQUAL TO 1.	The inputs for volatilization index parameters (VOLF1, VOLF2, VOLF3 and VOLF4) should be checked.	Application
WARNING -SOIL PERMEABILITY (K1) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check the intrinsic permeability value.	Soil

SESOIL Error Or Warning Message	**Description**	**SESOIL Input File**
WARNING -SOIL PERMEABILITY (K11) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check the intrinsic permeability value for the upper soil layer.	Application
WARNING -SOIL PERMEABILITY (K12) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check the intrinsic permeability value for the second soil layer.	Application
WARNING -SOIL PERMEABILITY (K13) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check the intrinsic permeability value for the third soil layer.	Application
WARNING -SOIL PERMEABILITY (K14) IS USUALLY ON THE ORDER OF 10**-7 OR LESS, IS: ?????	Check the intrinsic permeability value for the lower soil layer.	Application

[redacted]

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Appendix B

Introduction and Overview of the AT123D Model

Portions of this Appendix were originally presented as part of the
"Analytical Transient 1-, 2-, and 3-Dimensional Simulation of
Waste Transport in the Aquifer System User's Guide"
prepared for the
Wisconsin Department of Natural Resources

[redacted]

B1.0 Introduction to AT123D

AT123D is an acronym for **Analytical Transient 1-, 2-, and 3-Dimensional Simulation of Waste Transport in the Aquifer System**. It is a generalized three-dimensional groundwater model developed by G. T. Yeh (1981) at Oak Ridge National Laboratory. Significant modifications were made by John Seymor (1982), Darryl Holman (1984) and Howard Trussell, (1986) of the University of Wisconsin-Madison. AT123D was further modified by Robert A. Schneiker (1997) at Environmental Software Consultants, Inc. The model was developed to estimate concentrations of contaminants transported, dispersed, degraded and sorbed in one-dimensional groundwater flow. The transport mechanisms simulated by AT123D include advection, dispersion, sorption, decay/biodegradation and heat losses to the atmosphere. Model results can be used to estimate how far a contaminant plume will migrate and can be compared to groundwater standards to evaluate risks at specific locations and times. Contaminant transport in AT123D can be modeled using one of two methods:

1. Contaminant transport without decay, and
2. Contaminant transport with biodegradation as a first-order decay process.

The no biodegradation option is used to evaluate the transport and fate of non-degrading contaminants. Model results without biodegradation can also be compared to site conditions and/or modeling with biodegradation to evaluate the effects of remediation through natural attenuation (RNA).

When used with SEVIEW, AT123D produces monthly results and can simulate up to 1,000 years of contaminant transport. The AT123D program is written in FORTRAN. The results of a comparison between AT123D and analytical equations are presented in Section B3. A description of all AT123D input parameters including the data formats are presented in Section B4. An example AT123D input file is presented in Section B5. An example AT123D output file is presented in Section B6. A detailed description of the AT123D input parameters used in SEVIEW are presented in Section 7 of the SEVIEW User's Guide.

There are a total of 450 AT123D run options. The run options are defined by the varying combinations of the three contaminant types, eight source configurations, three source release types, and four types of aquifer dimensions. There are 288 run options for the three-dimensional case, 72 for the two- dimensional case in the X-Y plane, 72 for the two- dimensional case in the X-Z plane, and 18 for the one- dimensional case in the longitudinal direction. A list of the run options is presented in Table 13 below.

Table 13 AT123D Run Options

Contaminant Types	Source Configurations	Releases Type	Aquifer Dimensions
Chemical	Point source	Instantaneous	Infinite depth and infinite width
Heat	Line source, parallel to the x-, y-, or z-axis	Finite	Finite depth and infinite width
Radioactive	Plane (area) source, perpendicular to the x-, y-, or z-axis	Continuous	Infinite depth and finite width
	Volume source		Finite depth and finite width

The AT123D model can simulate four types of groundwater boundary conditions. The boundary conditions modeled by AT123D are; specified head, specified flow, head-dependent flow and radiation boundaries. A description of these boundary conditions is presented in Section B2.2.

The initial load can now be established as either a concentration or a mass. As the equation governing contaminant transport and fate is linear, AT123D employs a superposition of simple, analytical (point source) solutions to generate solutions for various types of source releases and configurations, and aquifer dimensions. Line sources are simulated by superimposing an infinite number of point sources along a line. Area sources are simulated by superimposing an infinite number of line sources. Volume source loads are simulated by superimposing an infinite number of area sources. Superposition, for source configurations and boundary conditions and initial conditions, are represented by Green's functions. Some of the solutions are in the form of an infinite series, whose terms must be evaluated and truncated at some finite point. A continuous source is evaluated by superimposing an infinite number of instantaneous source releases. The resulting spatial and temporal integrals of Green's functions are evaluated numerically by Simpson's rule. This means that AT123D performs numerous calculations to simulate contaminant transport and fate and borders on being a semi-analytical model.

B1.1 One- and Two-Dimensional Scenarios

AT123D can be used to model one-, two- and three-dimensional groundwater scenarios. To restrict AT123D to a one- or two-dimensional model the user must set the contaminant source width and/or depth to the width and/or depth of the aquifer. A description of this process is presented below.

B1.1.1 Two-Dimensional Scenarios

To restrict AT123D to a two-dimensional case the user must set the source width or depth to the width or depth of the aquifer. A two-dimensional model in the x-y plane is simulated by setting the starting coordinate of the source in the z-direction (RH1) to zero and the ending coordinate of the source in the z-direction (RH2) to the aquifer depth (DEPTH). A two-dimensional case in the x-z plane is simulated by setting the starting coordinate of the source in the y-direction (RB1) to zero and the ending coordinate of the source in the y-direction (RB2) to the aquifer width (WIDTH).

☞ *By setting the source coordinates along either the z- or y-axis to the aquifer depth or width, no variation in contaminant concentration in that direction can occur.*

B1.1.2 One-Dimensional Scenarios

To limit AT123D to a one-dimensional case the user must set source width and depth to the width and depth of the aquifer. A one-dimensional model in the x-y plane is simulated by setting the starting and ending coordinates of the source in the y- and z-directions (RB1 and RH1) to zero. The user must also set the ending coordinate of the source in the y-direction (RB2) to the aquifer width (WIDTH) and the ending coordinate of the source in the z-direction (RH2) to the aquifer depth (DEPTH).

☞ *By setting the source distance along the y- and z-axis to the aquifer width and depth, no variation in concentration in those directions can occur.*

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B2.0 AT123D Model Description

B2.1 Advection - Dispersion Equation

The AT123D model is based on the advection-dispersion equation which is used to determine the contaminant distribution in groundwater. Assuming incompressible flow the advection-dispersion equation is (Yeh, 1981):

$$\frac{\partial\left(n_e C\right)}{\partial t} = \nabla \bullet \left(n_e \overline{\overline{D}} \nabla C\right) - \nabla \bullet C\vec{q} + \overset{\bullet}{M} - K n_e C - \lambda\ n_e C - \left(\frac{\partial\left(\rho_b C_s\right)}{\partial t} + \lambda\ \rho_b C_s\right) \qquad \text{(B1)}$$

Where:

Parameter	Description
C	Dissolved contaminant concentration
C_s	Adsorbed contaminant concentration
$\overline{\overline{D}}$	Hydraulic dispersion coefficient tensor
K	Chemical degradation rate
$\overset{\bullet}{M}$	Contaminant source release rate
n_e	Effective porosity
$\vec{q}$	Darcy's velocity vector
t	Time
∇	Gradient (Del operator with respect to *x*, *y*, and *z*)
λ	Radioactive decay constant
ρ_b	Bulk density of the soil

By definition the ∇ is:

$$\nabla = \left(\vec{i}\ \frac{\partial}{\partial\ x} + \vec{j}\ \frac{\partial}{\partial\ y} + \vec{k}\ \frac{\partial}{\partial\ z}\right)$$

The term on the left side of advection-dispersion equation represents the time rate of change of dissolved contaminant mass per unit volume of the aquifer. The first term on the right side of the equation represents the combined effects of hydraulic dispersion and molecular diffusion. The second term on the right side represents the advection of the contaminant. The third term represents the contaminant source load to the aquifer system. The fourth term on the right side of the equation accounts for the chemical and biological degradation of the contaminant, while the fifth term represents radioactive decay. The last two terms the equation, in parentheses, represent the effects of ion exchange and sorption.

The initial condition for Equation B1 is

$$C = C_i\left(x, y, z, t = 0\right) \quad \text{in } R$$

Where:

Parameter	Description
C	Dissolved contaminant concentration
C_i	Initial contaminant concentration
R	A region with respect to x, y, and z (the region modeled)
t	Time
x	Longitudinal coordinate
y	Transfer coordinate
z	Vertical coordinate

This initial condition requires that the background concentration of the contaminant is known before the load is released into the aquifer.

B2.2 Boundary Conditions

AT123D can simulate four types of boundary conditions, depending on the physical situation being modeled. A description of these boundary conditions is presented in Table 14.

Table 14 AT123D Boundary Conditions

Boundary Condition	Description
Dirichlet	Specified head.
Neumann	Specified flow.
Cauchy or Mixed Type	Head-dependent flow.
Radiation Boundaries	

B2.2.1 Dirichlet Boundary Conditions

The Dirichlet boundary condition defines a specific head boundary. Contaminant concentrations are specified along the boundary of the modeled region (S) or a portion (S_1) as:

$$C = C_1(x, y, z, t) \text{ in } S_1$$

Where:

Parameter	Description
C	Dissolved contaminant concentration
C_1	Contaminant concentration on a portion of the boundary (S_1)
S	The boundary of the region modeled R
S_1	A portion of the boundary of the region modeled (S)
t	Time
x	Longitudinal coordinate
y	Transfer coordinate
z	Vertical coordinate

The concentration (C_1) is a given function of time and location on a portion of the boundary (S_1).

B2.2.2 Neumann Boundary Conditions

The Neumann boundary condition defines a specific flow boundary. Where the contaminant concentration gradient is normal to the boundary of the region modeled (S) or a portion of the boundary (S_2) of the boundary as:

$$-\left(n_e \overline{\overline{D}} \bullet \nabla C\right) \bullet \vec{n} = q_2(x, y, z, t) \text{ on } S_2$$

Where:

Parameter	Description
C	Dissolved contaminant concentration
$\overline{\overline{D}}$	Hydraulic dispersion coefficient tensor
∇	Gradient (Del operator with respect to x, y, and z)
n_e	Effective porosity
$\vec{n}$	Unit vector normal to a portion of the boundary (S_2)
q_2	Contaminant flux across the boundary at a given function of time and location on a portion of the boundary (S_2)
S_2	A portion of the boundary of the region modeled (S)
t	Time
x	Longitudinal coordinate
y	Transfer coordinate
z	Vertical coordinate

B2.2.3 Cauchy Boundary Conditions

The Cauchy boundary condition or mixed boundary condition is a head-dependent flow boundary. The Cauchy condition includes advective and dispersive transport through the boundary of the region modeled (*S*) or a portion of the boundary (S_3) and may be written:

$$-\left(n_e \overline{\overline{D}} \bullet \nabla C - \vec{q}C\right) \bullet \vec{n} = q_3(x, y, z, t) \text{ on } S_3$$

Where:

Parameter	Description
C	Dissolved contaminant concentration
$\overline{\overline{D}}$	Hydraulic dispersion coefficient tensor
∇	Gradient (Del operator with respect to *x, y*, and *z*)
n_e	Effective porosity
$\vec{n}$	Unit vector normal to a portion of the boundary (S_2)
$\vec{q}$	Darcy's velocity vector
q_3	Contaminant flux across the boundary at a given function of time and location on S_3
S_3	A portion of the boundary of the region modeled (*S*)
t	Time
x	Longitudinal coordinate
y	Transfer coordinate
z	Vertical coordinate

B2.2.4 Radiation Boundary Conditions

AT123D includes a radiation boundary condition for simulations involving thermal conduction. The radiation boundary condition within AT123D is defined as:

$$n_e \overline{\overline{D}} \bullet \nabla C \bullet \vec{n} + n_e K_e^* C = 0 \text{ on } S_4$$

Where:

Parameter	Description
C	Initial temperature
$\overline{\overline{D}}$	Hydraulic dispersion coefficient tensor
∇	Gradient (Del operator with respect to *x, y*, and *z*)
K_e^*	Modified heat exchange coefficient
n_e	Effective porosity
$\vec{n}$	Unit vector normal to S_4
S_4	The soil-air interface portion of the boundary of the region modeled (*S*).

