POLLUTEv7

Version 7
Reference Guide

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POLLUTEv7

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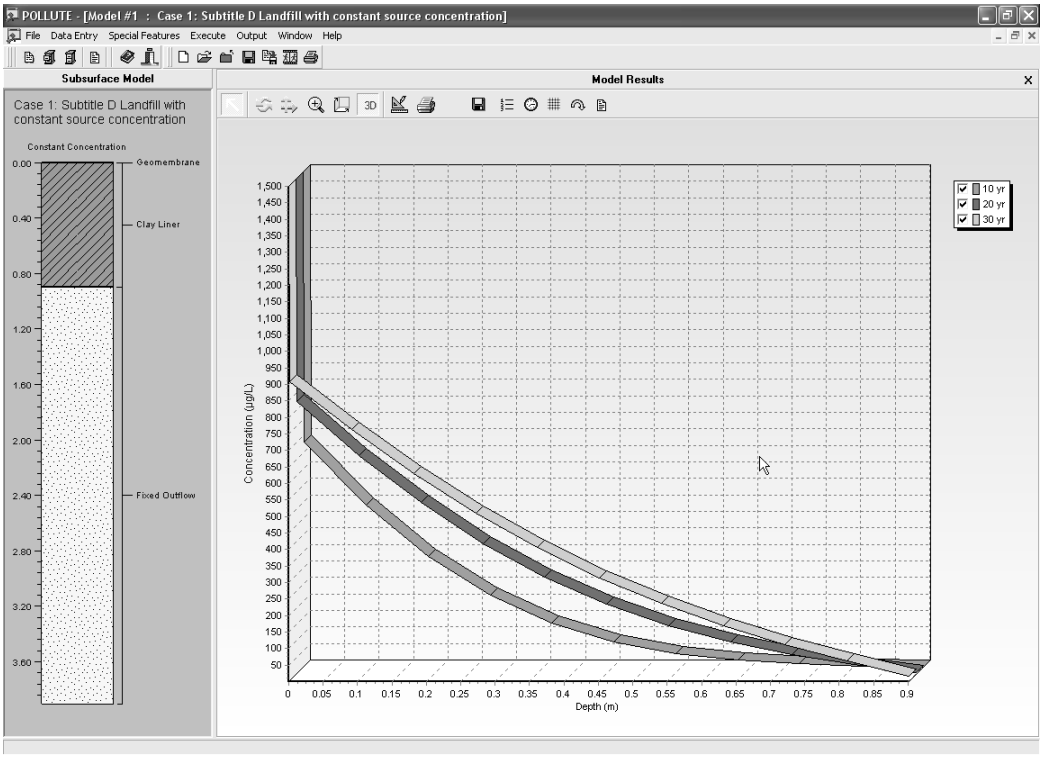
Introduction



Introduction

POLLUTEv7 can be used to provide fast, accurate, and comprehensive contaminant migration analysis capabilities. This program implements a one and a half dimensional solution to the advection-dispersion equation.

The new Windows Interface makes the creation, editing,, execution, printing and displaying of models easy and flexible. Models can be created from scratch, using the program Wizard, or by selecting one of the many pre-created models.

The program comes in two editions, Professional and Standard. The Professional edition is best suited for landfill design and the Standard edition is best suited for environmental remediation. Below is a comparison of the two versions:

Feature	Professional	Standard
Wizards and pre-created models	Yes	Yes
Unlimited number of models	Yes	Yes
Up to 200 layers	Yes	Yes
Constant concentration boundary conditions	Yes	Yes
Finite mass boundary condition	Yes	Yes
Fixed outflow boundary condition	Yes	Yes
Passive Sinks	Yes	Yes
Linear sorption	Yes	Yes
Non-linear sorption	Yes	No
Fractures in layers	Yes	No
Radioactive and biological decay	Yes	No
Initial concentration profile	Yes	No
Time-varying properties	Yes	No
Monte Carlo Simulation	Yes	Yes
Sensitivity Analysis	Yes	Yes

Unlike finite element and finite difference formulations, POLLUTEv7 does not require a time-marching procedure, and thus involves relatively little computational effort while also avoiding the numerical problems of alternate approaches.

With more then fifteen years utilization in industry, POLLUTEv7 is a well tested contaminant migration analysis program which is widely used internationally.

Models that can be considered range from simple systems on a natural clayey aquitard to landfill designs with composite liners, multiple barriers and multiple aquifers.

In addition to advective-dispersive transport, POLLUTEv7 can consider non-linear sorption, radioactive and biological decay, transport through fractures, passive sinks, time-varying properties, and phase changes.

The program is based upon the project concept for data storage, where the user has numerous projects and within each project there are numerous models. Using this method, a Microsoft Access database is used to store each project. Each project is stored in a separate directory, which can be on the same computer or spread across a network. A master database is used to keep track of projects and their locations, so that there is no need to remember the location of data files.

POLLUTEv7 is a Windows program and is compatible with Windows 98, 2000, NT, and XP. It supports all of the fonts and printers available in Windows.

Features

Project Features

POLLUTEv7 is based upon the project concept for data storage, where the user has numerous projects and within each project there are numerous models. Using this method, a Microsoft Access 2000 database is used to store each project. Each project is stored in a separate directory, which can be on the same computer or spread across a network. A master database is used to keep track of projects and their locations. This master project database is also used to store data (such as symbol libraries) that is common to all projects.

The creation and editing of projects is supported by the following features:

- Projects stored in Access 2000 databases.
- No limit to the number of projects.
- New projects can be easily created.
- Project directories are automatically created.
- Projects can be deleted, including project directories.
- Projects from other computers can be imported.
- Projects can be exported to other computers.
- Projects can be automatically backed up.
- Backed up projects can be restored.
- Model data from version 6 of the program can be imported into a project.

Model Features

Models are used to represent the subsurface lithology, containment systems, and contaminant source to be studied. These models can be used to study the effects of landfills, buried waste, spills, lagoons, barrier systems, etc. Each study area should be grouped into one or more projects. A project is used to store one or more models in a study area. After a model has been created it can be run to calculate the concentrations of a contaminant at specified depths and times.

The creation and editing of models is supported by the following features (features in italics are available in the Professional edition only):

- New models can be easily created using either a blank model, the wizard, or a quick entry model.
- There are four quick entry models: Primary Liner Landfill, Primary and Secondary Liner Landfill, Vertical Migration, and Horizontal Migration.
- A graphical diagram of the model is displayed as it is created.
- Models can contain up to 200 layers.
- The graphical symbol and color for a layer can be assigned and shown of the model diagram.
- *Layers can contain 1, 2, or 3 dimensional fractures.*
- The diffusion coefficient, distribution coefficient, and phase change parameter can be specified for each layer.
- The top boundary condition can be zero flux, constant concentration, or finite mass.
- The bottom boundary condition can be zero flux, constant concentration, fixed outflow, or infi nite thickness.
- The subsurface concentrations can be calculated at specified times or the time of the maximum concentration can be automatically found by the program.
- *Radioactive or biological decay of the contaminant can be modeled.*
- *An initial concentration profile at specified depths can be specified.*
- *Freundlich and Langmuir non-linear sorption can be modeled.*
- *Source, velocities, and layer properties can be varied with time (can be used model changes in the source, barriers, or flow patterns).*
- One or more passive sinks can be specified to model horizontal velocities in layers and the removal of contaminants.
- Monte Carlo simulation can be used to evaluate the effects of uncertainty of model parameters.
- Sensitivity analysis can be used to predict the expected range of concentration when parameter values are not known accurately.

Output Features

After a model has been run, the calculated concentrations can be displayed a number of ways. If they model did not use the Monte Carlo or Sensitivity Analysis special features these are:

- Concentration versus Depth Graph
- Concentration versus Time Graph
- Time versus Depth Graph
- Flux versus Time Graph
- Text Listing

If the model used the Monte Carlo or Sensitivity Analysis features they are:

- Distribution of the Maximum Concentration
- Distribution of the Time of the Maximum Concentration
- Distribution of the Variable Values
- Text Listing

In addition the output from the model can be exported into 19 different formats, including:

- ASCII
- Excel
- Access
- Rich text format
- Adobe pdf
- Lotus 123
- Paradox
- HTML

In addition to the calculated results of the model, imported output data can also be displayed on the concentration vs depth and concentration vs time graphs. This imported data can be from other models, experimental results, or theoretical results. The imported data can be extracted from a file, other models in the project, or created and entered directly. After the imported data has been entered in can be edited or deleted.

1. Getting Started

1. Getting Started

Before you begin working with the POLLUTEv7 program you should:

1. Check the contents of your distribution package;
2. Make sure you have the necessary equipment;
3. Run the installation program;
4. Read the README file;
5. Start the program.
6. Register the program.

The Distribution Package

The distribution package you received should include this User's Guide and a CD-ROM.

Required Equipment

POLLUTEv7 requires the following hardware and software to run efficiently:

1. Windows 98/2000/XP or NT;

2. At least 128 MB of RAM;

3. At least 32 MB of hard disk space;

4. A screen resolution of at least 600 x 800 with at least 16 bit color;

5. A CD-ROM drive.

Installation

To get POLLUTEv7 up and running, run the installation program setup.exe on the CD-ROM. For example, to install from drive D:

1. Start Windows

2. Insert the CD-ROM into drive D;

3. Choose Start and then Run and type “D:\POLLUTE\setup.exe”, or double-click on “D:\POLLUTE\setup.exe” in Windows Explorer, or double-click on the Add/Remove Programs icon in the Control;

4. Enter the requested information in the installation forms, discussed in the next section.

On some computer systems, depending on how they are configured, inserting the CD-ROM into the drive will automatically start the GAEA menu program. In this case select POLLUTEv7 from the menu screen. All of the programs listed on the menu screen can be installed and will run in demo mode until an unlock code is provided.

The SETUP program does the following:

1. Creates one or more directories on your hard disk and copies the contents of the POLLUTEv7 disk into them;

2. Creates a Windows application group and installs the POLLUTEv7 program and help icons.

Requested Information

The installation dialog boxes will request the directories to store the POLLUTEv7 program and databases, and the name of the application group for the POLLUTEv7 program icons.

README File

Any last-minute changes, additions or trouble-shooting tips are documented in the README file. When the SETUP program has finished installing the program, it will automatically install an icon for the README file in the application group. To view the README file click on this icon.

Uninstalling POLLUTEv7

The POLLUTEv7 program files can be removed from your hard disk using the Add/Remove programs option in the Windows Control Panel. Uninstalling the program will also remove the POLLUTEv7 icons, and application group.

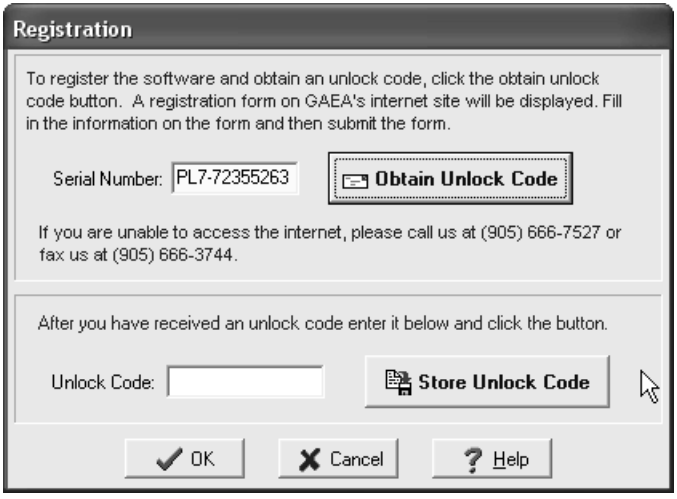
Registering and Unlocking POLLUTEv7

Before POLLUTEv7 can be used it must be registered. Prior to registration process the program will run in Demo mode. During the registration the program will be unlocked.

To register the program and obtain an unlock code, run the POLLUTEv7 program. Until the program is unlocked it will operate in Demo mode and the form below will be displayed.

To register the program press the Register button, the Registration form shown below will be displayed. This form can also be displayed using the Purchase menu item in the Help menu.In the middle of this form a unique serial number will be displayed. This serial number is unique for each computer.

To register the program an unlock code must be obtained using this serial number. If your computer is connected to the Internet, you can obtain this unlock code by clicking on the Obtain Unlock Code button. After the button is pressed a registration form on GAEA's web site will be displayed on your internet browser. Fill out the form and then click on the submit button. After your registration information has been received an unlock code will be emailed to you.



If your computer is not connected to the Internet, you can call or fax us the serial number. If you have problems emailing us the serial number or need an unlock code faster, call us and we will give it to you over the phone.

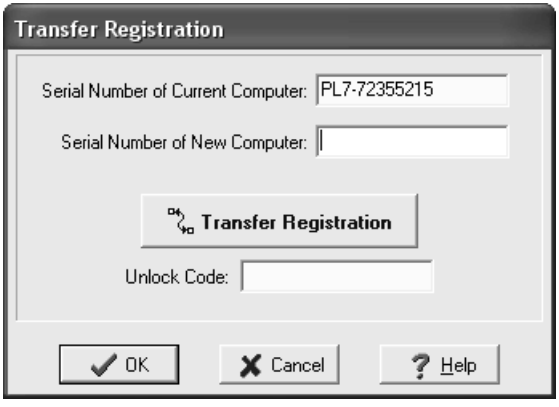
After GAEA has received your unique serial number, an unlock code will be generated and emailed or faxed to you. When you receive the unlock code enter it in the space at the bottom of the Registration form and then press the Store Unlock Code button. The program is now registered and the Demo form will no longer be displayed when the program is run.

Transferring the Registration

After the program has been registered, the unlocked program can be transferred to a different computer using the Transfer utility. This utility allows you to move the program between computers without requiring assistance from GAEA. After the registration has been transferred the program will only run on the new computer.

Step 1. The first step is to obtain the unique serial number of the new computer. Install and run POLLUTEv7 on the new computer. Initially the program will start in Demo mode and the Demo form will be displayed. Press the Register button and write down the unique serial number for the new computer.

Step 2. In the second step the Transfer utility is used to generate an unlock code for the new computer. Start POLLUTEv7 on the old PC and select the Transfer menu item from the Help menu. The Transfer Registration form below will be displayed.
Enter the serial number of the new computer and then press the Transfer Registration button. An unlock code for the new computer will be displayed. Enter this unlock code in the Registration form on the new computer, and then press the Store Unlock Code button.



After the Transfer Registration button has been pressed, POLLUTEv7 on the old PC will be set to run in demo mode. The Transfer utility should be used with caution, since if incorrect serial numbers are entered you will lose the registration on both computers. If this happens contact GAEA for a new unlock code. Transferring the registration is a two step process.

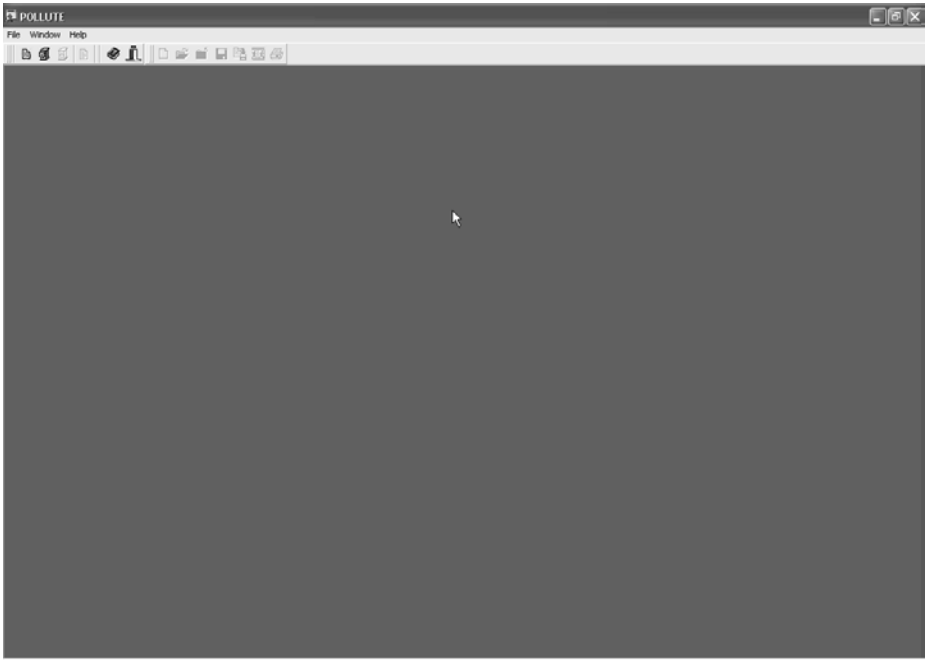
Using POLLUTEv7

This section explains how to interact with the various parts of the program. It discusses how to use the various toolbars and menus.