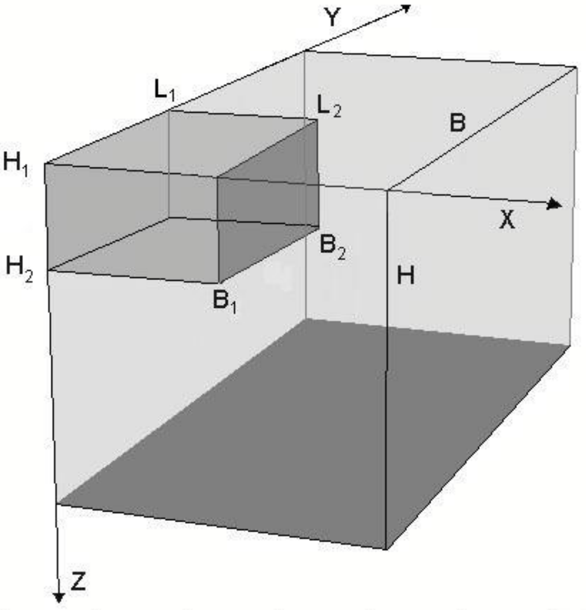
B2.3 Initial Conditions

To solve Equation B1, the initial and boundary conditions as defined above must be specified. Equation B1 is very difficult to solve analytically for typical groundwater situations. Assumptions must be made to simplify the aquifer geometry, boundary conditions, and the contaminant properties and load. These assumptions depend on the physical situation being modeled. Yeh (1981) made three assumptions to reduce Equation B1 to simplify the analytical solution.

1. The aquifer is assumed to be homogeneous and isotropic; thus, all of its properties (e.g., hydraulic conductivity, porosity, bulk density, aquifer thickness) are constant,
2. Groundwater flow is uniform along the positive x-axis (Figure B1), and
3. Sorption is in a state of instantaneous, linear, isothermal equilibrium so that $S = K_d C$.

☞ *Dispersivities are an exception which are assumed constant throughout the aquifer (homogeneous), but may differ in the longitudinal (direction of flow), lateral (perpendicular to flow direction in the horizontal plane), and vertical (perpendicular to flow direction in the vertical plane) directions.*

Figure B1: Sketch of source and aquifer dimensions. (after Yeh, 1981)



where

Parameter	Description
B	Aquifer width
H	Aquifer depth
L_1	Starting coordinate of the source in the x-direction
L_2	Ending coordinate of the source in the x-direction
B_1	Starting coordinate of the source in the y-direction
B_2	Ending coordinate of the source in the y-direction
H_1	Starting coordinate of the source in the z-direction
H_2	Ending coordinate of the source in the z-direction

Using these assumptions, Equation B1 can be reduced to (Robertson, 1974):

$$\frac{\partial C}{\partial t} = \nabla \bullet \left(\overline{\overline{K}} \bullet \nabla C\right) - \nabla \bullet \vec{U} C - \left(\frac{K}{R_d} + \lambda\right) C + \frac{\overset{\bullet}{M}}{n_e R_d} \qquad \text{(B2)}$$

Where:

Parameter	Description
C	Dissolved contaminant concentration
K	Chemical degradation rate
$\overline{\overline{K}}$	Retarded dispersion tensor
$\overset{\bullet}{M}$	Contaminant source release rate
n_e	Effective porosity
R_d	Retardation factor
t	Time
$\vec{U}$	Retarded seepage velocity vector
∇	Gradient (Del operator with respect to x, y, and z)
λ	Radioactive decay constant

The retardation factor $R_d = 1 + \frac{\rho_b K_d}{n_e}$.

Where:

Parameter	Description
K_d	Distribution coefficient
n_e	Effective porosity
ρ_b	Bulk density of the soil
R_d	Retardation factor

The retarded dispersion tensor $\overline{\overline{K}} = \frac{\overline{\overline{D}}}{R_d}$

Where:

Parameter	Description
$\overline{\overline{D}}$	Hydraulic dispersion coefficient tensor
$\overline{\overline{K}}$	Retarded dispersion tensor
R_d	Retardation factor

The retarded seepage velocity $\vec{U} = \left(\frac{\vec{q}}{n_e}\right) / R_d$.

Where:

Parameter	Description
n_e	Effective porosity
$\vec{q}$	Darcy's velocity vector
R_d	Retardation factor
$\vec{U}$	Retarded seepage velocity vector

The solution of Equation B2, subject to the initial and boundary conditions can be written:

$$C\left(x,y,z,t\right) = \int_o^t \int_R \frac{\overset{\bullet}{M}}{n_e R_d} G \, dR_o \, d\tau + \int_R \left(GC_i\right)\tau = 0^{dR_o} - \int_o^t \int_{S_1} \overline{\overline{K}} \bullet \nabla G \bullet \vec{n} C_1 dS_o \, d\tau - \int_o^t \int_{S_2} \frac{Gq_2}{n_e R_d} dS_o \, d\tau - \int_o^t \int_{S_3} \frac{Gq_3}{n_e R_d} dS_o \, d\tau \qquad \text{(B3)}$$

Where:

Parameter	Description
C	Dissolved contaminant concentration
C_i	Initial contaminant concentration
C_1	Concentration on the boundary S_1
G	Green's function
$\overline{\overline{K}}$	Retarded dispersion tensor
$\overset{\bullet}{M}$	Contaminant source release rate
n_e	Effective porosity
$\vec{n}$	Unit vector normal to S_2
q_2	The contaminant flux across the boundary at a given function of time and location on S_2
q_3	Contaminant flux across the boundary at a given function of time and location on S_3
R	A region with respect to x, y, and z (region modeled)
R_o	A region with respect to ξ, η, and ζ
S_1	A portion of S
S_2	A portion of S
S_3	A portion of S
S_o	The boundary of the region modeled R
t	Time
x	Longitudinal coordinate
y	Transfer coordinate
z	Vertical coordinate
∇	Gradient (Del operator with respect to x, y, and z)
τ	Duration of the contaminant release

☞ *The "o" subscript refers to the performance of the operation with respect to ξ, η, and ζ rather than x, y, z.*

Where $G(x, y, z, t: \xi, \eta, \zeta, \tau)$ is the Green's function which satisfies the following:

$$\lim_{t \to \tau} G = \delta(x-\xi)\delta(y-\eta)\delta(z-\zeta)$$

$$\begin{array}{rl}
G = 0 & \text{for } t < \tau \\
G = 0 & \text{on } S_1 \\
n_e \overline{\overline{D}} \bullet \nabla_o G \bullet \vec{n} = 0 & \text{on } S_2 \\
\left(n_e \overline{\overline{D}} \bullet \nabla_o G + \vec{q} G\right) \bullet \vec{n} = 0 & \text{on } S_3 \\
-\overline{\overline{D}} \bullet \nabla G \bullet \vec{n} + K_e^* G = D & \text{on } S_4
\end{array}$$

$$\text{and} \quad -\frac{\partial G}{\partial \tau} = \nabla_o \bullet \left(\overline{\overline{K}} \bullet \nabla_o G\right) + \vec{U} \bullet \nabla G - \left(\frac{K}{R_d} + \lambda\right) G \quad \text{for } t > \tau$$

Where:

Parameter	Description
D	Dispersion tension
$\overline{\overline{D}}$	Hydraulic dispersion coefficient tensor
δ	Dirac Delta function
G	Green's function
K	Chemical degradation rate
K_e^*	Modified heat exchange coefficient
$\overline{\overline{K}}$	Retarded dispersion tensor
n_e	Effective porosity
$\vec{n}$	Unit vector normal to S_2
$\vec{q}$	Darcy's velocity vector
R_d	Retardation factor
S_1	Part of S
S_2	Part of S
S_3	Part of S
S_4	Part of S (soil-air interface portion of the boundary)
t	Time
$\vec{U}$	Retarded seepage velocity vector
x	Longitudinal coordinate
y	Transverse coordinate
z	Vertical coordinate
∇	Gradient (Del operator with respect to x, y, and z)
∇_o	Del operator with respect to ξ, η, and ζ
λ	Radioactive decay constant
τ	Duration of the contaminant release
ξ	Longitudinal coordinate
η	Transverse coordinate
ζ	Vertical coordinate

Equation B3 represents the temporal and spatial distribution of the contaminant in terms of the source/sink term, $\dot{M}$, the initial condition, C_i, and the boundary conditions, C_1, q_2, and q_3. The only unknown is G, which is the Green's function. Thus the initial-boundary in Equation l is reduced to a homogeneous problem Equation 4 for G.

☞ *For a discussion of Green's functions, see De Wiest 1969.*

Green's functions can be determined for many simple geometries, such as separable coordinate systems. For these simple geometries, Green's function can be expressed as a product of three functions:

$$G(x, y, z, t{:}\, \xi, \eta, \zeta, \tau) = G_1(x, t; \xi, \tau)G_2(y, t; \eta, \tau)G_3(z, t; \zeta, \tau)$$

Parameter	Description
G	Green's function
G_1	Subgreen's function
G_2	Subgreen's function
G_3	Subgreen's function
t	Time
x	Longitudinal coordinate
y	Transverse coordinate
z	Vertical coordinate
τ	Duration of the contaminant release
ξ	Longitudinal coordinate
η	Transverse coordinate
ζ	Vertical coordinate

☞ *The derivations for G_1, G_2 and G_3 can be found in various references (see Yeh and Tsai, 1976, or Carslaw and Jaeger, 1959).*

To solve Equation B3, it is assumed that no contaminant flows across the impervious boundaries and that all flow passes through open boundaries which are located at infinity. Thus $C_1 = 0$, $q_2 = 0$ and $q_3 = 0$. Further, it is assumed that the initial (background) contaminant concentration, $C_i = 0$, Thus Equation B3 reduces to the following depending on the source duration:

a) For continuous source or finite duration release and $t < \tau$:

$$C(x, y, z, t) = \int_o^t \frac{\dot{M}}{n_e R_d} F_{ijk}(x, y, z, t; \tau)\, d\tau$$

Where:

Parameter	Description
C	Dissolved contaminant concentration
F_{ikj}	The integral of Green's function over contaminant source space
$\dot{M}$	Contaminant source release rate
n_e	Effective porosity
R_d	Retardation factor
t	Time
x	Longitudinal coordinate
y	Transfer coordinate
z	Vertical coordinate
τ	Duration of the contaminant release

b) For finite duration source and $t > \tau$:

$$C(x,y,z,t) = \int_o^T \frac{\dot{M}}{n_e R_d} F_{ijk}(x,y,z,t;\tau)\ d\tau$$

c) For instantaneous source:

$$C(x,y,z,t) = \frac{M}{n_e R_d} F_{ijk}(x,y,z,t;\tau)$$

Where:

Parameter	Description
M	Total instantaneous contaminant mass released

F_{ijk} is given by

$$F_{ijk} = X_i Y_j Z_k$$

Where:

Parameter	Description
i	l or 2
j	l, 2, 3 or 4
k	l, 2, 3 or 4
X_1	A function defined below
X_2	A function defined below
Y_1	A function defined below
Y_2	A function defined below
Y_3	A function defined below
Y_4	A function defined below
Z_1	A function defined below
Z_2	A function defined below
Z_3	A function defined below
Z_4	A function defined below

The selection of which X_i, Y_j, or Z_k to use depends on the contaminant source and aquifer configurations. The ten X_i, Y_j, or Z_k functions are as follows:

1) For a point source in the x-direction:

$$X_1 = \frac{1}{\sqrt{4\pi \ K_{xx}(t-\tau)}} \exp\left[-\frac{\left\{(x-x_s)-U(t-\tau)\right\}^2}{4K_{xx}(t-\tau)} - \left(\frac{K}{R_d}+\lambda\right)(t-\tau) \right]$$

2) For a line source in the x-direction:

$$X_2 = \frac{1}{2}\left\{ erf\left(\frac{x-L_1-U(t-\tau)}{\sqrt{4K_{xx}(t-\tau)}} \right) - erf\left(\frac{x-L_2-U(t-\tau)}{\sqrt{4K_{xx}(t-\tau)}} \right) \right\} \bullet \exp\left[-\left(\frac{K}{R_d}+\lambda\right)(t-\tau) \right]$$

3) For a finite width aquifer and point source in the y-direction:

$$Y_1 = \frac{1}{B} + \frac{2}{B}\sum_{i=1}^{\infty} \cos\left(\frac{i\pi y}{B}\right) \bullet \cos\left(\frac{i\pi y_s}{B}\right) \bullet \exp\left[-\left(\frac{i\pi}{B}\right)^2 K_{yy}(t-\tau) \right]$$

4) For a finite width aquifer and line source in the y-direction:

$$Y_2 = \frac{B_2-B_1}{B} + \frac{2}{B}\sum_{i=1}^{\infty} \cos\left(\frac{i\pi y}{B}\right) \bullet \frac{B}{i\pi}\left\{ \sin\left(\frac{i\pi B_2}{B}\right) - \sin\left(\frac{i\pi B_1}{B}\right) \right\} \exp\left[-\left(\frac{i\pi}{B}\right)^2 K_{yy}(t-\tau) \right]$$

5) For an infinitely wide aquifer and point source in the y-direction:

$$Y_3 = \frac{1}{\sqrt{4\pi \ K_{yy}(t-\tau)}} \exp\left[-\frac{(y-y_s)^2}{4K_{yy}(t-\tau)} \right]$$

6) For an infinitely wide aquifer and line source in the y-direction:

$$Y_4 = \frac{1}{2}\left[erf\left(\frac{y-B_1}{\sqrt{4K_{yy}(t-\tau)}} \right) - erf\left(\frac{y-B_2}{\sqrt{4K_{yy}(t-\tau)}} \right) \right]$$

7) For a finite depth aquifer and point source in the z-direction:

$$Z_1 = \sum_{i=1}^{\infty} \psi_i(\mathrm{z})\psi_i(z_s) \bullet \exp\left[-\kappa_i^2 K_{zz}(t-\tau) \right]$$

8) For a finite depth aquifer and line source in the z-direction:

$$Z_2 = \sum_{i=1}^{\infty} \psi_i(z)\left(\frac{a_i}{\kappa_i}\right)\left\{ \sin(\kappa_i H_2) - \sin(\kappa_i H_1) - \frac{K_e^*}{K_{zz}\kappa_i}\left[\cos(\kappa_i H_2) - \cos(\kappa_i H_1)\right] \right\} \bullet \exp\left[-\kappa_i^2 K_{zz}(t-\tau) \right]$$

9) For an infinitely deep aquifer and point source in the z-direction:

$$Z_3 = \frac{1}{\sqrt{4\pi\ K_{zz}(t-\tau)}}\left\{\exp\left[-\frac{(z-z_s)^2}{4K_{zz}(t-\tau)}\right]+\exp\left[-\frac{(z+z_s)^2}{4K_{zz}(t-\tau)}\right]\right\}-\frac{K_e^*}{K_{zz}}\exp\left[K_{zz}\left(\frac{K_e^*}{K_{zz}}\right)^2(t-\tau)+\left(\frac{K_e^*}{K_{zz}}\right)(z+z_s)\right]\bullet erfc\left[\frac{z+z_s}{\sqrt{4K_{zz}(t-\tau)}}+\frac{K_e^*}{K_{zz}}\sqrt{K_{zz}(t-\tau)}\right]$$

10) For an infinitely deep aquifer and line source in the z-direction:

$$Z_4 = \frac{1}{2}\left\{erf\left[\frac{z+H_2}{\sqrt{4K_{zz}(t-\tau)}}\right]-erf\left[\frac{z+H_1}{\sqrt{4K_{zz}(t-\tau)}}\right]-erf\left[\frac{z-H_2}{\sqrt{4K_{zz}(t-\tau)}}\right]+erf\left[\frac{z-H_1}{\sqrt{4K_{zz}(t-\tau)}}\right]\right\}-erf\left[K_{zz}\left(\frac{K_e^*}{K_{zz}}\right)^2(t-\tau)\right]$$

$$\bullet\left\{\exp\left[\left(\frac{K_e^*}{K_{zz}}\right)(z+H_2)\right]\bullet erfc\left[\frac{z+H_2}{\sqrt{4K_{zz}(t-\tau)}}+\left(\frac{K_e^*}{K_{zz}}\right)\sqrt{K_{zz}(t-\tau)}\right]-\exp\left[\left(\frac{K_e^*}{K_{zz}}\right)(z+H_1)\right]\bullet erfc\left[\frac{z+H_1}{\sqrt{4K_{zz}(t-\tau)}}+\left(\frac{K_e^*}{K_{zz}}\right)\sqrt{K_{zz}(t-\tau)}\right]\right\}-\left\{erf\left[\frac{z+H_2}{\sqrt{4K_{zz}(t-\tau)}}\right]-erf\left[\frac{z-H_1}{\sqrt{4K_{zz}(t-\tau)}}\right]\right\}$$

Where:

Parameter	Description
a_i	A coefficient defined below
B	Width of the aquifer
L_1	Starting coordinate of the source in the x-direction
L_2	Ending coordinate of the source in the x-direction
B_1	Starting coordinate of the source in the y-direction
B_2	Ending coordinate of the source in the y-direction
H_1	Starting coordinate of the source in the z-direction
H_2	Ending coordinate of the source in the z-direction
K	Chemical degradation rate
K_e^*	Modified heat exchange coefficient
K_{xx}	X-component of the retarded dispersion tensor
K_{yy}	Y-component of the retarded dispersion tensor
K_{zz}	Z-component of the retarded dispersion tensor
t	Time
U	The magnitude of $\vec{U}$ the retarded seepage velocity vector
x	Longitudinal coordinate
x_s	X-coordinate of a point source
y	Transverse coordinate
y_s	Y-coordinate of a point source
z	Vertical coordinate
z_s	Z-coordinate of a point source
λ	Radioactive decay constant
τ	Duration of the contaminant release
κ_i	i-th eigenvalue defined below
ψ_i	i-th eigenfunction defined below
erf	Error function
erfc	Complimentary error function

The eigenfunction parameter $\psi_i(z)$ is given by:

$$\psi_i(z) = a_i \left\{ \cos(\kappa_i z) + \frac{K_e^*}{K_{zz}\kappa_i} \sin(\kappa_i z) \right\}$$

The eigenvalue parameter κ_i is given by:

$$\tan(\kappa_i H) = \frac{K_e^*}{K_{zz}\kappa_i}$$

The parameter a_i is given by:

$$a_i^2 = \frac{2}{H\left\{1 + \left(\frac{K_e^*}{K_{zz}\kappa_i}\right)^2 + \left(\frac{K_e^*}{K_{zz}X_i}\right)\right\}}$$

Where:

Parameter	Description
H	Depth of the aquifer

For non-heat flow cases, K_e^* and $\kappa_i = -\frac{i\pi}{H}$ and $a_i^2 = \frac{2}{H}$.

For the three-dimensional cases, the applicable X_i, Y_j and Z_k are selected from the ten equations and multiplied together to obtain F_{ijk}. For two-dimensional cases, the unused dimension's coefficient is set equal to one (e.g., for a case involving the X-Z plane, $Y_j = 1$). For one-dimensional cases, the two unused dimensions have their coefficients set equal to one (e.g., for a case involving only x, $Y_j = Z_k = 1$).

For problems involving finite width aquifers, the Y_j equations (using equations 3 and 4) converge very slowly for small values of $K_{yy}(t-\tau)/B^2$ (Yeh, 1981). This situation occurs when the aquifer is very wide and the contaminant concentrations during the initial time steps (t is small) are being calculated. For this case the program uses alternate Y_j equations calculated by the method of images, to provide more rapid convergence. These equations are:

$$Y_1 = \frac{1}{\sqrt{4\pi K_{yy}(t-\tau)}} \left\{ \sum_{n=0}^{\infty} \exp\left[-\frac{\{(y-y_s)+2nB\}^2}{4K_{yy}(t-\tau)}\right] + \sum_{n=0}^{\infty} \exp\left[-\frac{\{(y-y_s)-2(n-1)B\}^2}{4K_{yy}(t-\tau)}\right] + \sum_{n=0}^{\infty} \exp\left[-\frac{\{(y-y_s)+2(n-1)B\}^2}{4K_{yy}(t-\tau)}\right] + \sum_{n=0}^{\infty} \exp\left[-\frac{\{(y-y_s)+2nB\}^2}{4K_{yy}(t-\tau)}\right] \right\}$$

and

$$Y_2 = \frac{1}{2}\sum_{n=0}^{\infty} \left\{ erf\left[\frac{(y-B_1)-2nB}{\sqrt{4K_{yy}(t-\tau)}}\right] - erf\left[\frac{(y-B_2)-2nB}{\sqrt{4K_{yy}(t-\tau)}}\right] + erf\left[\frac{(y-B_1)+2(n-1)B}{\sqrt{4K_{yy}(t-\tau)}}\right] - erf\left[\frac{(y-B_2)+2(n-1)B}{\sqrt{4K_{yy}(t-\tau)}}\right] + erf\left[\frac{(y+B_2)+2(n-1)B}{\sqrt{4K_{yy}(t-\tau)}}\right] - erf\left[\frac{(y+B_1)+2(n-1)B}{\sqrt{4K_{yy}(t-\tau)}}\right] + erf\left[\frac{(y+B_2)-2nB}{\sqrt{4K_{yy}(t-\tau)}}\right] - erf\left[\frac{(y+B_1)-2nB}{\sqrt{4K_{yy}(t-\tau)}}\right] \right\}$$

Where:

Parameter	Description
B	Width of the aquifer
B_1	Starting coordinate of the source in the y-direction
B_2	Ending coordinate of the source in the y-direction
K_{yy}	Y-component of the retarded dispersion tensor
t	Time
Y	Transverse coordinate
Y_s	Y-coordinate of a point source
τ	Duration of the contaminant release

The integral of Green's function, F_{ijk} can have 32 different equations using the ten equations for X_i, Y_j and Z_k (32 is the number of permutations of 2 X_i, 4 Y_j and 4 Z_k). Substituting these 32 equations into the three equations for the source release (continuous or finite duration release with $t < \tau$, finite duration release with $t > \tau$, and instantaneous release), 96 equations are obtained. As these equations are applicable to 3 types of contaminants (chemical, thermal or radioactive), there are 288 options for the three-dimensional case. Similarly, there are 144 options for the two-dimensional case, 72 involving the x-y plane and 72 involving the x-z plane [2 X_i times 4 Y_j (or 4 Z_k) times 3 source release types times 3 contaminant types]. For the one- dimensional case, in the x-direction, there are 18 options (2 X_i times 3 source release types times 3 contaminant types). Thus, there are a total of 450 run options in the AT123D model.

AT123D determines the concentration at (x, y, z, t) from a continuous or finite duration release by superimposing the contributions from instantaneous contaminant releases at τ (where $0 < \tau < t$). To carry out the integration necessary for computing concentrations resulting from continuous or finite duration source releases, AT123D uses Simpson's rule to numerically calculate the time integral. A source release rate that varies through time is modeled as a sequence of finite duration releases of varying load.

[redacted]

B3.0 Verification of AT123D

This section presents the results of a verification of the AT123D using analytical equations. A total of four verification scenarios were performed (Yeh et al., 1987). Three of the solutions were for infinite aquifers with instantaneous source releases under uniform flow (point source with three dimensional mixing, infinite line source lying along the z-axis, and a line source lying along the y-axis with a finite width aquifer). The fourth solution was for a continuous point source with three-dimensional mixing.

Identical concentrations were determined using AT123D and the analytical equations, although some concentrations differ in the final decimal place due to different rounding techniques. Identical results are anticipated as AT123D uses analytical equations to determine the predicted groundwater concentrations.

B3.1 Solution for an Instantaneous Point Source

The following equation was used to determine groundwater contaminant concentrations for an instantaneous point source with uniform groundwater flow parallel to the x-axis. The source is at the origin (x, y and z equal 0), and in an infinite aquifer (semi-infinite in z-direction):

$$C(x,y,z,t)=\frac{M}{4n_e(\pi t)^{\frac{3}{2}}\sqrt{D_xD_yD_z}}\exp\left\{-\frac{\left(x-\bar{v}t\right)^2}{4D_xt}-\frac{y^2}{4D_yt}-\frac{z^2}{4D_xt}\right\}$$

Where:

Parameter	Description	Units
M	Mass of contaminant introduced	Grams
D_x	Dispersion coefficients in x direction	Meters
D_y	Dispersion coefficients in y direction	Meters
D_z	Dispersion coefficients in z direction	Meters
$\bar{v}$	Average linear velocity	Meters/hour
n_e	Aquifer porosity	Fraction
t	Time after injection	Hours

From Freeze and Cherry, 1979.

Data for the solution

Mass contaminant load is 25,000 grams. Porosity is 0.25. Dispersivities (α) are 5 meters, 0.5 meters, and 0.5 meters in the *x, y, z* directions, respectively. Hydraulic conductivity is 3.6 meters/hour with a gradient of 0.02 meters/meter.

Results

Identical groundwater contaminant concentrations were determined using the analytical equation and the AT123D model. A summary of the results is presented in Table 15.

Table 15 Analytical Solution for an Instantaneous Point Source

Time (hours)	x (meters)	y (meters)	z (meters)	Analytical Concentration (mg/l)	AT123D Concentration (mg/l)
24	10	0	0	206.25	206.25
	11	0	0	195.82	195.82
	12	0	0	183.24	183.24
	13	0	0	169.01	169.01
	14	0	0	153.65	153.65
	15	0	0	137.67	137.67
	16	0	0	121.59	121.59
	17	0	0	105.84	105.84
	18	0	0	90.81	90.81
	19	0	0	76.79	76.79
	20	0	0	64.00	64.00
24	10	0	0	206.25	206.25
	10	1	0	191.86	191.86
	10	2	0	154.86	154.86
	10	3	0	107.56	107.56
	10	4	0	64.82	64.82
	10	5	0	33.81	33.81
	10	6	0	15.26	15.26
	10	7	0	5.96	5.96
	10	8	0	2.01	2.01
	10	9	0	0.59	0.59
24	10	0	0	206.25	206.25
	10	0	1	191.86	191.86
	10	0	2	154.86	154.86
	10	0	3	107.56	107.56
	10	0	4	64.82	64.82
	10	0	5	33.81	33.81
	10	0	6	15.26	15.26
	10	0	7	5.96	5.96
	10	0	8	2.01	2.01
	10	0	9	0.59	0.59
24	10	0	0	206.25	206.25
26	10	0	0	187.89	187.89
28	10	0	0	171.33	171.33
30	10	0	0	156.44	156.44
32	10	0	0	143.05	143.05
34	10	0	0	131.03	131.03
36	10	0	0	120.21	120.21
38	10	0	0	110.47	110.47
40	10	0	0	101.68	101.68
42	10	0	0	93.74	93.74
44	10	0	0	86.55	86.55

B3.2 Solution for an Instantaneous Semi-Infinite Line Source

The following equation was used to determine groundwater concentrations for a semi-infinite line source parallel to the z-axis. The source length was established such that the z-dimension is neglected (0, ∞). The source is at *x* and *y* equal 0 and the source release starts at *t* equal to 0:

$$C(x,y,z,t) = \frac{M}{n_e 4\pi t\sqrt{D_x D_y}} \exp\left\{-\frac{\left(x-\bar{v}t\right)^2}{4D_x t} - \frac{y^2}{4D_y t}\right\}$$

From Carslaw and Jaeger, 1959, p 258.

Where:

Parameter	**Description**	**Units**
M	Mass of contaminant load per unit length of line source.	Grams/meter
D_x	Dispersion coefficients in x direction	Meters
D_y	Dispersion coefficients in y direction	Meters
D_z	Dispersion coefficients in z direction	Meters
$\bar{v}$	Average linear velocity	Meters/hour
n_e	Aquifer porosity	Fraction
t	Time after injection	Hours

Within AT123D this scenario is simulated using a finite depth solution with a line source extending over the entire depth of aquifer.

Data for the solution

Hydraulic conductivity and gradient are 1 meters/hour and 0.02 respectively. Porosity is 0.25. Longitudinal and transverse dispersivities are 5 meters and 0.5 meters, respectively. Contaminant mass load is 1000 grams/meter. In AT123D the line source length was set to 25 meters. This length is arbitrary as long as it results in 1000 grams/meter of mass released from the line source.

Results

Identical groundwater contaminant concentrations were determined using the analytical equation and the AT123D model. However, some concentrations varied slightly due to different numerical rounding techniques. A summary of the results is presented in Table 16.

Table 16 Analytical Solution for an Instantaneous Semi-Infinite Line Source

Time (hours)	x (meters)	y (meters)	Analytical Concentration (mg/l)	AT123D Concentration (mg/l)
96	10	0	25.31	25.31
	11	0	24.40	24.40
	12	0	23.21	23.21
	13	0	21.80	21.80
	14	0	20.21	20.21
	15	0	18.49	18.49
	16	0	16.70	16.70
	17	0	14.89	14.89
	18	0	13.10	13.10
	19	0	11.38	11.38
	20	0	9.76	9.76
96	10	0	25.31	25.31
	10	0	23.72	23.72
	10	0	19.51	19.51
	10	0	14.09	14.09
	10	0	8.93	8.93
	10	0	4.97	4.97
	10	0	2.43	2.43
	10	0	1.04	1.04
	10	0	0.39	0.39
	10	0	0.13	0.13
72	10	0	29.90	29.90
78	10	0	28.81	28.81
84	10	0	27.65	27.65
90	10	0	26.48	26.48
96	10	0	25.31	25.31
102	10	0	24.16	24.17
108	10	0	23.05	23.05
114	10	0	21.98	21.98
120	10	0	20.95	20.95
126	10	0	19.97	19.97
132	10	0	19.04	19.04

B3.3 Solution for Instantaneous Line Source in a Finite Width Aquifer

The following equation was used to determine the groundwater concentrations for a line source along the y-axis at x and z equal to 0 in a semi-infinite depth aquifer. Groundwater mixing is in three-dimensions. This formula uses Green's functions and the method of images.

$$C(x,y,z,t) = \frac{M}{n_e} F_{ijk} = \frac{M}{n_e} X \bullet Y \bullet Z$$

Where:

Parameter	Description	Units
M	Mass of contaminant load introduced/unit length of line source	Grams /meter
X	Instantaneous point source at $x = 0$ (infinite medium) $= \frac{1}{\sqrt{4\pi D_x t}} \exp\left\{ -\frac{\left(x - \bar{v}t\right)^2}{4D_x t} \right\}$	
Y	Instantaneous line source in a finite aquifer $= \frac{1}{2}\sum_{n=0}^{\infty}\left\{\left[erf\left(\frac{y-B_1+2nB}{A}\right)-erf\left(\frac{y-B_2+2nB}{A}\right)\right]+\left[erf\left(\frac{y+B_2+2nB}{A}\right)-erf\left(\frac{y+B_1+2nB}{A}\right)\right]+\left[erf\left(\frac{y-B_1-2(n+1)B}{A}\right)-erf\left(\frac{y-B_2-2(n+1)B}{A}\right)\right]+\left[erf\left(\frac{y+B_2-2(n+1)B}{A}\right)-erf\left(\frac{y-B_1-2(n+1)B}{A}\right)\right]\right\}$	
Z	Instantaneous point source at $z = 0$ (semi-infinite depth) $= \frac{2}{\sqrt{4\pi D_z t}} \exp\left\{ -\frac{z^2}{4D_z t} \right\}$	
A	$4D_y t$	

Carslaw, Jaeger, 1959, p 358 and J. A. Hoopes for Yeh, (from Yeh et al., 1987)

Data for the solution

Hydraulic conductivity and gradient, porosity, and mass/unit length of the line source are 1.0 m/hr and 0.02, 25%, and 1000 grams/meter respectively. Dispersivities are 5 m, 0.5m and 0.5 m in the *x, y*, and *z* directions respectively. The aquifer width, *B*, is 100 m. End points of the line source are B_1 = -12.5 m and B_2 = 12.5 m.

Results

Identical groundwater contaminant concentrations were determined using the analytical equation and the AT123D model. However, some concentrations varied slightly due to different numerical rounding techniques. A summary of the results is presented in Table 17.