Starting POLLUTEv7

To begin working with POLLUTEv7 after you have installed the program, start it by double-clicking on the POLLUTEv7 icon in the application group.

When you first start the program the main window will be displayed. The main window of the program consists of a title bar, menu bar, optional toolbars and desktop. In addition, popup menus can be displayed by clicking the right mouse button.



This section explains how to interact with the various parts of the program.

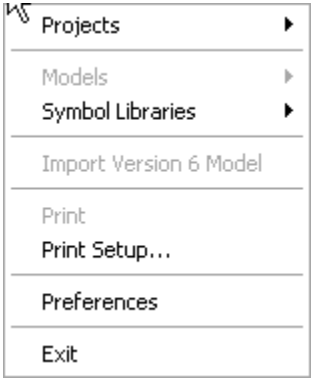
Menu Bar

The menu bar contains the main level of commands. It uses standard Windows pull-down menus. You can choose any menu item on any submenu that is not dimmed (POLLUTEv7 will know when certain menu commands are not available, and prevents you from choosing them). The majority of these commands can also be selected using the speed buttons on the toolbars (see below).

When the program is first started and no project is opened, the File, Window, and Help items will appear on the menu bar. After a model is opened there will also be an Data Entry, Special Features, Execute, and Output items on the menu bar.

File Menu

This menu contains commands similar to those in other Windows applications and contains the following submenu.



Projects - displays a submenu used to create, open, save, delete, close, import, export, backup and restore projects.

Models - displays a submenu used to create, open, save, close, and delete models.

Symbol Libraries - displays a submenu used to create, open, save, close, and delete lithologic symbol libraries.

Import Version 6 Data - used to import data created in version 6 of the program.

Print - used to print models.

Print Setup - used to adjust the printer settings.

Preferences - used to set program preferences.

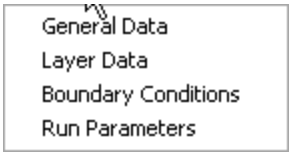
Exit - closes the program.

Data Entry Menu

After a model has been opened the Data Entry menu will appear on the menu bar. The contents of the menu will vary depending on the type of model.

General Model

If a general model (created using the blank model or wizard) is currently displayed on the desktop the data entry menu will contain the following commands.



General Data - used to edit the general data for the model (title, Darcy velocity, number of layers, and Laplace Transform parameters).

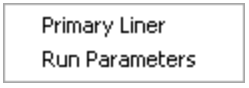
Layer Data - used to edit the data for each layer.

Boundary Conditions - used to edit the top and bottom boundary conditions.

Run Parameters - used to edit the depths and times to calculate the concentrations.

Primary Liner Model

If a primary liner model is currently displayed on the desktop the data entry menu will contain the following commands.

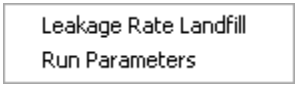


Primary Liner - used to edit the data for the layers and boundary conditions.

Run Parameters - used to edit the depths and times to calculate the concentrations.

Leakage Rate Model

If a leakage rate model is currently displayed on the desktop the data entry menu will contain the following commands.

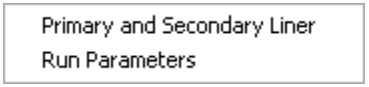


Leakage Rate Landfill - used to edit the data for the layers and boundary conditions.

Run Parameters - used to edit the depths and times to calculate the concentrations.

Primary and Secondary Liner Model

If a primary and secondary model is currently displayed on the desktop the data entry menu will contain the following commands.

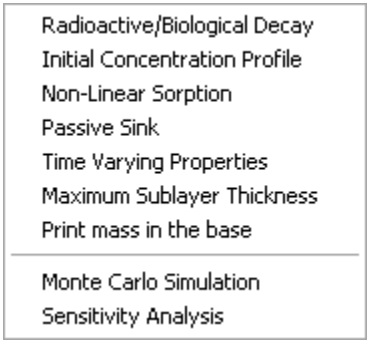


Primary and Secondary Liner - used to edit the data for the layers and boundary conditions.

Run Parameters - used to edit the depths and times to calculate the concentrations.

Special Features Menu

After a model has been opened the Special Features menu will appear on the menu bar.This menu contains commands for adding special features to the model.



Radioactive/Biological Decay - used to add either radiological or biological decay to the model.

Initial Concentration Profile - used to add an initial concentration profile to the model.

Non-linear Sorption - used to add either Freundlich or Langmuir Non-Linear Sorption to the model.

Passive Sink- used to add a passive sink to the model.

Time Varying Properties - used to enter time varying properties for the model.

Maximum Sublayer Thickness - used to change the maximum sub-layer thickness.

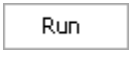
Print mass in the base - used to print the mass in the base when the concentrations are calculated.

Monte Carlo Simulation - used to perform a Monte Carlo simulation on the model.

Sensitivity Analysis - used to perform a Sensitivity Analysis on the model.

Execute Menu

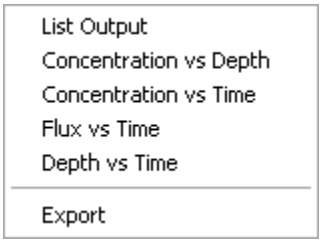
This menu is used to execute the the model and calculate the concentrations..



Run - used to execute the model.

Output Menu

This menu is used to display the results of the model after it has been executed.



List Output- displays the model output as text.
Concentration vs Depth - displays the model output as a graph of concentration vs depth.
Concentration vs Time - displays the model output as a graph of concentration vs time.
Flux vs Time - displays the model output as a graph of flux vs time.
Depth vs Time - displays the model output as a graph of depth vs time with the concentrations represented by various colors.
Export - used to export the model output to a variety of file formats.

Window Menu

This menu contains the standard Windows commands for selecting and arranging windows on the desktop.

Help Menu

This menu contains the following commands:

Contents - displays the contents of the online help.
Search for Help On... - displays help on a specified topic.
Transfer Registration - used to transfer the registration from one computer to another.
Email Technical Support - used to send an email to technical support.
Check for Upgrade - used to download and install the latest upgrade from the Internet.
GAEA's Web Site - used to display GAEA's web site in the default Internet browser.
About - used to display version information about the program.

Popup Menus

Popup menus can be displayed at any time by pressing the right mouse button. The menu that will be displayed depends upon what is currently displayed on the desktop.

Project Popup Menu

If there is no model open the Project Popup Menu will be displayed. This menu contains the following menu items:

New Project - used to create a new project.
Open Project - opens an existing project.
Save Project - saves the current project (disabled if no project is open) .
Close Project - closes the current project (disabled if no project is open).
New Model - used to create a new model (disabled if no project is open).
Open Model - used to open an existing model (disabled if no project is open).
Exit - exits the program.

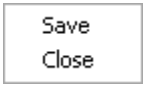
Model Popup Menu

If a model is currently open the Model Popup Menu will be displayed This popup menu contains the following commands.

Save - saves the model.
Run - runs the model and calculates the concentrations.
Close - closes the model.
General Data - used to edit the general data for the model.
Layer Data - used to edit the data for each layer.
Boundary Conditons - used to edit the top and bottom boundary conditions.
Run Parameters - used to edit the times and depths to calculate the concentrations..
Special Features - used to display a submenu to edit the special features for the model.

Symbol Library Popup Menu

If a symbol library is currently displayed on the desktop the Symbol Library Popup Menu will be displayed This popup menu contains the following commands.



Save - saves the symbol library.
Close - closes the symbol library.

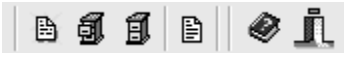
Toolbars

There are two toolbars that can be displayed on the desktop; they are the Project Toolbar and Model Toolbar. These toolbars can either float over top of the desktop or be docked to the top side or left side of the desktop.

To make the toolbar float click and hole down the left mouse button on the edge of the toolbar. Then drag the mouse to where you want the toolbar and release the button. The number of rows in the floating toolbar can be adjusted by changing the size of the toolbar with the mouse.

Each toolbar contains several speed buttons that can be used to perform the same tasks as the menu bar at the top of the desktop. These speed buttons are described below.

Project Toolbar



The Project Toolbar is used to create, open, and close projects. Each of the speed buttons on the toolbar is explained below.

The **New** button is used to create a new project.

The **Open** button is used to open an existing project.

The **Close** button is used to close an open project (this button will be dimmed if no project is currently opened).

The **Hide** button is used to toggle on and off the list of models in the project (this button will be dimmed if no project is currently opened).

The **Help** button is used to display help on using the program.

The **Exit** button is used to exit the program.

Model Toolbar

The Model Toolbar is used to create and edit models. Each of the speed buttons on the toolbar is explained below.

The **New** button is used to create a new model.

The **Open** button is used to open an existing model.

The speed buttons below will be dimmed if no model is currently opened.

The **Close** button is used to close a model.

The **Save** button is used to save changes to the model.

The **SaveAs** button is used to save the model under a different name.

The **Run** button is used to execute the model and calculate concentrations.

The **Print** button is used to print the model.

2. Theory

2. Theory

The movement or migration of contaminants through the soil is of interest in the prediction of contaminant impact from sources such as landfills and spills. There are three main mechanisms for contaminant transport, these are advection, diffusion, and dispersion. In many applications the movement of contaminants will be primarily in one direction, and can be predicted using the one-dimensional dispersion-advection equation for a layered deposit [Rowe and Booker, 1985, 1991b; Rowe et al, 1994].

POLLUTEv7 is a computer program that implements a solution to the one-dimensional dispersion-advection equation for a layered deposit of finite or infinite extent [Rowe & Booker, 1991b]. Using this solution POLLUTEv7 calculates the concentrations of a contaminant at user specified times and depths.

Unlike finite element and finite difference formulations, POLLUTEv7 does not require the use of a "time-marching" procedure. POLLUTEv7 uses a finite-layer formulation that provides numerically accurate results for a given idealization while requiring relatively little computational and data entry effort. Thus, in its basic mode of operation the concentration of contaminant can be directly determined at any specified time without calculating the concentration at earlier times.

Transport Mechanisms

The migration of dissolved contaminants through the subsurface involves different transport mechanisms depending upon the type of soil, presence of fractures, degree of saturation, and soil - contaminant interaction. For a saturated clay or silt the primary mechanisms are advection and diffusion, whereas for a saturated sand the primary mechanisms are advection and dispersion. In a fractured soil the primary mechanisms are advection and dispersion along the fractures and diffusion from the fractures in the matrix. Soils with clay particles or organic matter may also act to retard the migration of contaminants by adsorbing the contaminant. These transport mechanisms are described in detail below.

Advection

When water flows through the soil it will carry contaminants along with it in solution, this process is called advection. The amount of contaminant mass transported by advection is proportional to the groundwater (seepage) velocity, **v**, and the concentration, **c**, of the contaminant. This mass can be measured in a plane perpendicular to the direction of groundwater flow during a unit of time, this is called the flux, **f** . The flux is then the mass of contaminant transported per unit area per unit time and is given by:

$$\mathbf{f = n\ v\ c = v_a\ c}$$

where,

n = effective porosity of the soil,

v = groundwater (seepage) velocity,

$\mathbf{v_a}$ = Darcy velocity = **n v.**

c = concentration of the contaminant at the time of interest.

The total mass of contaminant transported from a contaminant source into the ground can then be obtained by integrating the flux over the time period of interest viz.

$$\mathbf{m_a = A \int_0^t n\ v\ c\ dt}$$

where,

$\mathbf{m_a}$ = total mass of contaminant transported,

A = cross-sectional area of the landfill.

It is should be noted that the velocity that the contaminant moves through the soil is the groundwater velocity and not the Darcy velocity. If the groundwater velocity is zero (i.e., there is no flow) then there would be no advection.

Diffusion

Diffusion is the process where chemicals contaminants in the soil will migrate from areas of high chemical concentration (potential) to areas of low chemical concentration (potential). The mass flux transported by diffusion is proportional to the concentration gradient and is given by:

$$f = - n \ D_e \ dc/dz$$

where,

n = effective porosity of the soil,
$\mathbf{D_e}$ = effective diffusion coefficient,
dc/dz = concentration gradient.

The negative sign in the above equation arises from the fact that contaminants move from areas of high concentration to areas of low concentrations. By integrating the above equation the total mass of contaminant transported by diffusion from a landfill can be obtained viz.:

$$m_d = A \int_0^t (- n \ D_e \ dc/dz) \ d\tau$$

Advective-Diffusive Transport

For unfractured clayey and silty soils the primary transport mechanisms will be generally be advection and diffusion (i.e., advective-diffusive transport). The flux of mass, **f**, is obtained by adding the advective flux and the diffusive flux viz.:

$$f = n \ v \ c - n \ D_e \ dc/dz$$

and the total mass, m, transported from the landfill is given by:

$$m_d = A \int_0^t (n \ v \ c - n \ D_e \ dc/dz) \ d\tau$$

where the parameters are the same as those defined previously. By convention if the velocity is positive the flow is out of the landfill, and if the velocity is negative the flow is into the landfill. The direction of transport for diffusion and advection can be in the same direction or in opposite directions. If the direction of diffusive transport is in the same direction as that of advective transport, then diffusion will increase the amount of contaminant transported and decrease the time taken for the contaminant to move to a given point. Diffusion can also occur in the opposite direction to advection.

For example, even if groundwater is flowing into a landfill, the high concentration of contaminant in the leachate can cause diffusive transport out from the landfill. Thus, even though the groundwater flow is into a landfill contaminants can still escape from the landfill by diffusion.

Dispersion

In a granular layer (eg. an aquifer) or a fractured layer there can be significant localized variations in the groundwater flow. These variations will cause mechanical mixing within the layer, this process is called dispersion [Freeze and Cherry, 1979]. Although the process is very different to diffusion it can be modelled mathematically in the same manner, and the two processes can be grouped together as the "coefficient of hydrodynamic dispersion", **D**, viz.:

$$D = D_e + D_{md}$$

where,
D_e = effective diffusion coefficient,
D_{md} = coefficient of mechanical dispersion.

In unfractured clayey soils the coefficient of hydrodynamic dispersion is often controlled by the diffusion coefficient, and the coefficient of mechanical dispersion is negligible. In sandy soils and fractured layers the opposite is generally true and dispersion dominates [Gillham and Cherry, 1982; Rowe, 1987; Rowe et al, 2004].

The mass flux for advective-dispersive transport (including diffusion) is given by:

$$f = n\ v\ c - n\ D\ dc/dz$$

where the parameters are the same as those defined previously and **D** is the coefficient of hydrodynamic dispersion.

Dispersion is often modelled as a linear function of velocity [Bear, 1979; Freeze and Cherry, 1979; Rowe et a;, 2004] given by:

$$D_{md} = \alpha\ v$$

where,

α = dispersivity,

v = groundwater (seepage) velocity.

The dispersivity tends to be scale dependent and is not a true material property [Gillham and Cherry, 1982].

Retardation Mechanisms

In addition to the transport mechanisms mentioned above, the migration of contaminants is also controlled by retardation mechanisms. There are two types of retardation mechanisms, sorption and radioactive or biological decay, that can be modelled in POLLUTEv7. These mechanisms both serve to slow the migration of contaminants by reducing the mass of contaminant available for transport. Both mechanisms are discussed below.

Sorption

Sorption is the process whereby contaminants are removed from solution by interaction with solid matter in the soil. Typical interactions are cation exchange in clays and the attraction of organic contaminants to organic matter in the soil. Sorption can be modelled as a function of the concentration of the contaminants in the soil. POLLUTEv7 can model three types of sorption; linear sorption, Freundlich non-linear sorption, and Langmuir non-linear sorption.

Radioactive or Biological Decay

Some contaminant species experience radioactive decay or biological degradation and the concentration of these contaminants may decay as a function of time. The rate of radioactive decay is very predictable and is controlled by the half-life of the contaminant species. Whereas, the rate of biological decay is a function of several factors, including the presence of the appropriate bacteria, the presence of a suitable substrate, and the temperature. Both types of decay are often modelled by first order decay, with the controlling parameter being the half-life of the species.

Phase Change

Many practical problems involve a phase change as a compound (eg. volatile organic compounds such as dichloromethane, benzene, toluene, etc.) migrate through a multiphased system. A common example is diffusion migration from a dissolved phase (eg. in contaminated water) into the gaseous phase (eg. in air in an unsaturated secondary leachate collection system). Under these conditions it is well known (eg. see Schwartzenbach et. al., 1993) that there is usually a concentration 'jump' at the interface between the contaminated water and the air, and that equilibrium is reached at the interface such that:

$$c_{a/w} = K_H' \; c_{w/a}$$

where

$\mathbf{c_{a/w}}$ = concentration in air at the interface,

$\mathbf{c_{w/a}}$ = concentration in water at the interface,

$\mathbf{K_H'}$ = *dimensionless* Henry's Law Constant, and is related to the Henry's Law Constant $\mathbf{K_H}$ by the relationship

$$\mathbf{K_H' = K_H / (R\ T)}$$

(**R** is the gas constant and **T** is the absolute temperature).

More generally, there is potential for phase change at interfaces other than air-water. For example, the migration of an organic compound from a dissolved phase in leachate through a "solid" geomembrane, may involve a phase change defined by [Rowe et al, 2004]:

$$\mathbf{c_g = S_{gf}\ c_f}$$

where $\mathbf{S_{gf}}$ is the dimensionless ratio of the concentration at the gemembrane and water interface, typical values have been reported by Rowe et al, 2004. Thus, in general the concentration ratio at an interface where there is a phase change can be written as:

$$\mathbf{c_{n/w} = \Delta\ c_{w/n}}$$

where $\mathbf{c_{n/w}}$ is the gas or solid concentration (mol. m^{-3}) in the n phase (i.e. gas or solid), $\mathbf{c_{w/n}}$ is the concentration (mol. m^{-3}) dissolved in the solvent of interest (eg. water), and $\mathbf{\Delta}$ is the dimensionless phase parameter (mol. m^{-3} $mol.^{-1}$ m^3).

One-Dimensional Contaminant Migration

The theory implemented by the POLLUTEv7 program, in its basic mode of operation, is described in detail by Rowe and Booker [1985, 1987, 1991b] and Rowe et al [1994]. According to this theory contaminant migration in one-dimension, for an intact material, is governed by:

$$n\ dc/dt = n\ D\ d^2c/dz^2 - n\ v\ dc/dz - \rho\ K_d\ dc/dt - n\ \lambda\ c$$

where,

c = concentration of contaminant at depth z at time t,
D = coefficient of hydrodynamic dispersion at depth z,
v = groundwater (seepage) velocity at depth z,
n = porosity of the soil at depth z,
ρ = dry density of the soil at depth z,
$\mathbf{K_d}$ = distribution/partitioning (sorption) coefficient at depth z,
$\mathbf{v_a} = \mathbf{nv}$ = Darcy velocity,
λ = decay constant of the contaminant species (i.e., the reciprocal of the species mean half life times ln 2).

Contaminant migration in a fractured layer is primarily in one direction along the fracture (e.g. either horizontally or vertically), but contaminants can migrate from the fractures into the intact material in all three co-ordinate directions. Thus contaminant migration along the fractures is governed by [Rowe et al, 2004]:

$$n_f\ dc_f/dt = n_f\ D_f\ d^2c_f/dz^2 - n_f\ v_f\ dc_f/dz - \Delta\ K_f\ dc_f/dt - q - n_f\ \lambda\ c_f$$

where,

$\mathbf{c_f}$ = concentration in a fracture at depth **z** and time **t**,
$\mathbf{D_f}$ = coefficient of hydrodynamic dispersion of the fractures,
$\mathbf{v_f}$ = fracture (groundwater) velocity in the fractures,
$\mathbf{n_f}$ = fracture porosity in the plane of flow = $\mathbf{h_1/H_1 + h_2/H_2}$,
Δ = surface area of fractures per unit volume of soil/rock,
$\mathbf{K_f}$ = fracture distribution coef. [Freeze and Cherry, 1979],
q = contaminant transported into the intact matrix material, from the fractures, by matrix diffusion,
λ = decay constant of the contaminant species.

Note: the program automatically calculates $\mathbf{n_f}$, $\mathbf{v_f}$, and **q** from other information provided by the user.

Boundary Conditions

The POLLUTEv7 program solves the one-dimensional contaminant migration equation subject to boundary conditions at the top and bottom of the soil deposit being modelled. There are three possible top boundary (i.e., the usually the point of contact between the contaminant source and the soil deposit), these are zero flux, constant concentration, and finite mass. The bottom boundary (i.e., the point of contact between the soil deposit and either a much more or much less permeable strata) may be either zero flux, constant concentration, fixed outflow, or infinite thickness.

Zero Flux Top Boundary

The top boundary may be assumed to not allow any transmission of contaminant (i.e. zero flux). This option has some highly specialized applications and will be rarely used. The surface flux passing into the soil is given by:

$$f(z=0) = 0 \quad \text{for all } t$$

Constant Concentration Top Boundary

In this boundary condition the top boundary is assumed to maintain a constant concentration. The concentration at the boundary is given by:

$$c(z=0) = c_s \quad \text{for all } t$$

where c_s is the constant concentration at the top boundary.

Finite Mass Top Boundary

The top boundary may be assumed to have a finite mass, in which case the source concentration starts at an initial value c_o, increases linearly with time at a rate c_r, and then decreases with time as contaminant is transported into the soil and collected by a leachate collection system, if present. In version 7, the gradual conversion of waste into leachate can also be considered by providing a conversion rate half-life.

The concentration at the top boundary is given by:

$$c(t) = c_0 + c_r t - \lambda \int_0^t c(\tau)\, d\tau - 1/H_r \int_0^t f(c, \tau)\, d\tau - q_c/H_r \int_0^t c(\tau)\, d\tau + R_s/WC\ (1 - e^{-Kt})$$

where,

c_o = initial source concentration at the start time.

c_r = rate of increase in concentration with time due to the addition of mass to the landfill.

$f(c, \tau, z=0)$ = the surface flux (mass per unit area per unit time) passing into the soil at the top boundary.

q_c = the volume of leachate collected per unit area of the landfill per unit time, if there is no leachate collection system $q_c=0$.

λ = first order decay coefficient calculated based on the half-life specified in the Special Features, Radioactive/Biological Decay option, such that $\lambda = \ln 2$ /(half-life for decay).

R_s = mass of contaminant in the waste available to be transformed into dissolved form over time (per unit volume of waste). The program calculates R_s as follows:

$$R_s = p\, \rho_w - c_0\, WC$$

where,

p = available (leachable) mass of contaminant in the waste per unit mass of waste (eg. mass of chloride in waste/total mass of waste);

ρ_w = apparent density of the waste (i.e. mass of waste per unit volume of the landfill);

WC = volumetric water content of the waste.

κ = generation coefficient calculated based on the conversion rate half-life K, such that $\kappa = \ln 2 / K$. A value of $\kappa = 0$ implies no generation of concentration with time. In the program $\kappa = 0$ is obtained by specifying $K = 0$ (this is the default case).

H_r = reference height of leachate, and represents the volume of leachate (per unit area of landfill) which would contain the total mass of contaminant at a concentration c_o. And may be defined in one of several ways depending on what other options are being used. Note that generally the program will calculate H_r (i.e. the user will generally not input any value for H_r, but the user does have the power to override the program).

Option (a). If the user specified K is not 0 and WC is not 0 then $H_r = WC\ H_w$ and represents the actual fluid in the landfill (generally WC corresponds to field capacity, but could vary with time).

Option (b). If the user specified **K** equals 0 or **WC** equals 0 then $H_r = p\ \rho_W\ H_w / c_0$ and this represents the volume of fluid (per unit area of landfill) required to dissolve the leachable mass of contaminant (i.e. $p\ \rho_W\ H_w$) at the initial concentration c_0.

Option (c). If the user specifies H_r is not 0 then the user specified value overrides the values calculated under option (a) or (b). This is an advanced feature of the program and should not be used without very carefully checking your calculations.

If the rate of increase in concentration c_r is zero and the reference height of leachate H_r is very large, this boundary condition reduces to a constant concentration boundary condition.

Zero Flux Bottom Boundary

The bottom boundary may be assumed to not allow any transmission of contaminant, which corresponds to an impermeable base strata. The flux across the boundary is given by:

$$f\ (z=H_b) = 0 \quad \text{for all t}$$

where H_b is the depth of the base strata.

Constant Concentration Bottom Boundary

In this boundary condition the bottom boundary is assumed to maintain a constant concentration. The concentration at the boundary is given by:

$$c\ (z=H_b) = c_b \quad \text{for all t}$$

where c_b is the constant concentration at the bottom boundary and H_b is the depth of the bottom boundary.

Fixed Outflow Velocity

The bottom boundary may be specified as fixed outflow to represent a base aquifer, where the concentration varies with time as mass is transported into the aquifer from the landfill and transported out from beneath the landfill by the base velocity v_b.

Consideration of the conservation of mass gives the base concentration as:

$$c(\tau, z = H_b) = \int_0^t [\, f(\tau, z=H_b, c)/n_b h_b - v_b\, c\, (\tau, z=H_b)/n_b\, L \,]\, d\tau$$

where,

$c(\tau, z=H_b)$ = the concentration in the base aquifer, averaged over the entire thickness of the base,

$f(\tau, z=H_b, c)$ = the mass flux into the aquifer,

n_b = porosity of the base aquifer,

h_b = thickness of the base aquifer,

v_b = Darcy velocity in the aquifer and down-gradient edge of the landfill,

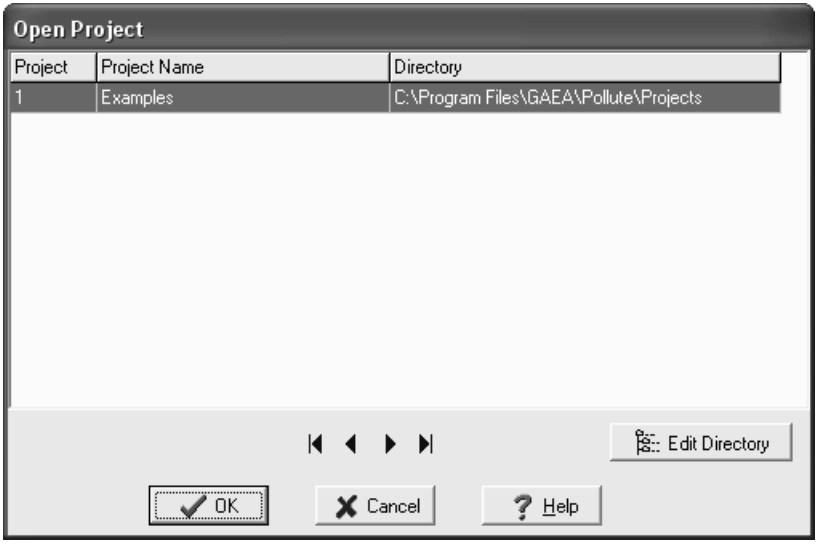
L = length of the landfill parallel to the velocity v_b.

Note that the use of a very large base velocity will give the same results at using a constant base concentration of zero. If the base velocity is zero and the porosity is zero the bottom boundary is effectively a zero flux boundary.

Infinite Thickness

The bottom boundary may also be of infinite extent, in this option the properties of the bottom most layer are adopted for the infinite layer.

3. Projects


Open Project
Project
Project Name
Directory
1
Examples
C:\Program Files\GAEA\Pollute\Projects
Edit Directory
OK
Cancel
Help

3. Projects

As discussed in the introduction, the POLLUTEv7 program is based upon the project concept for data storage. Using this method, a separate Microsoft Access 2000 database is used to store each project. Each project is stored in a separate directory, which can be on the same computer or spread across a network.

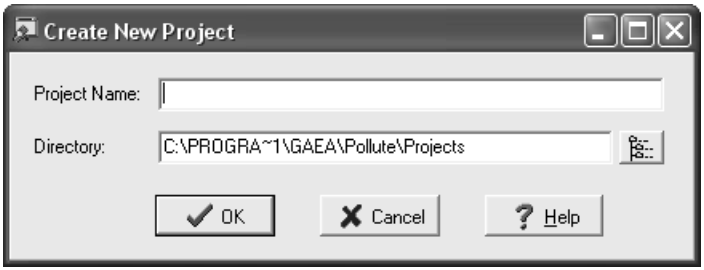
The names of the project databases are the project ID and name combined with the application name. For example, if the project ID is 25 and the project name is "980205" then the project database name for would be "25.980205.pollute.mdb". Typically, this project would be stored in the subdirectory "980205".

This chapter describes how to:

1. Create a new project.
2. Open an existing project.
3. Open the last project.
4. Close a project.
5. Delete a project.
6. Import a project.
7. Export a project
8. Backup a project
9. Restore a project
10. Import Version 6 Data
11. Set Program Preferences.

Creating a New Project

To create a new project either select the New Project menu item of the Projects sub menu, or click the New Project button on the Project Toolbar. After one of these tasks is performed, the New Project form below will be displayed.



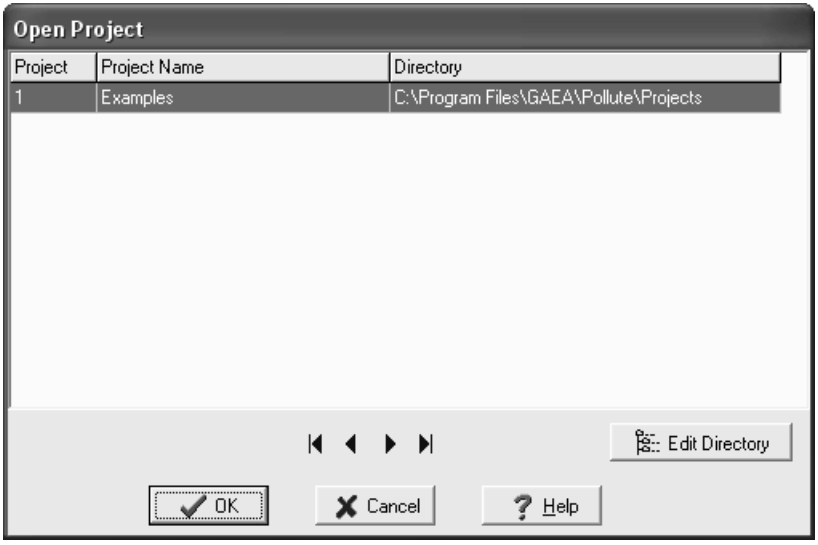
The following information can be entered for the project:

Project Name: The name of the project (up to 255 characters).

Directory: The directory to store the project database tables (up to 255 characters). This directory can be on a local computer or a network server. If the directory entered does not exist, the program will create it. It is recommended that each project reside in a separate directory (usually the same as the project ID). Typically, this directory is named after the Project Id or Name. This provides an efficient method to organizing your projects on a network or local computer.

Opening an Existing Project

To work with an existing project you can open it by selecting the Open Project menu item of the Projects submenu or clicking the Open button on the Project Toolbar. A list of available projects will be displayed in the Open Project Form as shown on the next page. The desired project can be selected by clicking on it in the list and then pressing the OK button.



The directory that a project is stored in can be changed by clicking on the Edit Directory button. This will display a Select Directory form that can be used to select the new directory for the project. Changing the directory will not move any of the project files. The purpose of this option is to allow for the movement of projects on a network.