Table 17 Analytical Solution for an Instantaneous Line Source in a Finite Width Aquifer

Time (hours)	x (meters)	y (meters)	z (meters)	Analytical Concentration (mg/l)	AT123D Concentration (mg/l)
96	10	0	0	101.24	101.24
	11	0	0	97.59	97.59
	12	0	0	92.86	92.86
	13	0	0	87.21	87.21
	14	0	0	80.84	80.85
	15	0	0	73.97	73.98
	16	0	0	66.81	66.81
	17	0	0	59.56	59.57
	18	0	0	52.41	52.42
	19	0	0	45.53	45.53
	20	0	0	39.03	39.03
96	10	0	0	101.24	101.24
	10	3	0	101.21	101.21
	10	6	0	100.28	100.28
	10	9	0	90.78	90.79
	10	12	0	57.87	57.87
	10	15	0	18.58	18.58
	10	18	0	2.39	2.39
	10	21	0	0.11	0.11
	10	24	0	0.00	0.00
	10	27	0	0.00	0.00
96	10	0	0	101.24	101.24
	10	0	1	94.86	94.86
	10	0	2	78.03	78.03
	10	0	3	56.35	56.35
	10	0	4	35.73	35.73
	10	0	5	19.88	19.88
	10	0	6	9.72	9.72
	10	0	7	4.17	4.17
	10	0	8	1.57	1.57
	10	0	9	0.52	0.52
72	10	0	0	119.60	119.60
78	10	0	0	115.23	115.24
84	10	0	0	110.61	110.62
90	10	0	0	105.92	105.92
96	10	0	0	101.24	101.24
102	10	0	0	96.66	96.65
108	10	0	0	92.21	92.20
114	10	0	0	87.92	87.92
120	10	0	0	83.81	83.80
126	10	0	0	79.88	79.87
132	10	0	0	76.13	76.13

B3.4 Solution for a Continuous Point Source in a Finite Depth Aquifer

The following equation was used to determine groundwater concentrations for a continuous point source at *x*, *y* and *z* equal to 0. The release was initiated at *t* equal to 0. The aquifer is infinite in x- and y-dimensions, and semi-infinite in z-dimension. Groundwater flow is uniform and is parallel to x-axis.

$$C(x,y,z,t) = 2 \bullet \frac{\dot{M} \exp\left[-\frac{\bar{v}}{2D_x}(R-x)\right]}{8\pi n_e R\sqrt{D_y D_z}} \left\{ erfc\left[\frac{R-\bar{v}t}{\sqrt{4D_x t}}\right] + \exp\left(\frac{\bar{v}R}{D_x}\right) \bullet erfc\left(\frac{R+\bar{v}t}{\sqrt{4D_x t}}\right) \right\}$$

From Yeh et al., 1987.

Where

Parameter	Description	Units
$\dot{M}$	Contaminant mass flow rate	Grams/hour
R	$\left(x^2 + \frac{D_x}{D_y}y^2 + \frac{D_x}{D_z}z^2\right)^{\frac{1}{2}}$	

Data for the solution

Contaminant mass flow rate is 25 g/hr. Porosity is 25%. Dispersivities are 5 m, 0.5 m and 0.5 m in the *x*, *y*, and *z* directions respectively. Hydraulic conductivity is 1.0 m/hr, while the gradient is 0.02.

Results

Identical groundwater contaminant concentrations were determined using the analytical equation and the AT123D model. However, some concentrations varied slightly due to different numerical rounding techniques. A summary of the results is presented in Table 18.

Table 18 Analytical Solution for a Continuous Point Source

Time (hours)	x (meters)	y (meters)	z (meters)	Analytical Concentration (mg/l)	AT123D Concentration (mg/l)
96	10	0	0	22.16	22.16
120	10	0	0	25.93	25.93

144	10	0	0	28.74	28.74
168	10	0	0	30.89	30.89
192	10	0	0	32.54	32.54
216	10	0	0	33.84	33.84
240	10	0	0	34.87	34.87
264	10	0	0	35.69	35.69
288	10	0	0	36.36	36.36
312	10	0	0	36.91	36.91
336	10	0	0	37.36	37.36
240	5	0	0	76.15	76.16
	6	0	0	62.61	62.61
	7	0	0	52.84	52.84
	8	0	0	45.43	45.43
	9	0	0	39.60	39.60
	10	0	0	34.87	34.87
	11	0	0	30.93	30.93
	12	0	0	27.60	27.60
	13	0	0	24.74	24.74
	14	0	0	22.24	22.24
240	10	0	0	34.87	34.87
	10	1	0	31.30	31.30
	10	2	0	23.42	23.42
	10	3	0	15.58	15.59
	10	4	0	9.68	9.68
	10	5	0	5.75	5.75
	10	6	0	3.29	3.29
	10	7	0	1.83	1.83
	10	8	0	0.98	0.98
	10	9	0	0.51	0.51
240	10	0	0	34.87	34.87
	10	0	1	31.30	31.30
	10	0	2	23.42	23.42
	10	0	3	15.58	15.59
	10	0	4	9.68	9.68
	10	0	5	5.75	5.75
	10	0	6	3.29	3.29
	10	0	7	1.83	1.83
	10	0	8	0.98	0.98
	10	0	9	0.51	0.51

B4.0 AT123D Data Input Guide

This appendix provides a description of the AT123D input parameters. AT123D uses ASCII text files to store the information used in the model scenarios. These files must be formatted so that the AT123D program correctly read the data. A description of the FORTRAN read format is also provided. The AT123D input file has been modified to read more than one load. The file format remains basically the same for the first load. Subsequent loads use a different format in that only the description, release coordinates, and load are required.

Input file format for the first load.

Title

Line 1

TITLE
80

Parameter	Format	Description
TITLE	A80	The title for the model scenario.

Basic Integer Parameters

Line 2

NX	NY	NZ	NROOT	NBGTI	NEDTI	NPRINT	INSTAN
5	10	15	20	25	30	35	40

NSOURS	ILOADS	ICASE	IDEP	IWID	IBUG ↓	ROC	RKOC
45	50	55	60	65	66	73	80

Parameter	Format	Description
NX	I5	Number of points in the x-direction (parallel to flow) where the concentration is desired. (Maximum = 15).
NY	I5	Number of points in the y-direction (perpendicular to flow in horizontal plane) where the concentration is desired. (Maximum = 10)
NZ	I5	Number of points in the z-direction (perpendicular to flow in the vertical plane) where the concentration is desired. (Maximum = 10)

☞ *An array of points for solution (NX, NY, NZ) is formed by these first three values. In other words, for each point in the x-direction, a solution will be generated for all possible x, y, z combinations using that x (e.g., if NX = NY = NZ = 3, then final concentrations will be calculated for 27 points.)*

Parameter	Format	Description
NROOT	I5	Number of eigenvalues required for series evaluation. The number of eigenvalues may not exceed 1000. NROOT represents the maximum number of terms that will be calculated for a series solution before truncation occurs. Start with 500 and increase it to a 1000 if a warning message is printed out with the solution.
NBGTI	I5	Starting time step where the solution is desired.

☞ *As AT123D counting loops start with 1 not 0, a 1 must be added to the values for NBGTI and NEDTI. For example, if you wanted a solution from year 10 to year 20, NBGTI should be set to 121 months and NEDTI should be set to 241 months.*

NEDTI	I5	Ending time step where the solution is desired.
NPRINT	I5	Print out time step in terms of DT.
INSTAN	I5	Integer parameter indicating if the contaminant release is instantaneous or continuous; = 0 for instantaneous release (slug), = 1 for continuous release.
NSOURS	I5	Integer parameter indicating if the source release is constant or changing over time; = 0 for constant source, > 0 for varying sources.

☞ *NSOURS must be set to the total number of contaminant releases.*

ILOADS	I5	Integer parameter indicating the total number of separate AT123D loads contained in the input file.
ICASE	I5	Integer parameter indicating the type of contaminant to be simulated: 1 for thermal, 2 for chemical and 3 for radioactive.
IWID	I5	Integer parameter indicating if the aquifer is infinite or not in the y-direction; = 0 for Yes, = 1 for No.
IDEP	I5	Integer parameter indicating if the aquifer is infinitely deep or not; = 0 for Yes, = 1 for No.
IBUG	I1	Integer parameter indicating if the diagnostic check is desired or not; no = 0, 1 for yes.
ROC	F7.2	Organic carbon content (percent)
RKOC	F7.2	Organic carbon adsorption coefficient (μg/g)/(μg/ml)

☞ *IBUG is typically set to 0.*

Aquifer Size and Source Size

Line 3

DEPTH	WIDTH	RL1	RL2	RB1	RB2	RH1	RH2
10	20	30	40	50	60	70	80

Parameter	Format	Description
DEPTH	F10.0	Aquifer depth (meters).
WIDTH	F10.0	Aquifer width (meters).
RL1	F10.0	Beginning coordinate of the source load in the x-direction (meters).
RL2	F10.0	Ending coordinate of the source load in the x-direction (meters).
RB1	F10.0	Beginning coordinate of the source load in the y direction (meters).
RB2	F10.0	Ending coordinate of the source load in the y direction (meters).
RH1	F10.0	Beginning coordinate of the source load in the z-direction (meters).
RH2	F10.0	Ending coordinate of the source load in the z direction (meters).

☞ *The F 10.0 format can read either exponential or real numeric formats.*

Soil and Waste Properties

Line 4

POR	HCOND	HGRAD	AELONG	ATRANV	AVERTI	AKD	CONC
10	20	30	40	50	60	70	80

Parameter	Format	Description
POR	F10.0	Porosity of the soil (decimal, dimensionless).
HCOND	F10.0	Hydraulic conductivity (meters/hour).
HGRAD	F10.0	Hydraulic gradient (meters/meters).
AELONG	F10.0	Longitudinal dispersivity (meters).
ATRANV	F10.0	Transverse dispersivity (meters).
AVERTI	F10.0	Vertical dispersivity (meters).
AKD	F10.0	Distribution coefficient, K_d (m^3/kg).
CONC	F10.0	Initial contaminant concentration, (mg/L).

Additional Soil and Waste Properties and Some Real Number Parameters

Line 5

AMTAU	RAMADA	RHOB	SOLH2O	SELMAX	DT	TDISP	Q
10	20	30	40	50	60	70	80

Parameter	Format	Description
AMTAU	F10.0	Molecular diffusion coefficient times tortuosity (m^2/hr).
RAMADA	F10.0	Decay constant (per hour).
RHOB	F10.0	Bulk density of the soil (kg/m^3).
SOLH2O	F10.0	Solubility in water (μg/ml)
SELMAX	F10.0	Maximum SESOIL leachate concentration (mg/L).
DT	F10.0	Time step size for calculating the solution (hours).
TDISP	F10.0	Total length of time over which the contaminant is to be released into the aquifer (hours)
Q	F10.0	Contaminant release in kg/hr, or the total instantaneous release in kg.

X-Axis Coordinates

Line 6

The number of lines in the file depends on the number of points in the x-direction (NX). There may be up to eight x-coordinate values on a line.

XDIM(1)	XDIM(2)	XDIM(3)	XDIM(4)	XDIM(5)	XDIM(6)	XDIM(7)	XDIM(8)
10	20	30	40	50	60	70	80

Parameter	Format	Description
XDIM(I)	F10.0	X-coordinate of the I-th point in the x-direction (direction of flow), where a concentration will be determined (meters).

Y-Axis Coordinates

The number of lines in the file depends on the number of points in the y-direction (NY). There may be up to eight y-coordinate values on a line.

YDIM(1)	YDIM(2)	YDIM(3)	YDIM(4)	YDIM(5)	YDIM(6)	YDIM(7)	YDIM(8)
10	20	30	40	50	60	70	80

Parameter	Format	Description
YDIM(I)	F10.0	Y-coordinate of the I-th point in the y-direction (horizontally perpendicular to flow), where a concentration will be determined (meters).

Z-Axis Coordinate

The number of lines in the file depends on the number of points in the z-direction (NZ). There may be up to eight z-coordinate values on a line.