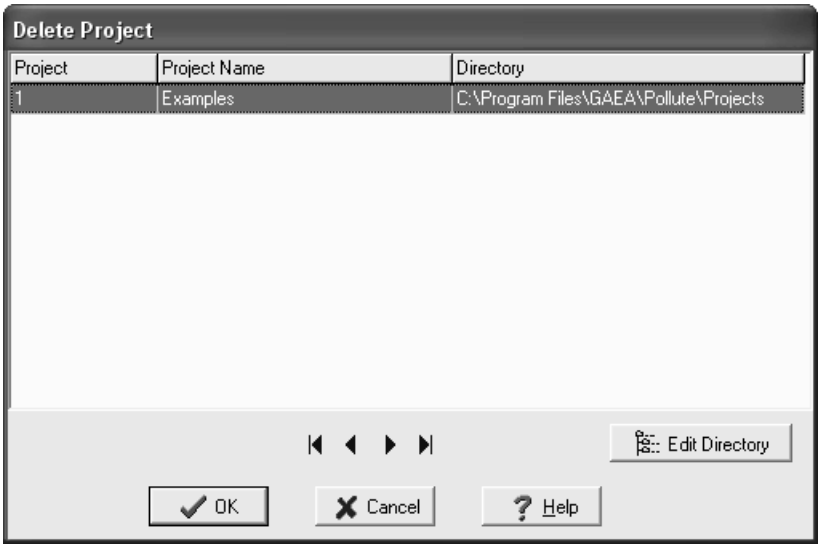
The arrow buttons at the bottom of the list can be used to move the selection to the start of the list, the previous record, the next record, or the end of the list.

Closing a Project

The current project can be closed so that no more changes can be made by selecting the Close Project menu item of the Projects submenu or· clicking the Close button on the Project Toolbar.

Deleting a Project

An existing project can be deleting by selecting the Delete Project menu item from the Projects submenu. When this is selected, a list of existing projects will be displayed.

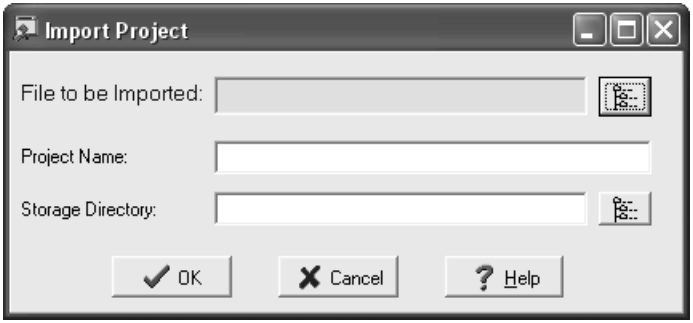


Select the project to be deleted, and then press Ok. **Note that once a project is deleted the data can not be recovered.**

The arrow buttons at the bottom of the list can be used to move the selection to the start of the list, the previous project, the next project, or the end of the list.

Importing a Project

Projects can be imported by selecting the Import Project menu item of the Projects submenu. When selected the Import Project form below will be displayed.



This form can be used to specify the following information:

File to be Imported: This is the database file to be imported. It must end with the ".mdb" extension. The Select button on the right can be used to select the file. If the Select button is used the Project Name and Directory will be filled in automatically.

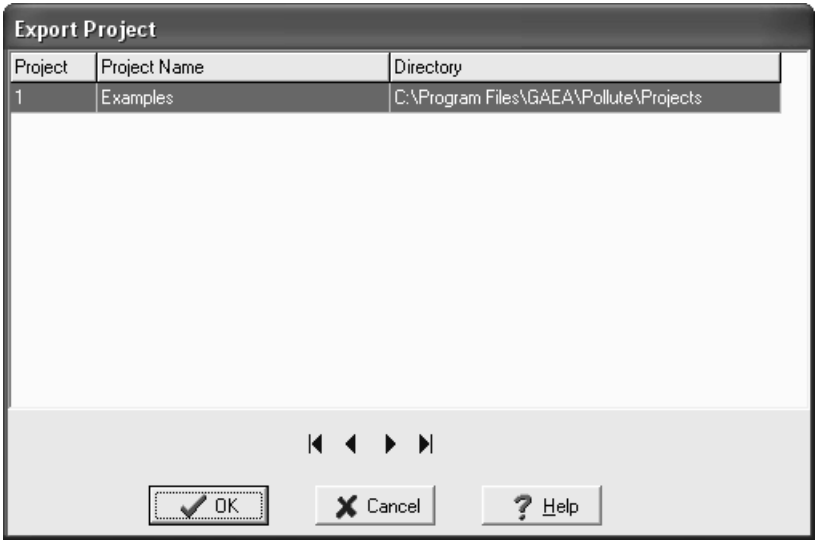
Project Name: The name of the project (up to 255 characters).

Directory: The directory to be used to store the project database tables (up to 255 characters). This directory can be on a local computer or a network server. The Select Directory button to the right of the directory name can be used to select an existing directory.

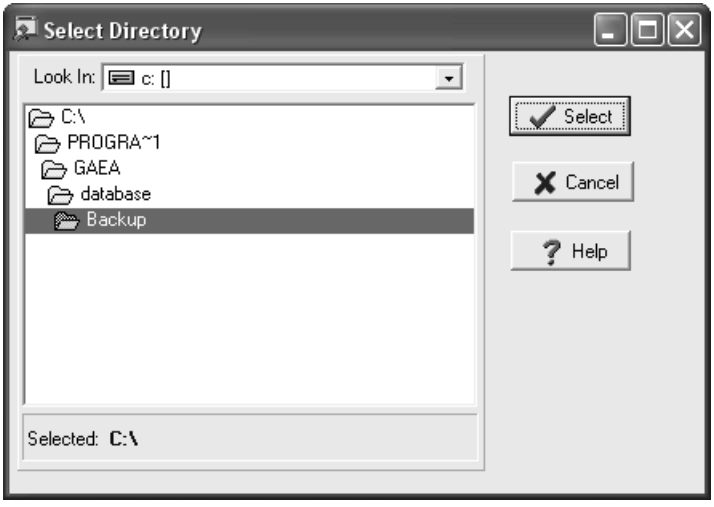
This option should be used to import projects that have been previously created but are not included in the Master Project database, such as a project that has been exported.

Exporting a Project

Existing projects can be exported by selecting the Export Project menu item from the Project submenu. When selected the Export Project form below will be displayed.



To export a project, select the project from the form and press the Ok button The Select Directory form below will be displayed. Select the directory to store the exported project database and then press the Ok button.



Backing Up a Project

POLLUTEv7 has the ability to automatically backup all databases at regular intervals while the user is editing and creating models and projects.You can decide how often you would like to backup your data. To set the time intervals between backups, select the Preferences menu item from the File menu.

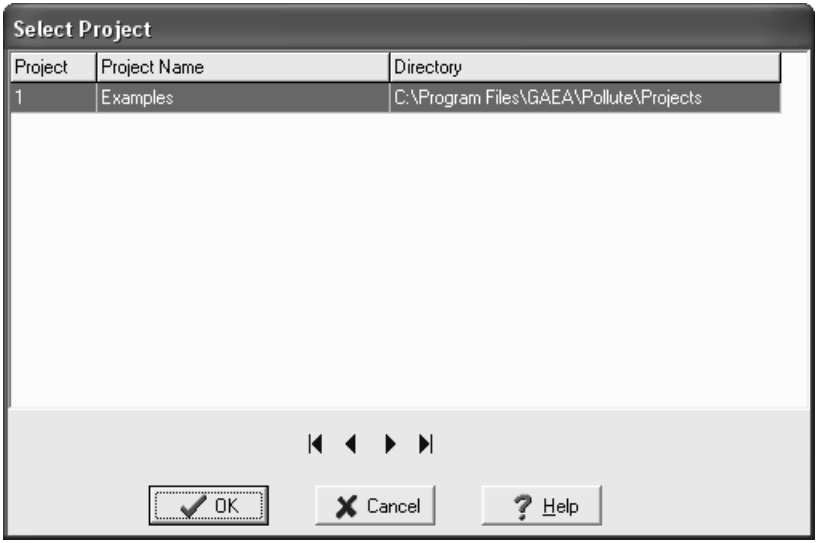
In addition to the auto-backups of the project databases and main database. The current project database and main database can be backed up at any time using the Backup Project menu item from the Projects submenu. This feature is useful for creating an archive copy of the POLLUTEv7 data. The backed up data will be stored in the Backup Directory that is set in the program's Preferences.

Restoring a Database

Restoration of a backed up POLLUTEv7 database is very simple. Select the either the Project Database or Main Database menu item from the Restore Backup submenu of the Projects submenu.

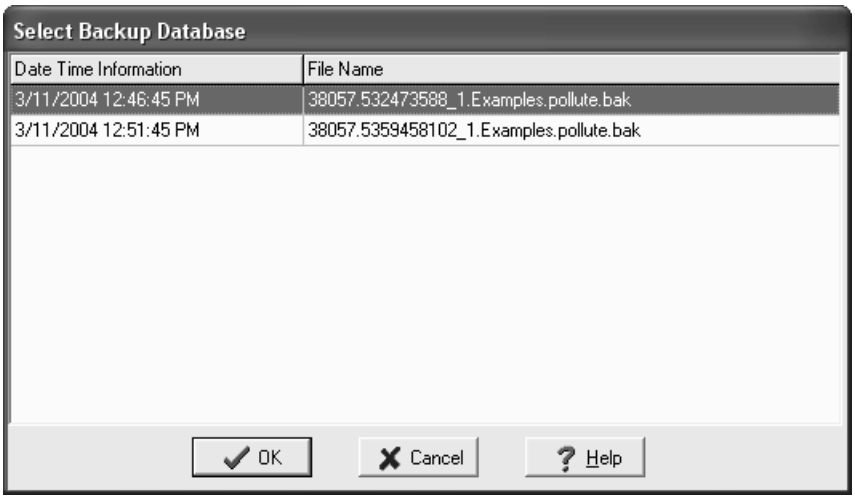
Restoring a Project Database

When the Project Database menu item is selected from the Restore Backup submenu, the Select Project form below will be displayed. This form allows you to select the project that your would like to restore.



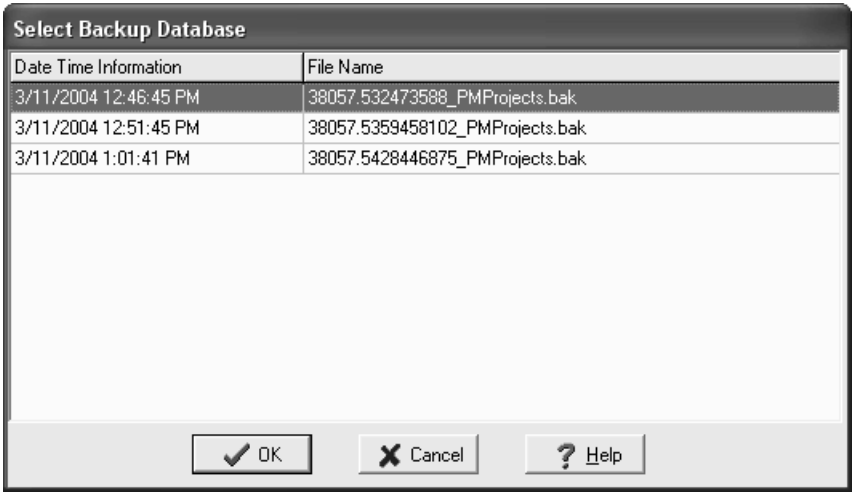
After a project has been selected the Select Backup Database form on the next page will be displayed. This form lists all the backup databases for an individual project. The date and time information indicates the date and exact time at which the project databases were backed up.

Select the database you wish to restore and then press the Ok button. The project database will then be restored.



Restoring the Main Database

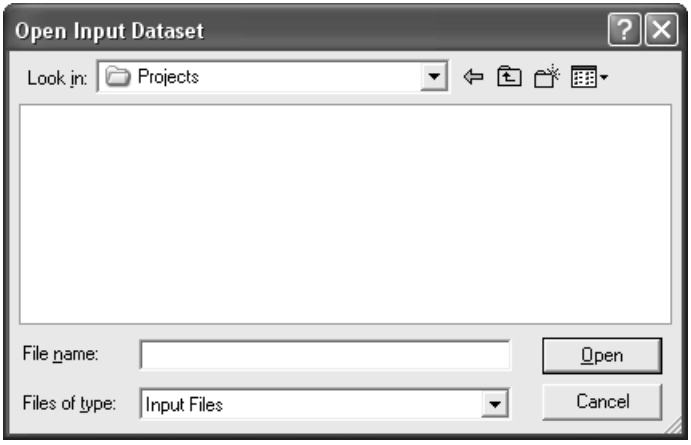
To restore a backup of the Main Database select the Main Database menu item from the Restore Backup submenu. A confirmation form will be displayed, select yes to continue and the Select Backup Database form will be displayed.



The Select Backup Database form lists all the backup databases for the main database. The date time information indicates the date and exact time at which the project list database was backed up. Select the database you wish to restore and then press the Ok button.

Importing Version 6 Data

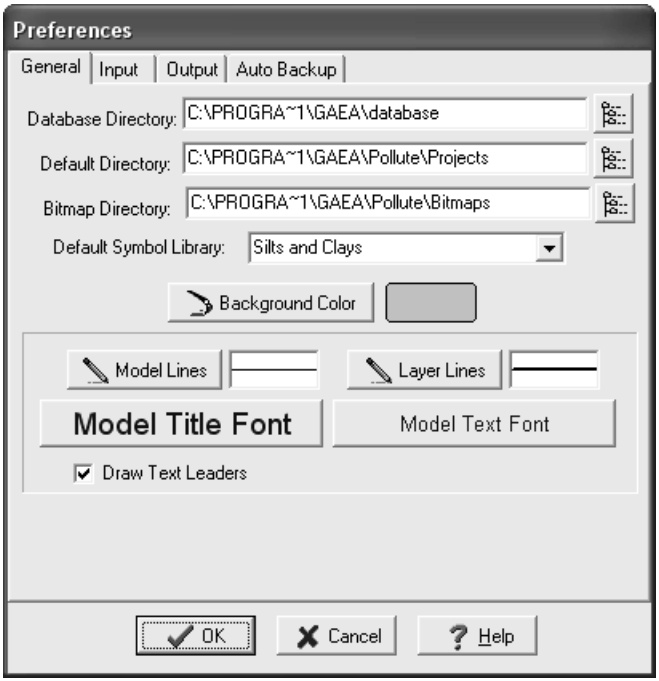
Model input data files that have been previously created in version 6 of the program can be imported into a project using the Import Version 6 Model menu item from the File menu. To use this menu item a project must be opened. The Open Input Dataset form below will be displayed.



Select the file containing the model input dataset and then press the Ok button. After the Ok button is pressed the model will be imported into the current project.

Setting Program Preferences

Using the Preferences menu item of the File menu, preferences for file directories, input, output, and back-ups can be set for the program. When this menu item is selected the Preferences form below is displayed.



General Tab

The following parameters can be set on the General tab shown above:

Database Database: This is the directory where the Main Database is located. It should only be changed if the database has been moved. The directory can be changed by entering the new directory or pressing the Select Directory button to the right of the input line.

Default Directory: This is the default directory that will be used when importing version 6 files.

Bitmap Directory: This is the directory where the bitmaps for lithologic symbols are stored. This directory should only be changed if these symbols have been moved.

Default Symbol Library: This is the default symbol library that will be used when adding a layer to a model. The library can be easily changed when the layer is added.

Background Color: This is the background color of the screen.

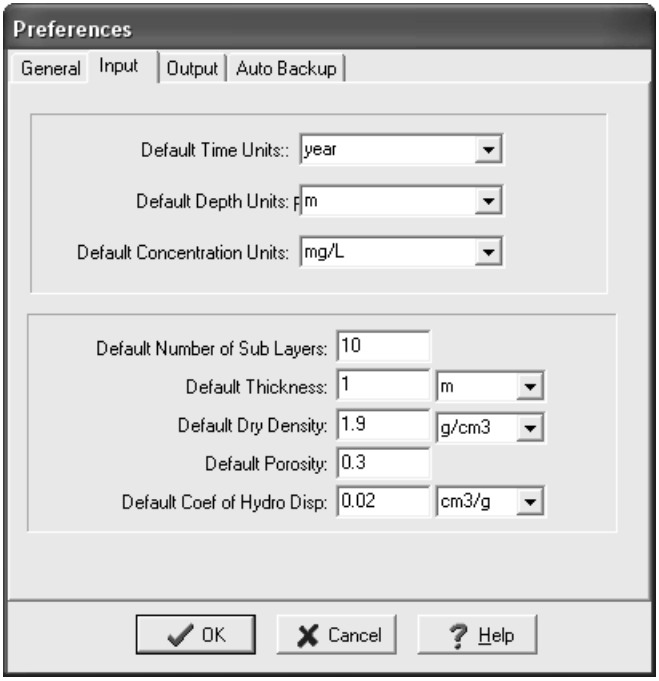
Model Lines: The line type, thickness and color of the lines used to draw the model can be changed by clicking on this button.