ZDIM(1)	ZDIM(2)	ZDIM(3)	ZDIM(4)	ZDIM(5)	ZDIM(6)	ZDIM(7)	ZDIM(8)
10	20	30	40	50	60	70	80

Parameter	Format	Description
ZDIM(I)	F10.0	Z-coordinate of the I-th point in the z-direction (vertically perpendicular to flow), where a concentration will be determined (meters).

Number of Point of Compliance

NPOC							
10	20	30	40	50	60	70	80

Parameter	Format	Description
NPOC	I10	Integer parameter indicating the total number of separate POCs contained in the input file.

Point of Compliance Coordinates

Users can define a maximum of 15 points of compliance. The number of lines in the file depends on the number of points of compliance and the number of coordinates in the z-direction (NZPOC).

First POC Line

POCT(I)
80

Parameter	Format	Description
POCT(I)	A80	The description of the POC.

Second POC Line

POC(I,1)	POC(I,2)	NZPOC	POC(I,4)	POC(I,5)	POC(I,6)	POC(I,7)	POC(I,8)
10	20	30	40	50	60	70	80

Parameter	Format	Description
POC(I,1)	F10.0	X-coordinate of the POC in the x-direction (direction of flow), where a concentration will be determined (meters).
POC(I,2)	F10.0	Y-coordinate of the POC in the y-direction (horizontally perpendicular to flow), where a concentration will be determined (meters).
NZPOC	I10	Number of points in the z-direction for the POC (perpendicular to flow in the vertical plane) where the concentration is desired. (Maximum = 10)
POC(I,4 - 8)	F10.0	Z-coordinate of the POC in the z-direction (vertically perpendicular to flow), where a concentration will be determined (meters). (Maximum = 10)

Third POC Line

POC(I,9)	POC(I,10)	POC(I,11)	POC(I,12)	POC(I,13)			
10	20	30	40	50	60	70	80

Parameter	Format	Description
POC(I,9 - 13)	F10.0	Z-coordinate of the POC in the z-direction (vertically perpendicular to flow), where a concentration will be determined (meters). (Maximum = 10)

Variable Source Release Time Steps

Used to define the number of varying contaminant loads (not used in constant release scenarios). The number of lines depends on the total number of contaminant loads (NSOURS). There may be up to 16 time step values on a line.

ITS(1)	ITS(2)	ITS(3)	. . . . ITS(NSOURS)
5	10	15	

Parameter	Format	Description

ITS(I)	I5	Integer number for the I-th time step number (in terms of DT) at which the release rate changes. Begin with 1 (remember AT123D loops start at 1, not 0), and continue with an integer in each field of 5 spaces, There should be a total of NSOURS ITS(I) entries.

Variable Source Release Rates

Used to specify the varying contaminant release loads (not used in constant release scenarios). The number of lines depends on the total number of contaminant loads (NSOURS). There may be up to six contaminant load values on a line.

QSA(1)	QSA(2)	QSA(3)	. . . . QSA(NSOURS)
12	24	36	

Parameter	Format	Description
QSA(I)	F12.0	Waste release rate at time step corresponding to the variable source release time step [ITS(I)]

☞ *Use same units as the constant release rate (Q) in kg/hr, kcal/hr, or CI/hr.*

☞ *There must be as many variable source release rates [QSA(I)'s] as variable source release time steps [ITS(I)'s] and NSOURS entries.*

Input file format for all subsequent loads.

Title

The first line of any subsequent loads.

TITLE
80

Parameter	Format	Description
TITLE	A80	The title for the model scenario.

The second line of any subsequent loads.

INSTAN	NSOURS	SELMAX
5	10	20

Parameter	Format	Description

INSTAN	I5	Integer parameter indicating if the contaminant release is instantaneous or continuous; = 0 for instantaneous release (slug), = 1 for continuous release.
NSOURS	I5	Integer parameter indicating if the source release is constant or changing over time; = 0 for constant source, > 0 for varying sources.

☞ *NSOURS must be set to the total number of contaminant releases.*

SELMAX	F10.0	Maximum SESOIL leachate concentration (mg/L).

Aquifer Size and Source Size

The third line of any subsequent loads.

CONC	Q	RL1	RL2	RB1	RB2	RH1	RH2
10	20	30	40	50	60	70	80

Parameter	Format	Description
CONC	F10.0	Initial contaminant concentration, (mg/L).
Q	F10.0	Contaminant release in kg/hr, or the total instantaneous release in kg.
RL1	F10.0	Beginning coordinate of the source load in the x-direction (meters).
RL2	F10.0	Ending coordinate of the source load in the x-direction (meters).
RB1	F10.0	Beginning coordinate of the source load in the y direction (meters).
RB2	F10.0	Ending coordinate of the source load in the y direction (meters).
RH1	F10.0	Beginning coordinate of the source load in the z-direction (meters).
RH2	F10.0	Ending coordinate of the source load in the z direction (meters).

Variable Source Release Time Steps

Used to define the number of varying contaminant loads (not used in constant release scenarios). The number of lines depends on the total number of contaminant loads (NSOURS). There may be up to 16 time step values on a line.

ITS(1)	ITS(2)	ITS(3)	. . . . ITS(NSOURS)
5	10	15	

Parameter	Format	Description

ITS(I)	I5	Integer number for the I-th time step number (in terms of DT) at which the release rate changes. Begin with 1 (remember AT123D loops start at 1, not 0), and continue with an integer in each field of 5 spaces, There should be a total of NSOURS ITS(I) entries.

Variable Source Release Rates

Used to specify the varying contaminant release loads (not used in constant release scenarios). The number of lines depends on the total number of contaminant loads (NSOURS). There may be up to six contaminant load values on a line.

QSA(1)	QSA(2)	QSA(3)	. . . . QSA(NSOURS)
12	24	36	

Parameter	Format	Description
QSA(I)	F12.0	Waste release rate at time step corresponding to the variable source release time step [ITS(I)]

☞ *Use same units as the constant release rate (Q) in kg/hr, kcal/hr, or CI/hr.*

☞ *There must be as many variable source release rates [QSA(I)'s] as variable source release time steps [ITS(I)'s] and NSOURS entries.*

B5.0 AT123D Example Input Data File

RUN01.ATI

```
Benzene in Sand
    7    5    2500     25  2411        1  2401    2        0    005.00E-13.10E+1
       0.0       0.0-1.581E+00 1.581E+00-1.581E+00 1.581E+00       0.0       0.0
 2.500E-01 3.600E-02     0.003      2.16       0.2      0.02 1.550E-04 .0000E+00
 3.528E-06 0.000E+00 1.700E+03 .1000E+04      0.010.7300E+03 1.752E+050.7300E+03
       0.0       5.0      10.0      15.0      20.0      25.0      30.0
     -10.0      -5.0       0.0       5.0      10.0
       0.0       1.0
         2
       0.0       5.0         7        0.0      1.0       2.0       3.0       4.0
       5.0       6.0
      11.0      -3.0        10        0.0      1.0       2.0       3.0       4.0
       5.0       6.0       7.0        8.0      9.0
    1    2    3    4    5    6    7    8    9   10   11   12   13   14   15   16
   17   18   19   20   21   22   23   24   25   26   27   28   29   30   31   32
   33   34   35   36   37   38   39   40   41   42   43   44   45   46   47   48
   49   50   51   52   53   54   55   56   57   58   59   60   61   62   63   64
   65   66   67   68   69   70   71   72   73   74   75   76   77   78   79   80
   81   82   83   84   85   86   87   88   89   90   91   92   93   94   95   96
   97   98   99  100  101  102  103  104  105  106  107  108  109  110  111  112
  113  114  115  116  117  118  119  120  121  122  123  124  125  126  127  128
  129  130  131  132  133  134  135  136  137  138  139  140  141  142  143  144
  145  146  147  148  149  150  151  152  153  154  155  156  157  158  159  160
  161  162  163  164  165  166  167  168  169  170  171  172  173  174  175  176
  177  178  179  180  181  182  183  184  185  186  187  188  189  190  191  192
  193  194  195  196  197  198  199  200  201  202  203  204  205  206  207  208
  209  210  211  212  213  214  215  216  217  218  219  220  221  222  223  224
  225  226  227  228  229  230  231  232  233  234  235  236  237  238  239  240
   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
   1.061E-09   3.764E-08   4.469E-08   4.058E-08   2.573E-08   3.576E-08
   3.971E-08   3.021E-08   3.831E-08   3.961E-08   3.305E-08   3.063E-08
   2.465E-08   2.784E-08   3.169E-08   2.839E-08   1.791E-08   2.480E-08
   2.746E-08   2.086E-08   2.639E-08   2.726E-08   2.271E-08   2.102E-08
   1.691E-08   1.909E-08   2.171E-08   1.945E-08   1.227E-08   1.698E-08
   1.879E-08   1.427E-08   1.805E-08   1.863E-08   1.553E-08   1.436E-08
   1.156E-08   1.304E-08   1.484E-08   1.329E-08   8.386E-09   1.160E-08
   1.284E-08   9.750E-09   1.233E-08   1.273E-08   1.061E-08   9.821E-09
   7.901E-09   8.916E-09   1.014E-08   9.082E-09   5.730E-09   7.928E-09
   8.775E-09   6.661E-09   8.428E-09   8.701E-09   7.250E-09   6.710E-09
   5.398E-09   6.091E-09   6.930E-09   6.205E-09   3.915E-09   5.417E-09
   5.995E-09   4.552E-09   5.758E-09   5.945E-09   4.954E-09   4.584E-09
   3.689E-09   4.163E-09   4.735E-09   4.239E-09   2.675E-09   3.701E-09
   4.097E-09   3.110E-09   3.935E-09   4.063E-09   3.384E-09   3.132E-09
   2.520E-09   2.843E-09   3.235E-09   2.897E-09   1.827E-09   2.530E-09
   2.800E-09   2.126E-09   2.689E-09   2.775E-09   2.313E-09   2.141E-09
   1.721E-09   1.943E-09   2.210E-09   1.979E-09   1.249E-09   1.728E-09
   1.913E-09   1.452E-09   1.836E-09   1.897E-09   1.580E-09   1.463E-09
   1.176E-09   1.328E-09   1.510E-09   1.352E-09   8.534E-10   1.181E-09
   1.307E-09   9.923E-10   1.255E-09   1.296E-09   1.080E-09   9.995E-10
   8.041E-10   9.073E-10   1.032E-09   9.242E-10   5.831E-10   8.069E-10
   8.931E-10   6.780E-10   8.579E-10   8.856E-10   7.379E-10   6.830E-10
   5.494E-10   6.200E-10   7.053E-10   6.315E-10   3.984E-10   5.513E-10
   6.102E-10   4.632E-10   5.861E-10   6.050E-10   5.042E-10   4.667E-10
   3.754E-10   4.236E-10   4.819E-10   4.315E-10   2.721E-10   3.767E-10
   4.169E-10   3.165E-10   4.005E-10   4.134E-10   3.445E-10   3.189E-10
   2.564E-10   2.894E-10   3.291E-10   2.947E-10   1.860E-10   2.573E-10
   2.849E-10   2.163E-10   2.735E-10   2.824E-10   2.353E-10   2.178E-10
   1.752E-10   1.976E-10   2.249E-10   2.013E-10   1.270E-10   1.758E-10
   1.946E-10   1.476E-10   1.868E-10   1.928E-10   1.608E-10   1.487E-10
   1.196E-10   1.350E-10   1.536E-10   1.375E-10   8.679E-11   1.201E-10
   1.329E-10   1.009E-10   1.276E-10   1.317E-10   1.098E-10   1.016E-10
   8.175E-11   9.224E-11   1.049E-10   9.395E-11   5.927E-11   8.202E-11
```