Layer Lines: The line type, thickness and color of the lines used to draw the layers in the model can be changed by clicking on this button.

Model Title Font: The font of the title for the model can be changed by clicking on this button.

Model Text Font: The font of the text in the model can be changed by clicking on this button.

Draw Text Leaders: If checked leaders (lines) will be drawn from the text to the layers for a model.



Input Tab

The Input tab shown on the previous page is used to specify the following parameters:

Default Time Units: This is used to select the default time units to be used when creating a model. The units can be easily changed within the model.

Default Depth Units: This is used to select the default depth units to be used when creating a model. The units can be easily changed within the model.

Default Concentration Units: This is used to select the default concentration units to be used when creating a model. The units can be easily changed within the model.

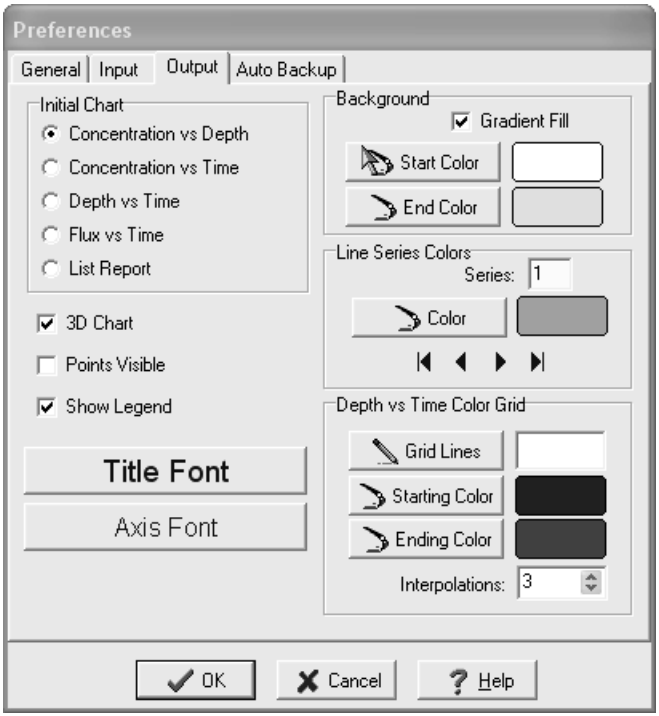
Default Number of Sublayers: This is used to specify the default number of sublayers to be used when creating a layer. The units can be easily changed within the model.

Default Thickness: This is used to specify the default thickness to be used when creating a layer. The units can be easily changed within the model.

Default Dry Density: This is used to specify the default dry density to be used when creating a layer. The units can be easily changed within the model.

Default Porosity: This is used to specify the default porosity to be used when creating a layer. The units can be easily changed within the model.

Default Coef. of Hydro. Disp.: This is used to specify the default coefficient of hydrodynamic dispersion to be used when creating a layer. The units can be easily changed within the model.



Output Tab

The Output tab shown above is used to specify the following parameters:

Initial Chart: This is used to select the initial type of output display when a model is run. The chart type can later be changed when viewing the output.

3D Chart: Check this to display the chart in 3D. The chart display can later be changed when viewing the output.

Points Visible: Check this to display the data points on the chart.The chart display can later be changed when viewing the output.

Show Legend: Check this to display a legend on the chart. The chart display can later be changed when viewing the output.

Title Font: Press this button to change the font for the chart title.

Axis Font: Press this button to change the font for the chart axis.

Background Gradient Fill: Check this box to display a gradient fill in the background of the chart.

Background Start Color: Press this button to change the start color of the background gradient fill.

Background End Color: Press this button to change the end color of the background gradient fill.

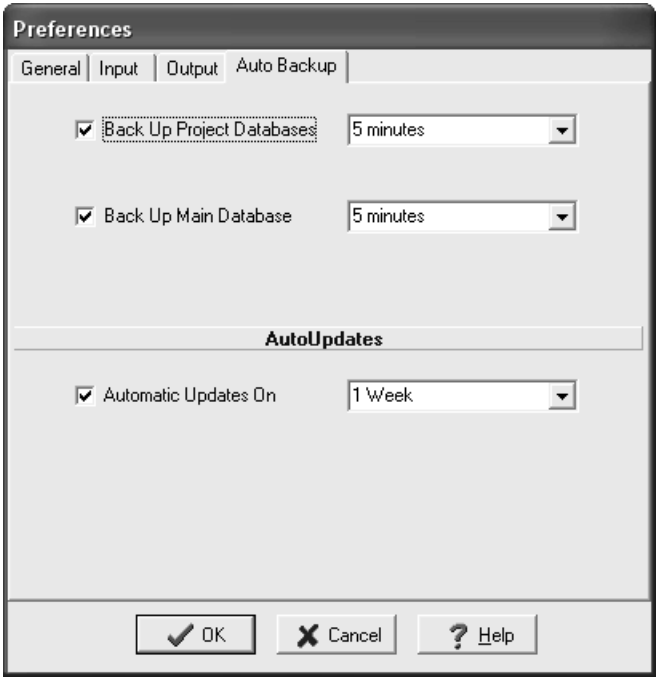
Interpolations: This is the number of interpolations to use on the data to create the color grid. A value of 0 will result in no interpolation being done and only the data being used for the grid. A value of 3 is recommended for the best results.

Lines Series Color: Press this button to change the color used to display a line series. Each lines series will be used to represent a time or depth depending upon the chart type. The line series can be changed using the arrow buttons.

Depth vs Time Chart Grid Lines: Press this button to change the line type, width, and color of the grid lines in the Depth vs Time chart.

Depth vs Time Chart Starting Color: Press this button to change the starting color of the Depth vs Time chart.

Depth vs Time Chart Ending Color: Press this button to change the ending color of the Depth vs Time chart.



Auto Backup Tab

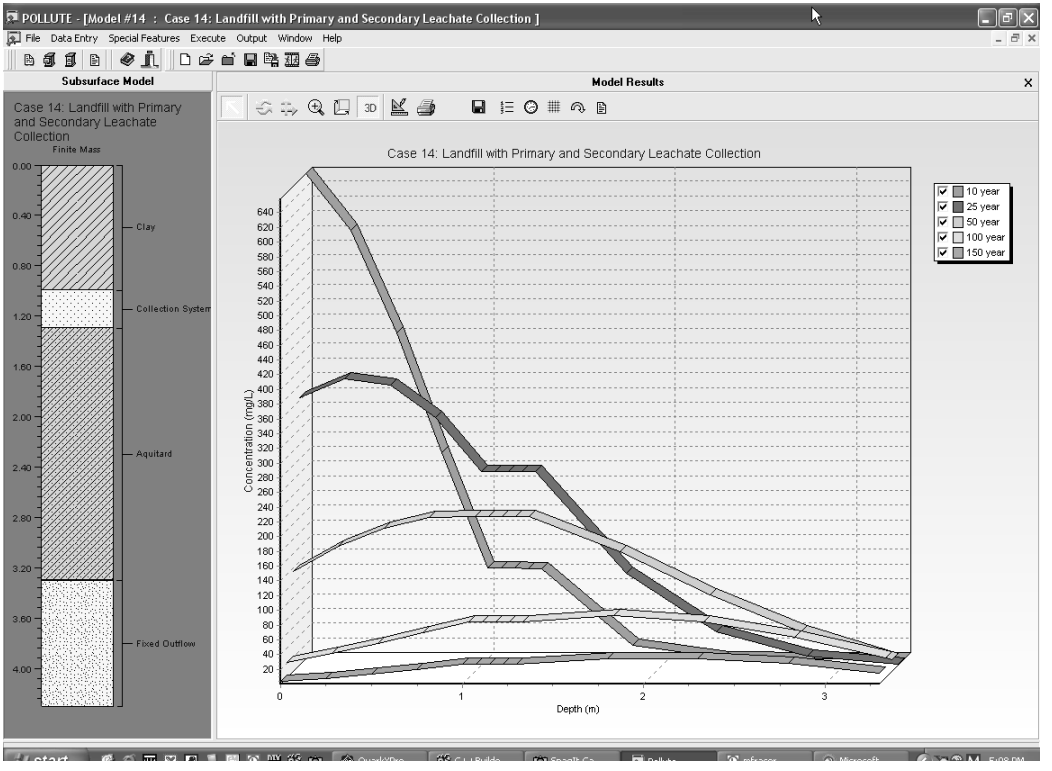
The Auto Backup tab shown above is used to specify the following parameters:

Back Up Project Database: If this checkbox is checked then the currently open project will be backed up at a regular interval defined by the combobox to the right. If this checkbox is not selected then the currently open project will not be backed up.

Back Up Main Database: If this checkbox is checked then the main database will be backed up at a regular interval defined by the combobox to the right. If this checkbox is not selected then the main database will not be backed up.

Automatic Updates On: Check this to have the program automatically check for updates on the Internet. The period between checks for updates can be set using the combobox to the right, If this checkbox is not selected then the program will not check for updates on the Internet.

4. Models


POLLUTE - [Model #14 : Case 14: Landfill with Primary and Secondary Leachate Collection]
File Data Entry Special Features Execute Output Window Help
Subsurface Model
Case 14: Landfill with Primary and Secondary Leachate Collection
Finite Mass
Clay
Collection System
Aquitard
Fixed Outflow
Model Results
Case 14: Landfill with Primary and Secondary Leachate Collection
10 year
25 year
50 year
100 year
150 year
Concentration (mg/L)
Depth (m)

4. Models

Models are used to represent the subsurface lithology, containment systems, and contaminant source to be studied. These models can be used to study the effects of landfills, buried waste, spills, lagoons, barrier systems, etc. After a model has been created it can be run to calculate the concentrations of a contaminant at specified depths and times.

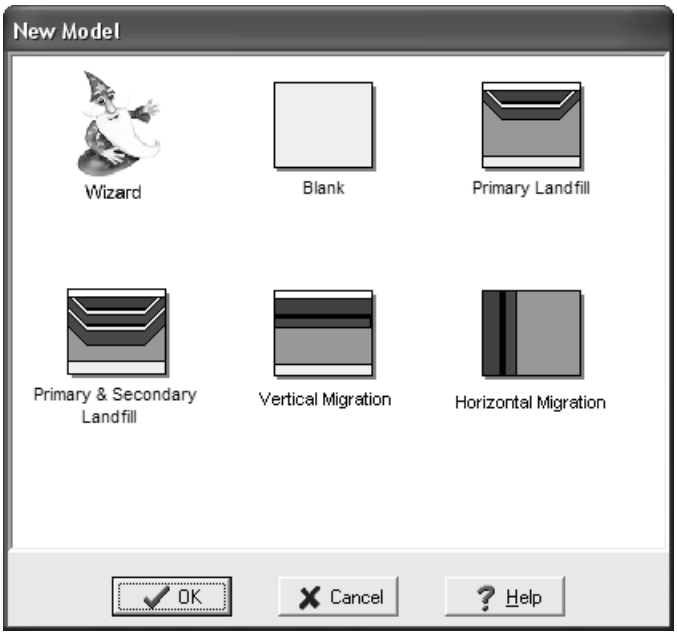
Each study area should be grouped into one or more projects. A project is used to store one or more models in a study area.

This chapter describes how to:

- create a model,
- edit a model,
- run a model,
- save a model,
- display model output,
- print a model,
- export a model,
- delete a model.

Creating a New Model

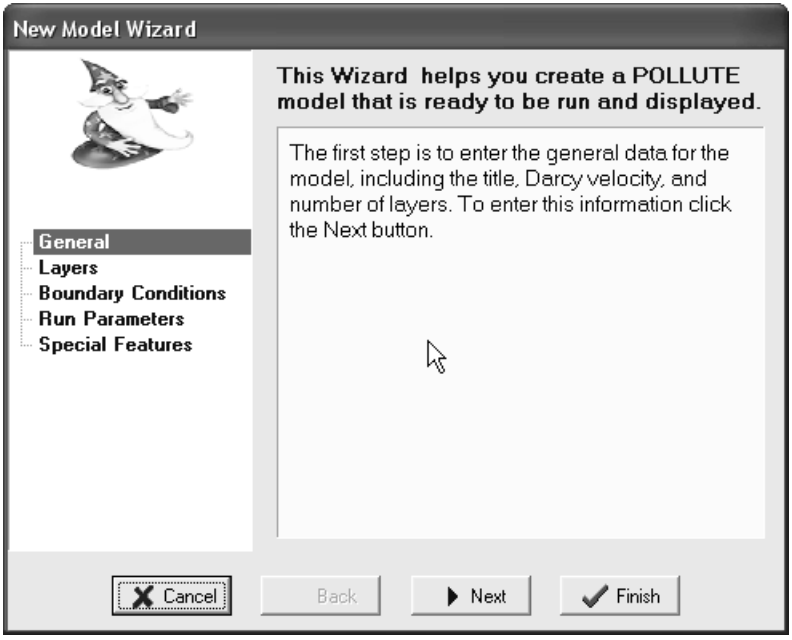
After a project has been created or opened (see Chapter 3), a model can be created either by clicking on the New Model button on the Model toolbar or selecting the New Model menu item from the Models submenu of the File menu. The New Model form below will be displayed.



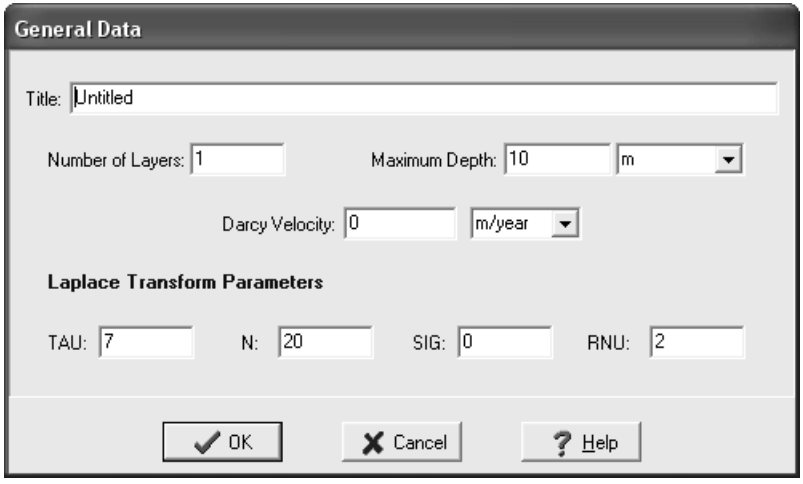
This form allows you to select one of several methods to create a new model; using a wizard, a blank model, or the following quick entry models: Primary Liner Landfill, Primary and Secondary Liner Landfill, Vertical Migration, and Horizontal Migration. Each of these methods is described in detail in the sections below.

Using the Wizard to Create a Model

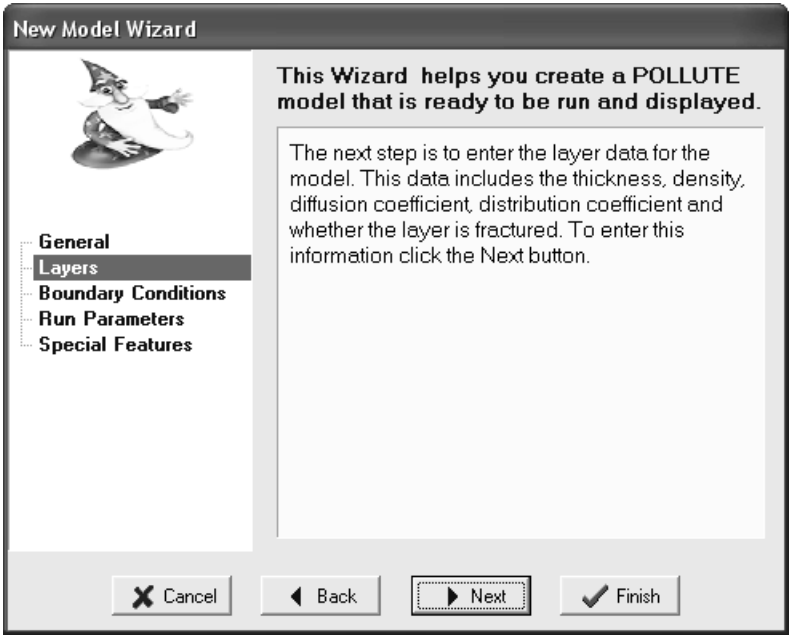
To use the Wizard to create a model, click on the Wizard button on the New Model form and then press the Ok button. The New Model Wizard form on the next page will be displayed. There are five steps to creating a model using this wizard. Each step can be moved to using the Next and Previous buttons.



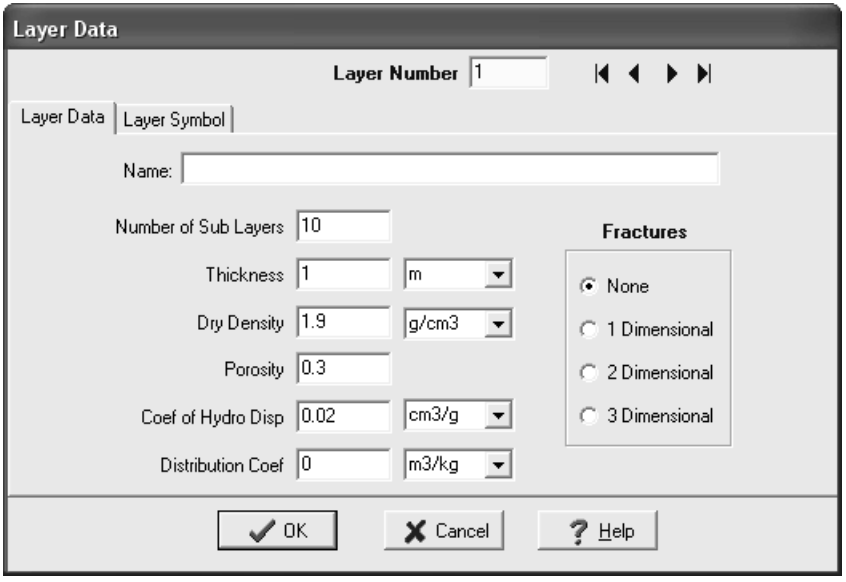
To begin creating the model, press the Next button and the General Data form below will be displayed. This form is used to enter the title, number of layers, maximum depth, Darcy Velocity, and Laplace Transform parameters. All of this data is explained in detail in the section on Editing a Model below.

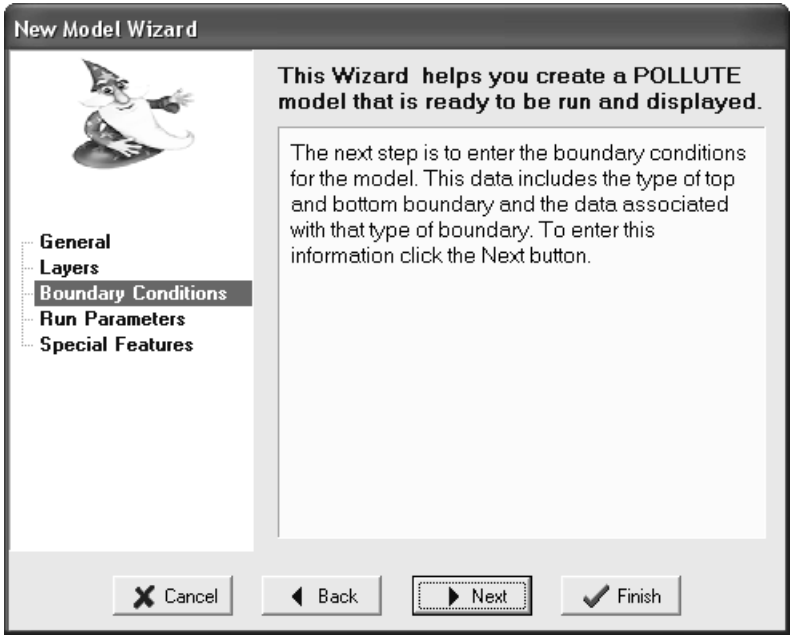


After the General Data has been entered press the Ok button to continue. The Wizard will then take you to the next step, entering Layer Data.

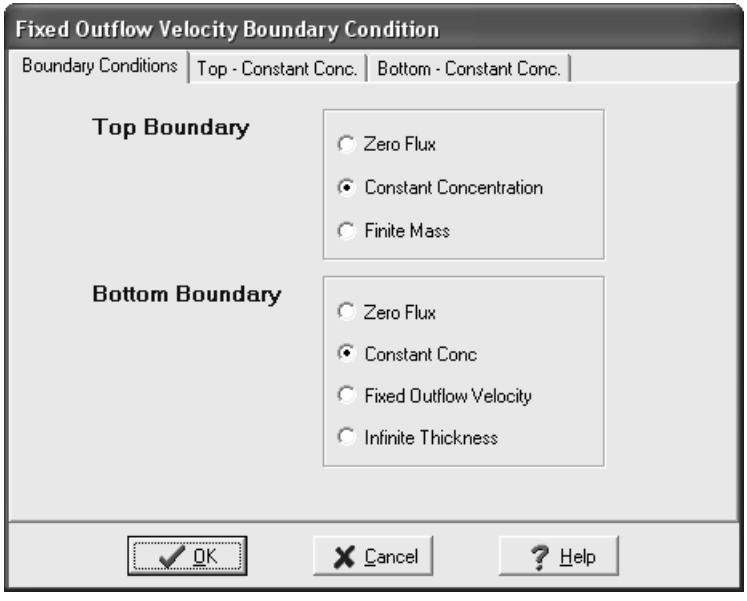


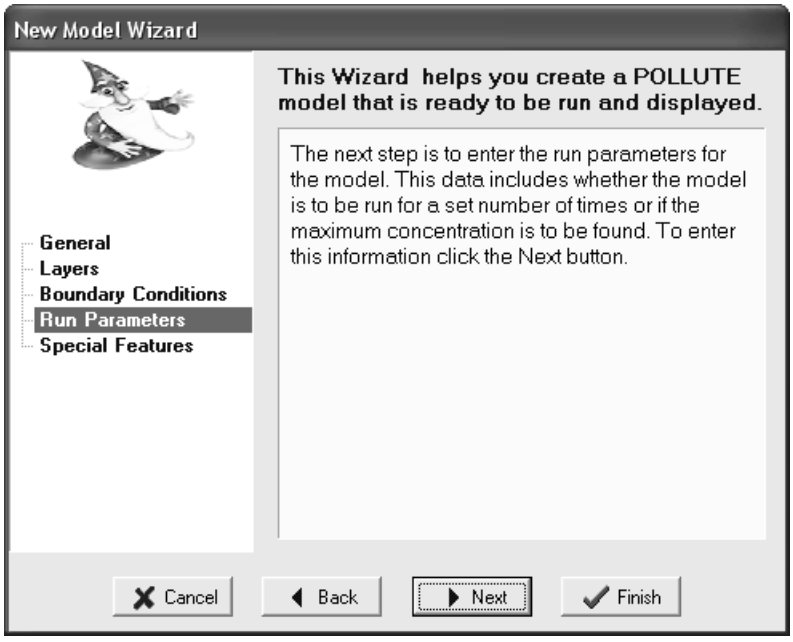
To enter the layer data, press the Next button on the Wizard form. The Layer Data form below will be displayed. This form is used to enter the data for each layer in the model. The data for each layer is described in detail in the section on Editing a Model below. After the layer data has been entered, press the Ok button to proceed to the next step on the Wizard form.



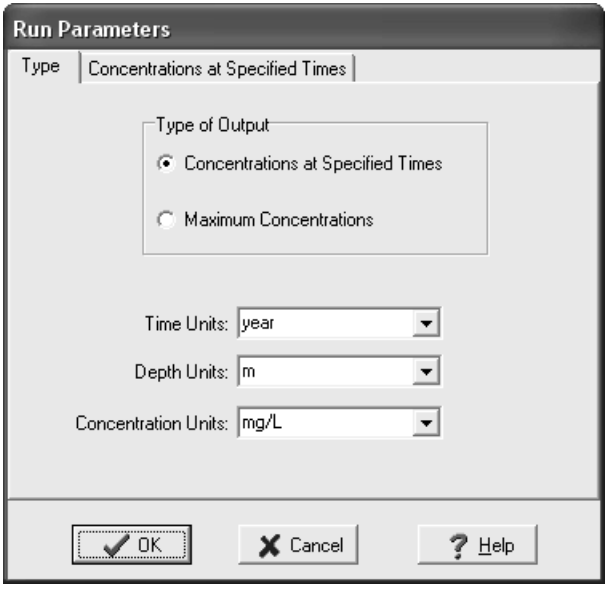


To enter the Boundary Conditions, press the Next button on the Wizard form.The Boundary Condition form below will be displayed. This form is used to enter the data for the top and bottom boundary conditions. The boundary condition data is explained in detail in the section on Editing Models below. After the boundary conditions have been entered, press the Ok button.

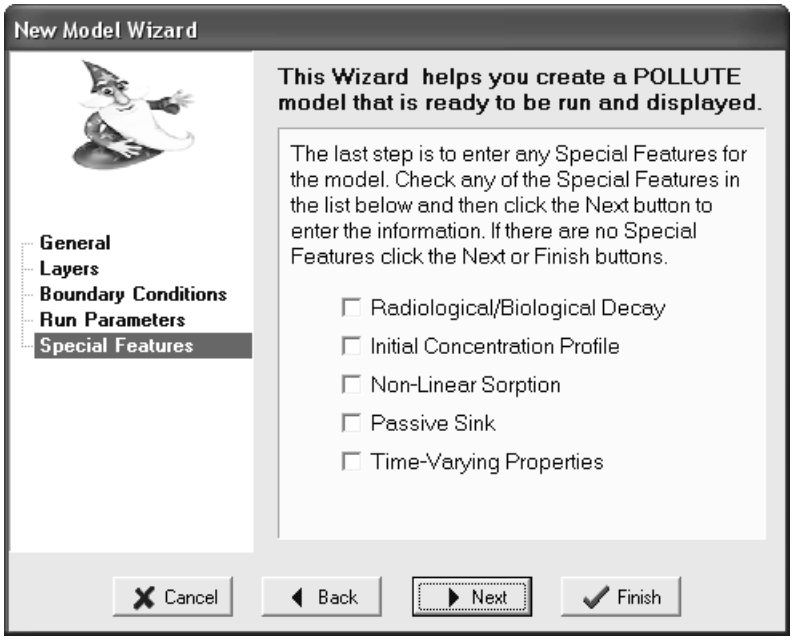




The next step is to enter the Run parameters for the model, press the Next button on the Wizard form to display the Run Parameters form below. This form is used to enter the depths and t times to calculate the concentrations. The parameters are described in detail in the section on Editing a Model below.



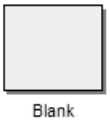
When the Run parameters have been entered press the Ok button to continue with the Wizard.



The last step is to enter any special features; such as, radioactive or biological decay, initial concentration profile, non-linear sorption, passive sink, or time-varying properties. To enter the data for one of these features check the box beside the feature. After the special features have been selected, press the Next button to enter the data for the features. For each special feature selected a form will be displayed to enter the data for that feature. The data for these features is described in detail in the section on Editing a Model below.

When all of the data for the model has been entered, press the Finish button on the Wizard form to create the model. The new model will then be displayed and can be edited as described in the section on Editing a Model below.

Creating a Blank Model



To create a blank model and fill in the data when editing the model, select the Blank model button and then press the Ok button. A blank model will be created and can be edited as described in the section, Editing a Model below.

Creating a Primary Liner Landfill


Primary Landfill

The Primary Liner (Subtitle D) Landfill option is used to quickly enter a landfill that may contain a leachate collection system, primary composite liner, aquitard, and aquifer. In this option the primary composite liner can be composed of a geomembrane and a primary liner. If the geomembrane is present the leakage through the geomembrane can be calculated using either equations by Rowe et. al., 2004; equations by Giroud et. al., 1992; or by specifying and equivalent hydraulic conductivity for the geomembrane.

To create a Primary Liner Landfill model, select the Primary Landfill button on the New Model form and then press the Ok button. The model will be created and can be edited as described in the section, Editing a Primary Liner Landfill Model below.

Creating a Primary and Secondary Liner Landfill


Primary & Secondary Landfill

The Primary and Secondary Liner Landfill option is used to quickly enter a landfill that may contain a primary leachate collection system, primary composite liner, secondary leachate collection system, secondary composite liner, aquitard, and aquifer. In this option the composite liners can be composed of a geomembrane and/or compacted clay or GCL. The leakage through the geomembrane can be calculated using either equations by Rowe et. al., 2004; equations by Giroud et. al., 1992; or by specifying and equivalent hydraulic conductivity for the geomembrane.

To create a Primary and Secondary Liner Landfill model, select the Primary and Secondary Liner Landfill button on the New Model form and then press the Ok button. The model will be created and can be edited as described in the section, Editing a Primary and Secondary Liner Landfill Model below

Creating a Vertical Migration Model


Vertical Migration

The Vertical Migration option is used to quickly enter a model for the vertical migration of a contaminant from a waste mass into an aquifer. The model may contain a primary composite liner, aquitard, and aquifer. In this option the primary composite liner can be composed of a geomembrane and a clay liner. If the geomembrane is present the leakage through the geomembrane is calculated using equations by Rowe et. al., 2004.

To create a Vertical Migration model, select the Vertical Migration button on the New Model form and then press the Ok button. The model will be created and can be edited as described in the section, Editing a Vertical Migration Model below.

Creating a Horizontal Migration Model


Horizontal Migration

The Horizontal Migration option is used to quickly enter a model for the horizontal migration of a contaminant from a waste mass to the site boundary. The model may contain a primary composite liner and an aquitard. In this option the primary composite liner can be composed of a geomembrane and a clay liner. If the geomembrane is present the leakage through the geomembrane is calculated using equations by Rowe et. al., 2004.

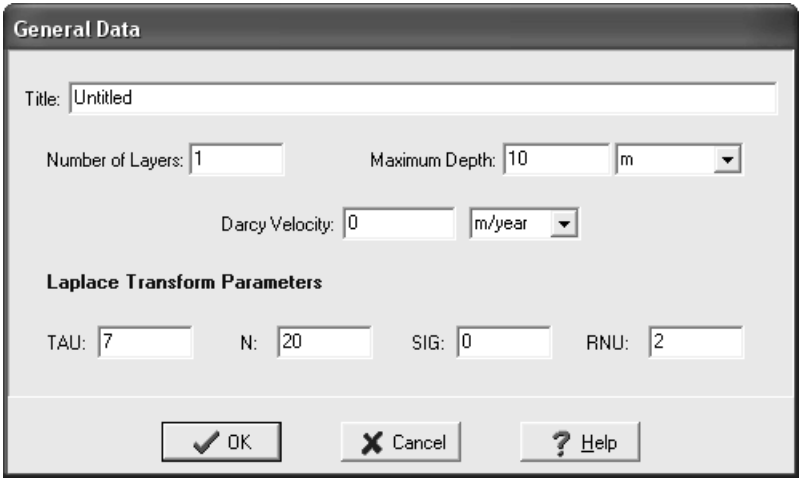
To create a Horizontal Migration model, select the Horizontal Migration button on the New Model form and then press the Ok button. The model will be created and can be edited as described in the section, Editing a Horizontal Migration Model below.

Editing a Model


After a model has been created it can be edited using the methods below. If the model is not open it will first need to be opened by double-clicking on it in the Project form or by pressing the Open Model button on the Model toolbar.

After the model is opened a Data Entry menu will appear on the menu bar. The menu items in the Date Entry menu will depend on the type of model. If the model was created using the Wizard or a Blank model then the normal editing method below will be used. If the model was created using one of the other options, such as Primary Landfill, then that editing method will be used.