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   9.078E-11   6.891E-11   8.719E-11   9.000E-11   7.498E-11   6.941E-11
   5.582E-11   6.300E-11   7.165E-11   6.416E-11   4.047E-11   5.601E-11
   6.198E-11   4.705E-11   5.953E-11   6.143E-11   5.119E-11   4.738E-11
```

[redacted]

B6.0 AT123D Example Output File

```
**************************************************************************
*****                                                                *****
*****                          A T 1 2 3 D                           *****
*****                                                                *****
*****           AT123D Version 6.2 -- March, 2005                    *****
*****   Copyright 2005 Environmental Software Consultants, Inc.      *****
*****                                                                *****
*****                                                                *****
*****     Developed by: G. T. Yeh, 1979                              *****
*****     Oak Ridge National Laboratory                              *****
*****     Oak Ridge, Tennessee, 37830                                *****
*****                                                                *****
**************************************************************************
*****                                                                *****
*****     Modified by : John Seymor, 1982                            *****
*****             and : Darryl Holman, 1984                          *****
*****     University of Wisconsin-Madison                            *****
*****     Department of Engineering & Applied Science                *****
*****                                                                *****
**************************************************************************
*****                                                                *****
*****     Modified by : Howard Trussell, 1986                        *****
*****     Department of Civil & Environmental Engineering            *****
*****     University of Wisconsin-Madison                            *****
*****                                                                *****
*****                                                                *****
**************************************************************************
*****                                                                *****
*****     Modified by: Robert A. Schneiker, 1999-2005                *****
*****     Environmental Software Consultants, Inc.                   *****
*****     P.O. Box 2622                                              *****
*****     Madison, Wisconsin 53701-2622                              *****
*****     Phone: (608) 240-9878                                      *****
*****     FAX:  (608) 241-3991                                       *****
*****                                                                *****
**************************************************************************
*****     Modified by: Robert A. Schneiker, October 2001             *****
*****     TO FIX STEADY STATE SOLUTION ERROR                         *****
*****                                                                *****
**************************************************************************

   Benzene in Sand

    NO. OF POINTS IN X-DIRECTION .....................     7
    NO. OF POINTS IN Y-DIRECTION .....................     5
    NO. OF POINTS IN Z-DIRECTION .....................     2
    NO. OF ROOTS & NO. OF SERIES TERMS ...............   500
    NO. OF BEGINNING TIME STEPS ......................    25
    NO. OF ENDING TIME STEP ..........................   241
    NO. OF TIME INTERVALS FOR PRINTED OUT SOLUTION ....   48
    INSTANTANEOUS SOURCE CONTROL = 0 FOR INSTANT SOURCE    1
    SOURCE CONDITION CONTROL = 0 FOR STEADY SOURCE ....  240
    INTERMITTENT OUTPUT CONTROL = 0 NO SUCH OUTPUT ....    1
    CASE CONTROL =1 THERMAL, = 2 FOR CHEMICAL, = 3 RAD     2

    SOIL ORGANIC CARBON CONTENT (OC) .................    0.50000
    ORGANIC CARBON ADSORPTION COEFFICIENT (KOC) ......   0.3100E+02
    INITIAL CONTAMINANT LOAD (MG/KG) .................   0.0000E+00
    INITIAL CONTAMINANT LOAD (KG) ....................   0.7300E+03

    AQUIFER DEPTH, = 0.0 FOR INFINITE DEEP (METERS) ...   0.00000
    AQUIFER WIDTH, = 0.0 FOR INFINITE WIDE (METERS) ...   0.00000
    BEGIN POINT OF X-SOURCE LOCATION (METERS) ........   -1.58100
    END POINT OF X-SOURCE LOCATION (METERS) ..........    1.58100
    BEGIN POINT OF Y-SOURCE LOCATION (METERS) ........   -1.58100
    END POINT OF Y-SOURCE LOCATION (METERS) ..........    1.58100
    BEGIN POINT OF Z-SOURCE LOCATION (METERS) ........    0.00000
```

```
   END POINT OF Z-SOURCE LOCATION (METERS) ..........   0.00000

   POROSITY .........................................   0.25000
   HYDRAULIC CONDUCTIVITY (METER/HOUR) ..............   0.03600
   HYDRAULIC GRADIENT ...............................   0.00300
   LONGITUDINAL DISPERSIVITY (METER) ................   2.16000
   LATERAL DISPERSIVITY (METER) .....................   0.20000
   VERTICAL DISPERSIVITY (METER) ....................   0.02000
   DISTRIBUTION COEFFICIENT, KD (M**3/KG) ...........   0.00016
   SOURCE CONCENTRATION (mg/L) ......................   0.00000

   MOLECULAR DIFFUSION MULTIPLY BY TORTUOSITY(M**2/HR)  0.3528E-05
   DECAY CONSTANT (PER HOUR) ........................  0.0000E+00
   BULK DENSITY OF THE SOIL (KG/M**3) ...............  0.1700E+04
   DENSITY OF WATER (KG/M**3) .......................  0.1000E+04
   ACCURACY TOLERANCE FOR REACHING STEADY STATE ......  0.1000E-01
   TIME INTERVAL SIZE FOR THE DESIRED SOLUTION (HR) ..  0.7300E+03
   DISCHARGE TIME (HR) ..............................  0.1752E+06
   WASTE RELEASE RATE (KCAL/HR), (KG/HR), OR (CI/HR) .  0.7300E+03

             X COORDINATES ...

     0.00      5.00     10.00     15.00     20.00     25.00     30.00

             Y COORDINATES ...

   -10.00     -5.00      0.00      5.00     10.00

             Z COORDINATES ...

     0.00      1.00

   NUMBER OF POCs ...................................    2

   POC-1 X COORDINATE ...............................        0.00
   POC-1 Y COORDINATE ...............................        5.00
   NUMBER OF POC-1 Z COORDINATES ....................    6

             POC-1 Z COORDINATES ...

     0.00      0.50      1.00      1.50      2.00      2.50

   POC-2 X COORDINATE ...............................       11.00
   POC-2 Y COORDINATE ...............................       -3.00
   NUMBER OF POC-2 Z COORDINATES ....................    5

             POC-2 Z COORDINATES ...

     0.00      0.25      0.50      0.75      1.00

   LIST OF TRANSIENT SOURCE RELEASE RATE
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.1061E-08  0.3764E-07  0.4469E-07  0.4058E-07  0.2573E-07  0.3576E-07
0.3971E-07  0.3021E-07  0.3831E-07  0.3961E-07  0.3305E-07  0.3063E-07
0.2465E-07  0.2784E-07  0.3169E-07  0.2839E-07  0.1791E-07  0.2480E-07
0.2746E-07  0.2086E-07  0.2639E-07  0.2726E-07  0.2271E-07  0.2102E-07
0.1691E-07  0.1909E-07  0.2171E-07  0.1945E-07  0.1227E-07  0.1698E-07
0.1879E-07  0.1427E-07  0.1805E-07  0.1863E-07  0.1553E-07  0.1436E-07
0.1156E-07  0.1304E-07  0.1484E-07  0.1329E-07  0.8386E-08  0.1160E-07
0.1284E-07  0.9750E-08  0.1233E-07  0.1273E-07  0.1061E-07  0.9821E-08
0.7901E-08  0.8916E-08  0.1014E-07  0.9082E-08  0.5730E-08  0.7928E-08
0.8775E-08  0.6661E-08  0.8428E-08  0.8701E-08  0.7250E-08  0.6710E-08
0.5398E-08  0.6091E-08  0.6930E-08  0.6205E-08  0.3915E-08  0.5417E-08
0.5995E-08  0.4552E-08  0.5758E-08  0.5945E-08  0.4954E-08  0.4584E-08
0.3689E-08  0.4163E-08  0.4735E-08  0.4239E-08  0.2675E-08  0.3701E-08
0.4097E-08  0.3110E-08  0.3935E-08  0.4063E-08  0.3384E-08  0.3132E-08
0.2520E-08  0.2843E-08  0.3235E-08  0.2897E-08  0.1827E-08  0.2530E-08
0.2800E-08  0.2126E-08  0.2689E-08  0.2775E-08  0.2313E-08  0.2141E-08
```

```
  0.1721E-08  0.1943E-08  0.2210E-08  0.1979E-08  0.1249E-08  0.1728E-08
  0.1913E-08  0.1452E-08  0.1836E-08  0.1897E-08  0.1580E-08  0.1463E-08
  0.1176E-08  0.1328E-08  0.1510E-08  0.1352E-08  0.8534E-09  0.1181E-08
  0.1307E-08  0.9923E-09  0.1255E-08  0.1296E-08  0.1080E-08  0.9995E-09
  0.8041E-09  0.9073E-09  0.1032E-08  0.9242E-09  0.5831E-09  0.8069E-09
  0.8931E-09  0.6780E-09  0.8579E-09  0.8856E-09  0.7379E-09  0.6830E-09
  0.5494E-09  0.6200E-09  0.7053E-09  0.6315E-09  0.3984E-09  0.5513E-09
  0.6102E-09  0.4632E-09  0.5861E-09  0.6050E-09  0.5042E-09  0.4667E-09
  0.3754E-09  0.4236E-09  0.4819E-09  0.4315E-09  0.2721E-09  0.3767E-09
  0.4169E-09  0.3165E-09  0.4005E-09  0.4134E-09  0.3445E-09  0.3189E-09
  0.2564E-09  0.2894E-09  0.3291E-09  0.2947E-09  0.1860E-09  0.2573E-09
  0.2849E-09  0.2163E-09  0.2735E-09  0.2824E-09  0.2353E-09  0.2178E-09
  0.1752E-09  0.1976E-09  0.2249E-09  0.2013E-09  0.1270E-09  0.1758E-09
  0.1946E-09  0.1476E-09  0.1868E-09  0.1928E-09  0.1608E-09  0.1487E-09
  0.1196E-09  0.1350E-09  0.1536E-09  0.1375E-09  0.8679E-10  0.1201E-09
  0.1329E-09  0.1009E-09  0.1276E-09  0.1317E-09  0.1098E-09  0.1016E-09
  0.8175E-10  0.9224E-10  0.1049E-09  0.9395E-10  0.5927E-10  0.8202E-10
  0.9078E-10  0.6891E-10  0.8719E-10  0.9000E-10  0.7498E-10  0.6941E-10
  0.5582E-10  0.6300E-10  0.7165E-10  0.6416E-10  0.4047E-10  0.5601E-10
  0.6198E-10  0.4705E-10  0.5953E-10  0.6143E-10  0.5119E-10  0.4738E-10
  0.4738E-10

     RETARDATION FACTOR ...............................  0.2054E+01
     RETARDED DARCY VELOCITY (M/HR) ...................  0.2103E-03
     RETARDED LONGITUDINAL DISPERSION COEF. (M**2/HR) ..  0.4612E-03
     RETARDED LATERAL DISPERSION COEFFICIENT (M**2/HR) .  0.4893E-04
     RETARDED VERTICAL DISPERSION COEFFICIENT (M**2/HR)   0.1108E-04

    DISTRIBUTION OF CHEMICALS IN PPM AT    730.00 DAYS

                    Z =       0.00
                                                          X
   Y        0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
 -5.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
  0.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
  5.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
 10.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00

                    Z =       1.00
                                                          X
   Y        0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
 -5.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
  0.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
  5.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00
 10.00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00

POC-1                   Z
   X        Y            0.00        0.50        1.00        1.50        2.00        2.50
  0.00     5.00      0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00

POC-2                   Z
   X        Y           0.00        0.25        0.50        0.75        1.00
 11.00    -3.00      0.000E+00   0.000E+00   0.000E+00   0.000E+00   0.000E+00

    DISTRIBUTION OF CHEMICALS IN PPM AT   2190.00 DAYS

                    Z =       0.00
                                                          X
   Y        0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.510E-08   0.103E-07   0.913E-08   0.365E-08   0.663E-09   0.555E-10   0.215E-11
 -5.00   0.252E-03   0.461E-03   0.335E-03   0.108E-03   0.164E-04   0.119E-05   0.416E-07
  0.00   0.558E-01   0.327E-01   0.133E-01   0.326E-02   0.425E-03   0.283E-04   0.933E-06
  5.00   0.252E-03   0.461E-03   0.335E-03   0.108E-03   0.164E-04   0.119E-05   0.416E-07
 10.00   0.510E-08   0.103E-07   0.913E-08   0.365E-08   0.663E-09   0.555E-10   0.215E-11

                    Z =       1.00
```

```
                                                                    X
   Y         0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.253E-08   0.509E-08   0.455E-08   0.183E-08   0.334E-09   0.281E-10   0.110E-11
 -5.00   0.108E-03   0.201E-03   0.153E-03   0.514E-04   0.801E-05   0.593E-06   0.209E-07
  0.00   0.597E-02   0.925E-02   0.532E-02   0.147E-02   0.203E-03   0.139E-04   0.466E-06
  5.00   0.108E-03   0.201E-03   0.153E-03   0.514E-04   0.801E-05   0.593E-06   0.209E-07
 10.00   0.253E-08   0.509E-08   0.455E-08   0.183E-08   0.334E-09   0.281E-10   0.110E-11


    DISTRIBUTION OF CHEMICALS IN PPM AT   3650.00 DAYS

                    Z =       0.00
                                                                    X
   Y         0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.938E-06   0.232E-05   0.373E-05   0.393E-05   0.276E-05   0.130E-05   0.414E-06
 -5.00   0.397E-03   0.917E-03   0.127E-02   0.115E-02   0.701E-03   0.295E-03   0.863E-04
  0.00   0.150E-01   0.138E-01   0.122E-01   0.882E-02   0.475E-02   0.185E-02   0.514E-03
  5.00   0.397E-03   0.917E-03   0.127E-02   0.115E-02   0.701E-03   0.295E-03   0.863E-04
 10.00   0.938E-06   0.232E-05   0.373E-05   0.393E-05   0.276E-05   0.130E-05   0.414E-06

                    Z =       1.00
                                                                    X
   Y         0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.649E-06   0.161E-05   0.259E-05   0.275E-05   0.194E-05   0.915E-06   0.293E-06
 -5.00   0.247E-03   0.581E-03   0.832E-03   0.770E-03   0.480E-03   0.205E-03   0.604E-04
  0.00   0.312E-02   0.630E-02   0.721E-02   0.568E-02   0.319E-02   0.127E-02   0.358E-03
  5.00   0.247E-03   0.581E-03   0.832E-03   0.770E-03   0.480E-03   0.205E-03   0.604E-04
 10.00   0.649E-06   0.161E-05   0.259E-05   0.275E-05   0.194E-05   0.915E-06   0.293E-06


    DISTRIBUTION OF CHEMICALS IN PPM AT   5110.00 DAYS

                    Z =       0.00
                                                                    X
   Y         0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.326E-05   0.866E-05   0.171E-04   0.253E-04   0.283E-04   0.242E-04   0.158E-04
 -5.00   0.239E-03   0.606E-03   0.107E-02   0.141E-02   0.141E-02   0.110E-02   0.671E-03
  0.00   0.386E-02   0.455E-02   0.565E-02   0.621E-02   0.562E-02   0.411E-02   0.240E-02
  5.00   0.239E-03   0.606E-03   0.107E-02   0.141E-02   0.141E-02   0.110E-02   0.671E-03
 10.00   0.326E-05   0.866E-05   0.171E-04   0.253E-04   0.283E-04   0.242E-04   0.158E-04

                    Z =       1.00
                                                                    X
   Y         0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.253E-05   0.673E-05   0.133E-04   0.198E-04   0.222E-04   0.190E-04   0.125E-04
 -5.00   0.172E-03   0.441E-03   0.798E-03   0.107E-02   0.109E-02   0.855E-03   0.525E-03
  0.00   0.113E-02   0.256E-02   0.387E-02   0.455E-02   0.426E-02   0.317E-02   0.187E-02
  5.00   0.172E-03   0.441E-03   0.798E-03   0.107E-02   0.109E-02   0.855E-03   0.525E-03
 10.00   0.253E-05   0.673E-05   0.133E-04   0.198E-04   0.222E-04   0.190E-04   0.125E-04

 STEADY STATE SOLUTION HAS NOT BEEN REACHED BEFORE FINAL SIMULATING TIME

    DISTRIBUTION OF CHEMICALS IN PPM AT   6570.00 DAYS

                    Z =       0.00
                                                                    X
   Y         0.00        5.00       10.00       15.00       20.00       25.00       30.00

-10.00   0.390E-05   0.108E-04   0.237E-04   0.419E-04   0.596E-04   0.691E-04   0.655E-04
 -5.00   0.110E-03   0.293E-03   0.593E-03   0.952E-03   0.124E-02   0.134E-02   0.120E-02
  0.00   0.993E-03   0.142E-02   0.218E-02   0.305E-02   0.368E-02   0.376E-02   0.324E-02
  5.00   0.110E-03   0.293E-03   0.593E-03   0.952E-03   0.124E-02   0.134E-02   0.120E-02
 10.00   0.390E-05   0.108E-04   0.237E-04   0.419E-04   0.596E-04   0.691E-04   0.655E-04

                    Z =       1.00
                                                                    X
```

```
   Y         0.00        5.00        10.00       15.00       20.00       25.00       30.00

-10.00   0.322E-05   0.890E-05   0.196E-04   0.347E-04   0.496E-04   0.576E-04   0.548E-04
 -5.00   0.856E-04   0.230E-03   0.473E-03   0.770E-03   0.102E-02   0.111E-02   0.994E-03
  0.00   0.373E-03   0.910E-03   0.163E-02   0.240E-02   0.297E-02   0.308E-02   0.268E-02
  5.00   0.856E-04   0.230E-03   0.473E-03   0.770E-03   0.102E-02   0.111E-02   0.994E-03
 10.00   0.322E-05   0.890E-05   0.196E-04   0.347E-04   0.496E-04   0.576E-04   0.548E-04
```

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Appendix C

SEVIEW Text Editor Commands

C1.0 SEVIEW Text Editor Commands

Command	<Alt> SEVIEW Menu Commands	Function
File Commands		
<ESCAPE>	**File Close** Double click on file handle	Closes the file and exits the SEVIEW editor without savings any changes. Will prompt you if you want to discard the changes.
<F5>	**File Save**	Saves the file and exits the SEVIEW editor.
	File Save As...	Saves the file with a new name.
Cursor Movement Commands		
<←→↑↓>		The arrow keys move the cursor within the document.
<Control + →>		Moves the cursor one word to the right.
<Control + ←>		Moves the cursor one word to the left.
<Page Down>		Moves the cursor down one page.
<Page Up>		Moves the cursor up one page.
<Home>		Moves the cursor to the start of the line.
<End>		Moves the cursor to the end of the line.
<Control + Home> or <Control + Page Up>		Moves the cursor to the start of the document.
<Control + Page Down>		Moves the cursor to the end of the document.
	Edit Go to Line	Moves cursor to specified line number.
Block Commands		
<Shift + *Cursor Movement Commands*>		Highlights text to be copied or deleted
	Edit Select All	Highlights the entire document.
Block Copy Commands		
<Control + C>	**Edit Copy**	Copies the selected block to the clipboard.
<Control + X>	**Edit Cut**	Copies the selected block to the clipboard and deletes the highlighted text.
<Control + V>	**Edit Paste**	Copies the contents of the clipboard to the document.

SEVIEW Text Editor Commands
(Continued)

Command	<Alt> SEVIEW Menu Commands	Function
Delete Commands		
<Delete>		Deletes the current character.
Undo / Redo Command		
<Control + Z>	**Edit Undo**	Undo - Un does the last command and restores the document.
<Control + R>	**Edit Redo**	Redo - Restores the previous Undo command.
Insert / Type Over Commands		
<Insert>		Toggles between insert and type over mode. OVR is displayed near the lower right portion of the screen.
Find / Replace Commands		
<Control + F>	**Edit Find**	Finds a specified text string with the document.
<Control + G>	**Find Again**	Repeats the previous Find command.

Appendix D

SEVIEW Technical Support

D1.0 SEVIEW Technical Support

ESCI will provide 30 days of free technical support to registered users. The 30 days of support begins when you receive your SEVIEW activation key. After the 30 days of free support registered users may obtain additional technical support.

D1.1 Technical Support

ESCI provides a one or two-year support plan. This plan includes the following services:

- Priority response
- Discount pricing on continued support
- Special mailings, including discounts on products and services

ESCI support is available for $500 per year (or $900 for two years).

D1.2 Contacting Technical Support

Environmental Software Consultants, Incorporated (ESCI) provides technical support for the SEVIEW data management program. If you have difficulty installing SEVIEW or have questions regarding the program, please consult this User's Guide for assistance. If after consulting the User's Guide you are still experiencing problems, contact our Technical Support Department. We will gladly assist you in the operation or configuration of the SEVIEW program. Please have the following information available.

- Version numbers of SEVIEW, SESOIL, AT123D, BIOSCREEN and Windows.
- Amount of RAM and free disk space.
- A brief description of the problem, including any error messages.
- Procedures necessary to duplicate the problem.

Technical support is available to registered users from 9:00 AM to 4:00 PM (Central Standard Time) Monday through Friday at (608) 240-9878. Technical support will be provided free for 30 days following the installation of SEVIEW.

Written correspondence may sent to our Technical Support Department at:

Environmental Software Consultants Inc, LLC
P.O. Box 2622
Madison, Wisconsin 53701-2622

You may also fax your request for technical support to ESCI at (608) 241-3991. Please follow the guidelines presented above in any correspondence.

A feedback form is included in Appendix E. ESCI would appreciate any feedback registered users may have concerning the software, including additional features you want to see in future versions.

Appendix E

SEVIEW Feedback Form

E1.0 SEVIEW Feedback Form

Please complete and return this for to Environmental Software Consultants Inc, LLC Attach additional pages if necessary.

Mail to: Environmental Software Consultants Incorporated
P.O. Box 2622
Madison, Wisconsin 53701-2622

Date: ______________________________
Name: ______________________________
Company Name: ______________________________
Company Address: ______________________________
____
____

Data Entry Problems

Please describe the problem you found. Indicate what you were doing when you discovered the problem.

____
____
____

Documentation

Please provide the SEVIEW User's Guide page number and describe any problems or errors you find.

____
____
____

Additional Documentation or Features You Would Like to See

Please describe the additional features you would like to see included in the Documentation/Manual.

____
____
____

Additional Comments

____
____
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