In addition to the Data Entry menu, a Special Features menu will also appear on the menu bar. The menu items for the Special Features will be the same for all of the model types. The editing of these Special Features is described at the end of this section.



Editing a Normal Model

If the model was created using the Wizard or Blank model options then the Data Entry menu will contain items for editing the General Data, Layer Data, Boundary Conditions and Run Parameters. The editing of each of types of data is described below.

Editing General Data

To edit the general data for a model either select the General Data item from the Data Entry menu or click on the title of the model. The General Data form below will be displayed.
This form can be used to edit the following data for the model:

Title: The title of the model is used to describe the model, and may be up to 255 characters long.

Number of Layers: The model or deposit is divided into layers where each layer has different parameters. The total number of layers is entered with this parameter.

Maximum Depth: This is the maximum depth of the model including the bottom boundary condition. It is used only for drawing purposes and will not affect the calculations within the model.

Darcy Velocity: The Darcy Velocity is defined as: $v_a = n\ v$ where, n = the effective porosity, v = the seepage (groundwater) velocity. If zero is entered for the Darcy velocity the transport mechanism will be purely diffusive. When the Variable Properties or Passive Sink options have been selected the Darcy Velocity parameter is omitted, since it is entered in these options.

Laplace Transform Parameters: The solution of the contaminant migration equations involves the inversion of a Laplace Transform. In this inversion the accuracy depends upon four parameters: TAU, N, SIG, and RNU. The user may adopt the default values (TAU=7, SIG=0, N=20, and RNU=2) or specify other values. It has been found that a value of TAU between 7 and 10, and a value of SIG = 0 is satisfactory in most cases. The more critical parameters, RNU and N, typically yield accurate results when:

$$RNU = \frac{0.1\ (\text{Layer Thickness})\ (\text{Darcy Velocity})}{\text{Minimum Diffusion/Dispersion Coefficient}}$$

and

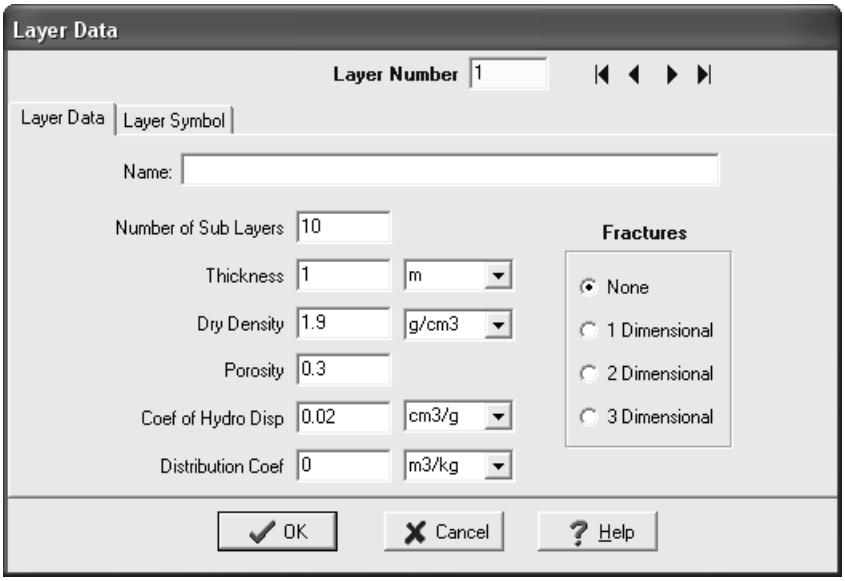
$N = 10 * RNU$ if RNU is greater than 1.0.

These values of RNU and N will work extremely well but will often require more integration than is necessary. If the computation times seem excessive smaller values of RNU and N should be tried, and the accuracy of the results compared.

The program will detect grossly unreasonable results and automatically repeat the calculation with the values suggested above, in this circumstance the value of RNU is limited to 40.

Editing Layer Data

To edit the layer data either select the Layer Data menu item from the Data Entry menu or click on a layer on the screen. The Layer Data form below will be displayed. This form has two tabs, one for entering the data for the layer and the other for selecting a symbol for the layer. If the layer is fractured, a third tab will appear for the fracture data.



Layer Data Tab

The following data can be edited on the Layer Data tab:

Name: This is the name of the layer. It is used only for drawing.

Number of Sublayers: The number of sublayers in each layer is primarily used in the output of the calculated concentrations with depth; a concentration will be calculated at each sublayer interface. If the Freundlich Non-Linear Sorption, Langmuir Non-Linear Sorption, or Variable Properties Special Feature is selected, the accuracy of the results will depend on the number of sublayers.

Thickness: This is the thickness of the layer, this is the total thickness of all the sublayers in the layer.. The maximum thickness of each sublayer is 5 units. This maximum can be adjusted using the Maximum Sublayer Thickness option of the Special Features menu. If the maximum sublayer thickness is not changed then the number of sublayers is automatically increased if required to keep their thickness to less than 5.

Dry Density: The dry density of the layer.

Porosity: This is the porosity of the layer, which must be greater than 0 and less than or equal to 1. If the layer is being used to represent a geomembrane the porosity should be set to 1.

Coefficient of Hydrodynamic Dispersion: This is the coefficient of hydrodynamic dispersion for the layer:

$$D = D_e + D_{md}$$

where,

D_e = the diffusion coefficient for the species,

D_{md} = the coefficient of mechanical dispersion.

For intact clayey layers, diffusion will usually be the controlling factor and dispersion will often be negligible [Gillham and Cherry, 1982, Rowe, 1987; Rowe et al, 2004]. In sandy layers, dispersion will tend to be the controlling factor.

If the Variable Properties option of the Special Features submenu is selected the dispersivity can be specified separately.

Distribution Coefficient: This is the distribution coefficient for the layer. In the basic mode (ie. where Langmuir Non-linear sorption and Freundlich Non-linear sorption have not been selected) the sorption-desorption of a conservative species of contaminant is assumed to be linear such that:

$$S = K_d \; c$$

where,

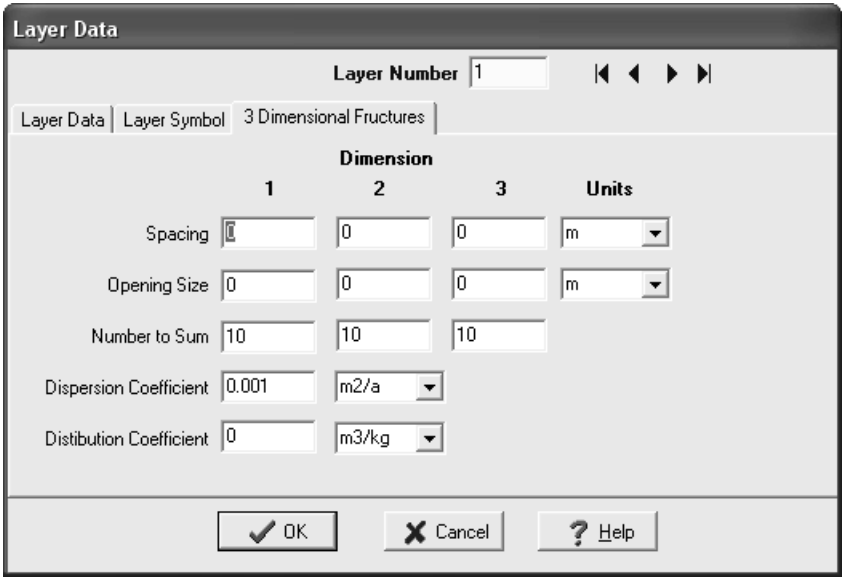
S = solute sorbed per unit weight of soil,

K_d = distribution (sorption) coefficient,

c = concentration of contaminant.

This is a reasonable approximation for low concentrations of contaminant, however at high concentrations sorption is generally not linear and more complex relationships should be used. If there is no sorption (i.e., a conservative species) the distribution coefficient is zero. Two types of non-linear sorption can be used if desired, these are Langmuir Non-Linear Sorption and Freundlich Non-Linear Sorption. Both options can be selected in the Special Features submenu.

Fractures: Any or all of the layers may be fractured. These fractures may be 1, 2, or 3 dimensional. Where the first dimension is for one set of vertical fractures, the second is for a second set of (orthogonal) vertical fractures, and the third is for horizontal fractures (ie. for a 3D block, dimension 1 is length, dimension 2 is width, and dimension 3 is depth). If 1, 2, or 3 dimensional fractures are specified for the layer, an additional tab will appear to enter the fracture data.



Fracture Tab

Continuity of concentration and flux is assumed at the boundary between layers. If a fractured layer is in contact with an unfractured layer, it is assumed that all fluid flow is transported along the fractures that intersect the unfractured layers (i.e., it is equivalent to having a very thin sand layer between unfractured and fractured layers).

In a fractured model the program can consider advective-dispersive transport along the fractures coupled with diffusion into the matrix on either side of the fracture. However, if the Darcy velocity is zero, or small, then the transport mechanism will be essentially diffusive through the matrix, the fractures will have no effect and should not be considered in modelling the migration of contaminants. Users planning to model migration in fractured media are warned that they should first see Rowe and Booker, 1990, 1991a, 1991b, and Rowe et al, 2004 for a discussion of modelling of fractured systems.

The following information about the fractures in each dimension can be specified on the Fracture tab:

Fracture Spacing: The spacing of fractures is the distance between fractures in each dimension.

Fracture Opening Size: The fracture opening size is the width of the gap between the fracture walls.

Number to sum: This is the number of terms to sum in the evaluation of the advective-dispersive equation for contaminant migration [Rowe and Booker, 1990, 1991a, 1991b]. For blocks where the fracture spacing is of the same order in all directions, 8 to 10 terms is usually adequate.

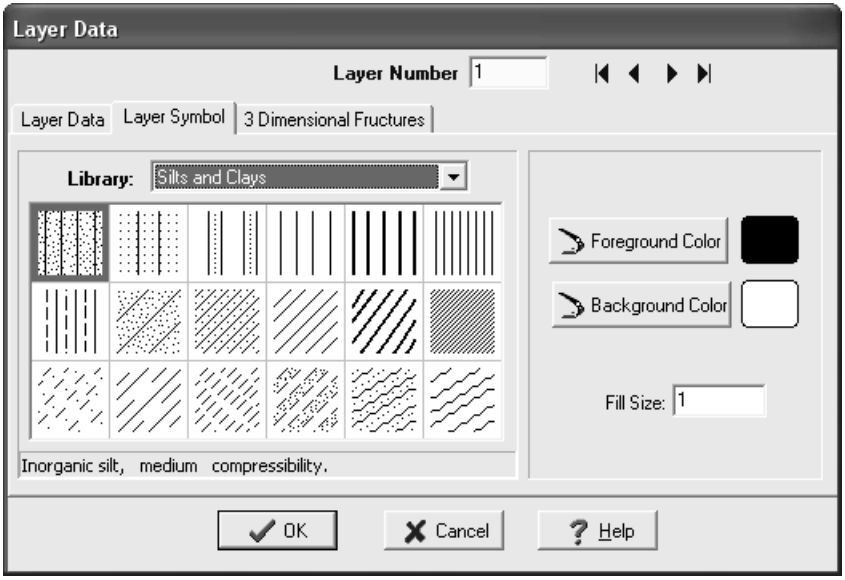
As the aspect ratio (horizontal spacing/vertical spacing or vertical spacing/vertical spacing) increases more terms are required in the summation. When the aspect ratio is large, the problem can usually be reduced to a lower order (eg. from 3D to 2D or 2D to 1D). For example, if the spacing between fractures in one vertical direction is 50 units, and in the other vertical and horizontal directions is 2 units. The widely spaced fractures can be ignored and the problem reduced to a 2D problem [Rowe and Booker, 1990].

In addition the following can be specified for the fractures:

Dispersion coefficient: This is the dispersion coefficient along the fracture. For a more complete description of dispersion coefficient see the Diffusion/ Dispersion Coefficient for a layer.

Distribution coefficient: This is the distribution coefficient along the fracture as defined by Freeze and Cherry (1979). This is often assumed to be zero.

Layer Symbol Tab



This tab is used to define how the layer will be drawn. The following information can be edited using this tab:

Library: This combo box is used to select the symbol library to use to draw the layer. When the arrow at the right is pressed a list will display the available symbol libraries. After a library has been selected, the symbols displayed in the tab will be updated.

Symbol: The symbol from the library can be selected by clicking on one of the 18 symbols displayed for the current library. The selected symbol is highlighted with a blue border.

Foreground Color: This is the color to use for the shaded parts of the symbol. The foreground color can be changed by pressing the Foreground Color button. When this button is pressed a Color form is displayed. Using this form, a basic color can be selected or a custom color can be specified.

Background Color: This is the color to use for the unshaded parts of the symbol. The background color can be changed by pressing the Background Color button. When this button is pressed a Color form is displayed. Using this form, a basic color can be selected or a custom color can be specified.

Fill Size: The fill size is used to expand or condense the symbol The size of the symbol is multiplied by the fill size and then the symbol is drawn. For example, a fill size of 2 will result in the symbol being doubled in size. The fill size must be greater than 0.

After the data for the layer is entered, the user can go to the next layer by selecting the Next button, go back to the previous layer by selecting the Previous button, go to the first layer using the First button, or go to the last layer using the Last button. When the data for all the layers has been edited, the user can save the information by selecting the OK button.

Editing Boundary Conditions

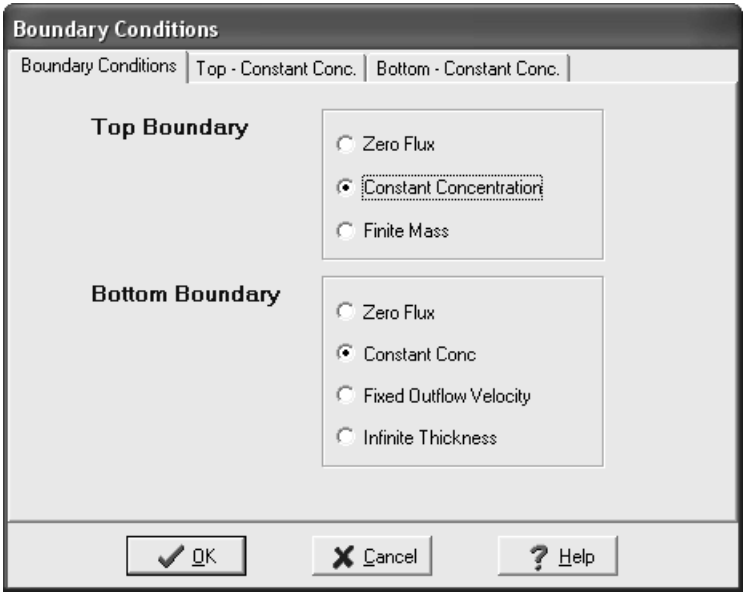
For every model there are two boundary conditions, one at the top and one at the bottom. The top boundary condition is usually the point of contact between the contaminant source (eg. a landfill) and the subsurface layers (deposit), and can be either:

- **Zero Flux**,
- **Constant Concentration**, or
- **Finite Mass**.

The bottom boundary condition is usually the point of contact between the deposit and either a much more or much less permeable strata (eg. an aquifer or bedrock) and can be either:

- **Zero Flux**,
- **Constant Concentration**,
- **Fixed Outflow**, or
- **Infinite Thickness**.

To edit the boundary conditions either select the Boundary Condition menu item from the Data Entry menu or click on the top or bottom boundary condition. The Boundary Condition form below will then be displayed.

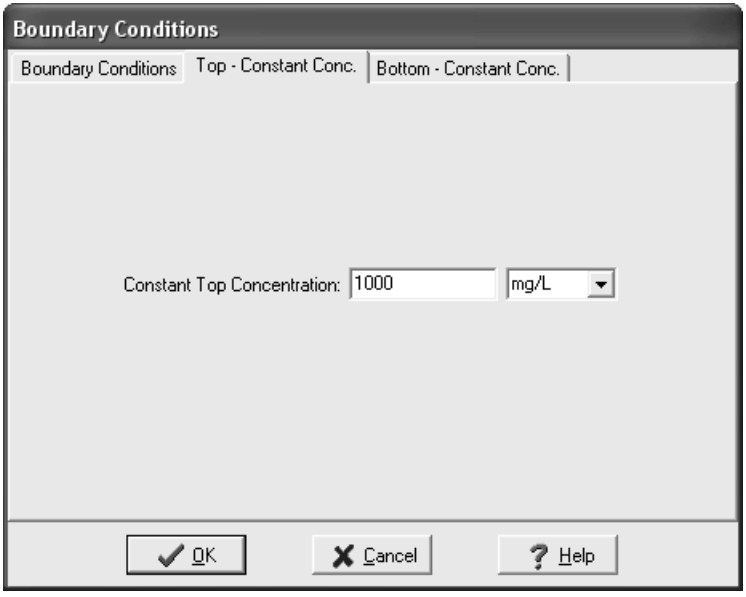


Depending upon the top and bottom boundary conditions selected, additional tabs will appear to enter the relevant data.

Zero Flux Top Boundary Condition

The zero flux top boundary condition represents the case where there is no transmission of contaminant across the top boundary. This option is for highly specialized applications and is rarely used.

If the top boundary is specified as zero flux no additional tab will be displayed, since there is no data to enter for the top boundary.



Constant Concentration Top Boundary Condition

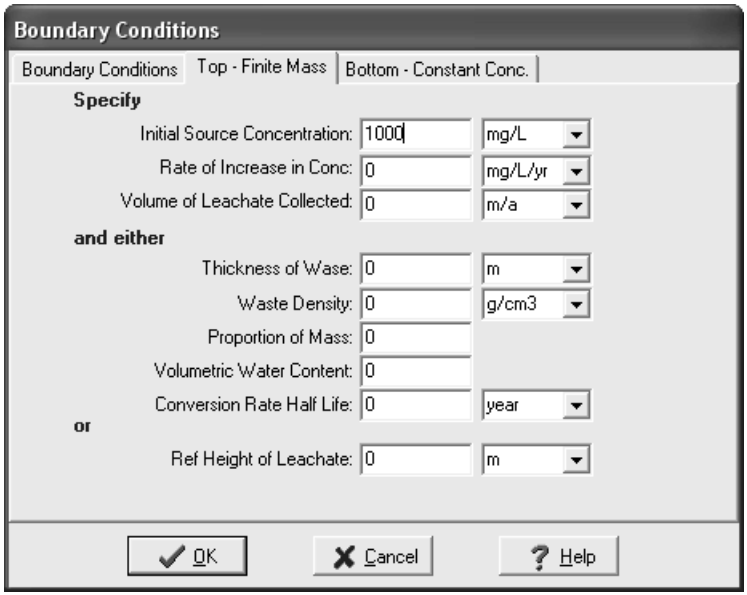
The constant concentration top boundary condition represents the case where the concentration of contaminant in the landfill remains constant throughout time, and is equivalent to the assumption of an infinite mass of contaminant in the landfill.

If the top boundary condition is specified as constant concentration an additional tab will be displayed as shown below. On this tab the contaminant concentration at the top boundary can be specified.

Finite Mass Top Boundary Condition

The finite mass top boundary condition is most representative of a landfill, where the concentration of contaminant starts at an initial value, increases with time, and then declines as contaminant is transported into the subsurface and is removed by leachate collection systems.

When the top boundary is specified as finite mass the Finite Mass tab will be displayed as shown on the next page. If the Variable Properties option has been selected from the Special Features menu, the values for the finite mass parameters will be specified in the Variable Properties entry and the tab will not appear.



When the top boundary is finite mass the user must specify:

- **Initial Source Concentration**,
- **Rate of Increase** in concentration,
- **Volume of Leachate Collected**.

and either:

- **Thickness of Waste**,
- **Waste Density**,
- **Proportion of Mass**,
- **Volumetric Water Content** of the waste,
- **Conversion Rate Half-Life** of the contaminant.

or:

- **Reference Height of Leachate**.

These parameters are described below.

Initial Source Concentration: This is the initial concentration of the source of contaminants, usually at time zero.

Rate of Increase: This is the rate of increase in concentration with time due to increasing mass entering the landfill. If the peak concentration is reached early in the landfill's life and the analysis starts at this time, the rate of increase would be zero.

Volume of Leachate Collected: This is the volume of leachate collected per unit area of landfill per unit time, usually by the leachate collection system. Thus, the average volume of leachate collected is equal to the average infiltration through the landfill cover less the average exfiltration through the base of the landfill (assuming the waste is at field capacity). For example, if the average infiltration is 0.3 m/a and the average exfiltration is 0.03 m/a, then the average volume of leachate collected is 0.3-0.03 = 0.27 m/a.
Thickness of Waste: This is the vertical thickness of the waste, and is used to calculate the mass of contaminant per unit area of waste. Either the thickness of waste or reference height of leachate must be specified.

Waste Density: This is the apparent density of the waste (i.e. mass of waste per unit volume of the landfill). Either the waste density or reference height of leachate must be specified.

Proportion of Mass: The available (leachable) mass of contaminant in the waste per unit mass of waste (eg. mass of chloride in waste/total mass of waste). Either the proportion of mass or reference height of leachate must be specified. Rowe et al (2004) report some published values for leachable mass.

Volumetric Water Content: This is the volumetric water content of the waste. Either the volumetric water content or reference height of leachate must be specified.

Conversion Rate Half-Life: The generation coefficient is calculated based on the conversion rate half-life K, such that = ln 2 / K. A value of = 0 implies no generation of concentration with time. In the program = 0 is obtained by specifying K = 0 (this is the default case).

Reference Height of Leachate: The reference height of leachate represents the volume of leachate that would contain the total leachable mass of a contaminant of interest at the initial source concentration. Thus, the reference height (H_r) is equal to the mass of contaminant (M) per unit area divided by the initial source concentration (c_o) (i.e. $H_r = M/c_o$).

Either the reference height of leachate or the waste thickness, waste density, proportion of mass, volumetric water content, and conversion rate half-life must be specified. If the reference height of leachate is zero then the mass of contaminant is calculated using the above parameters. If the reference height of leachate is not zero than the mass of contaminant is calculated using this value, and the above parameters are ignored.

For example, if there is an average of 12.5 m of waste at a density of 600 kg/m^3 and the contaminant represents 0.2% of the total waste mass, is then:

M = (0.2/100) (600) (12.5) = 15 kg/m^2

And, if the initial source concentration is 1000 mg/L (i.e., 1 kg/m^3) then the reference height is H_r = 15/1 = 15 m.

Zero Flux Bottom Boundary Condition

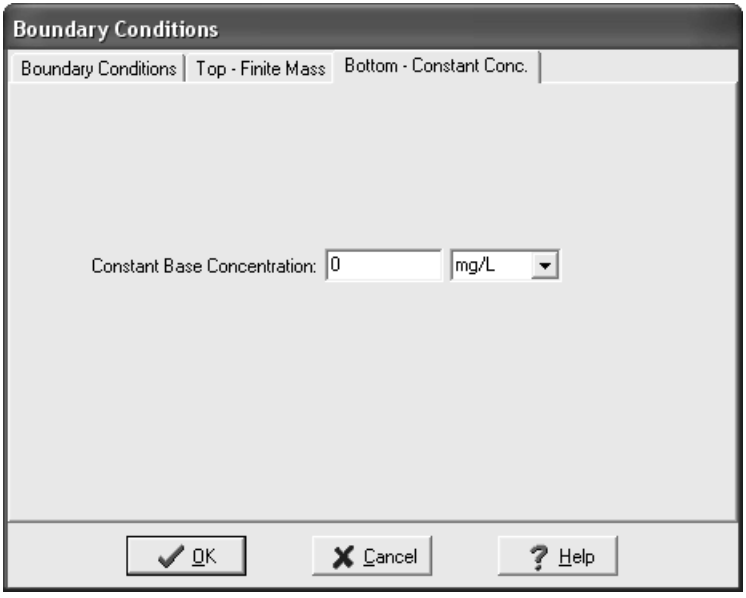
The zero flux bottom boundary condition represents the case where no mass is transported into or out of the bottom of the deposit. This condition can be used to represent the case of a deposit underlain by an impermeable base stratum (e.g., intact bedrock that is impermeable relative to the overlying layer or deposit).

If the bottom boundary is specified as zero flux no additional tab will be displayed, since there is no data to enter for the bottom boundary.

Constant Concentration Bottom Boundary Condition

The constant concentration bottom boundary condition represents the case where the concentration of contaminant remains constant in the base strata. The user will be prompted to specify the constant concentration in the base strata.

If the bottom boundary condition is specified as constant concentration an additional tab will be displayed as shown below. On this tab the contaminant concentration at the bottom boundary can be specified.

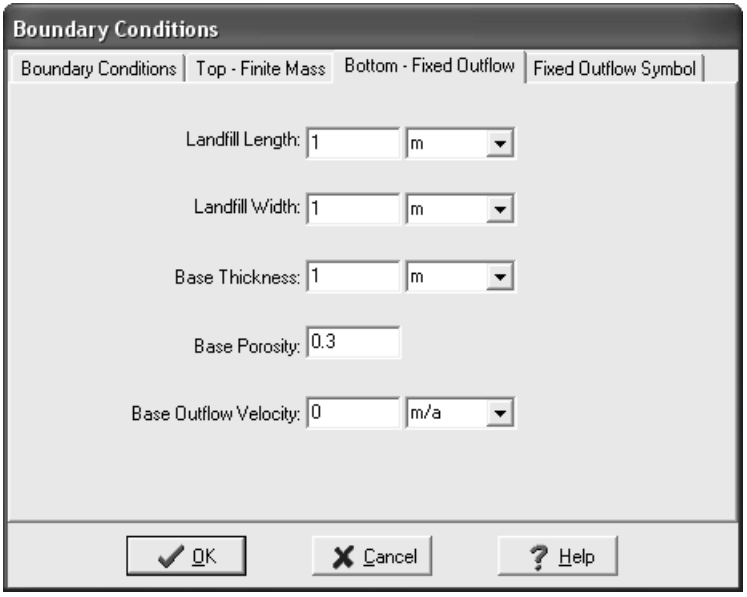


Fixed Outflow Bottom Boundary Condition

The fixed outflow bottom boundary condition is most representative of the case where the model is underlain by an aquifer (permeable base strata). The concentration in the base strata (aquifer) varies with time as mass is transported into the aquifer from the deposit, and then transported away by the horizontal velocity in the base strata.

The base aquifer is modelled as a boundary condition (not a separate layer) and the concentration at the bottom of the model is the concentration at the top of the base aquifer. This boundary condition assumes that there is sufficient dispersion/mixing such that the concentration is uniform across the thickness of the aquifer being considered. Thus the concentration at the bottom of the aquifer thickness modelled is the same as reported at the top of the aquifer. If the actual aquifer is very thick, normally only the upper portion (3 - 6 m depending on conditions) should be considered in modelling (see Example 3).

When the bottom boundary is specified as fixed outflow the Fixed Outflow tab will be displayed as shown below.



The following parameters can be entered on this tab:

Landfill Length: This is the length of the landfill in the direction of groundwater flow.

Landfill Width: This is the width of the landfill in a direction perpendicular to groundwater flow. The width is usually set to 1, since it has no influence on the results.

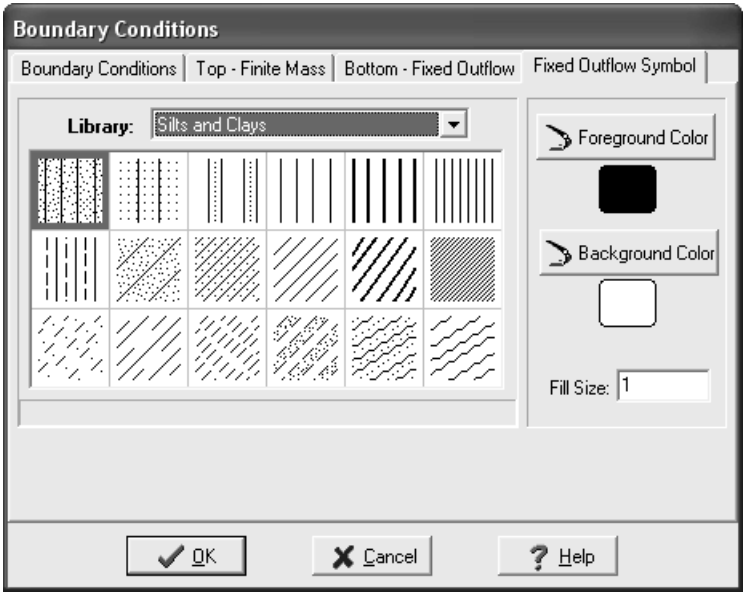
Thickness: This is the vertical thickness of the base strata that is being modelled as a boundary condition.

Porosity: This is the porosity of the base strata, between 0 and 1.

Base Outflow Velocity: This is the horizontal Darcy outflow velocity within the base strata at the down-gradient edge of the landfill. If the outflow velocity is set very high the results will be equivalent to setting a constant base concentration of zero. If the Variable Properties option has been selected from the Special Features submenu, the value of the Outflow Velocity will be specified in the Variable Properties option.

Warning: The user should read Example 3 before using this boundary condition.

In addition to the Fixed Outflow tab, the Fixed Outflow Symbol tab, shown below, will also appear if the bottom boundary condition is fixed outflow. This tab is used to select the symbol that will be used to draw the bottom boundary condition.



The following information can be edited using this tab:

Library: This combo box is used to select the symbol library to use to draw the boundary condition. When the arrow at the right is pressed a list will display the available symbol libraries. After a library has been selected, the symbols displayed in the tab will be updated.

Symbol: The symbol from the library can be selected by clicking on one of the 18 symbols displayed for the current library. The selected symbol is highlighted with a blue border.

Foreground Color: This is the color to use for the shaded parts of the symbol. The foreground color can be changed by pressing the Foreground Color button. When this button is pressed a Color form is displayed. Using this form, a basic color can be selected or a custom color can be specified.

Background Color: This is the color to use for the unshaded parts of the symbol. The background color can be changed by pressing the Background Color button. When this button is pressed a Color form is displayed. Using this form, a basic color can be selected or a custom color can be specified.

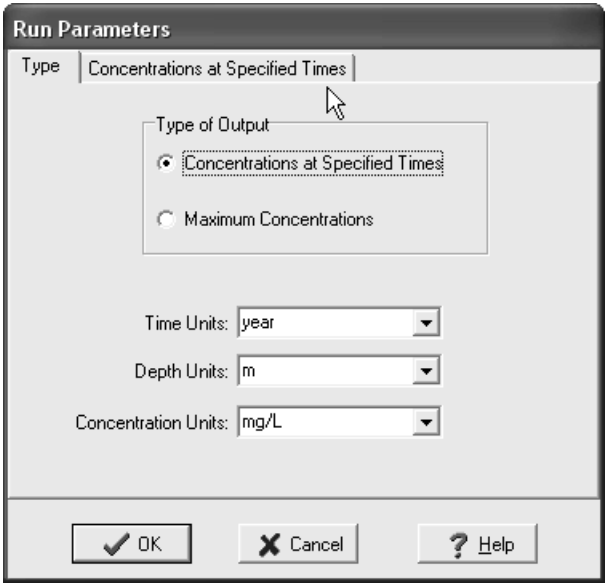
Fill Size: The fill size is used to expand or condense the symbol The size of the symbol is multiplied by the fill size and then the symbol is drawn. For example, a fill size of 2 will result in the symbol being doubled in size. The fill size must be greater than 0.

Infinite Thickness Bottom Boundary Condition

The infinite thickness bottom boundary condition represents the case where the deposit extends infinitely in depth. This condition can be used to model lateral migration within the deposit. If the bottom boundary is specified as infinite thickness no additional tab will be displayed, since there is no data to enter for the bottom boundary.

Editing Run Parameters

The run parameters specify the depths and times to calculate the concentrations for the model. To edit the run parameters select the Run Parameters menu item from the Data Entry menu. The Run Parameters form below will be displayed.



The following parameters can be specified on the Type tab:

Type of Output: There are two types of output that can be generated, either concentrations at specified times or maximum concentrations.

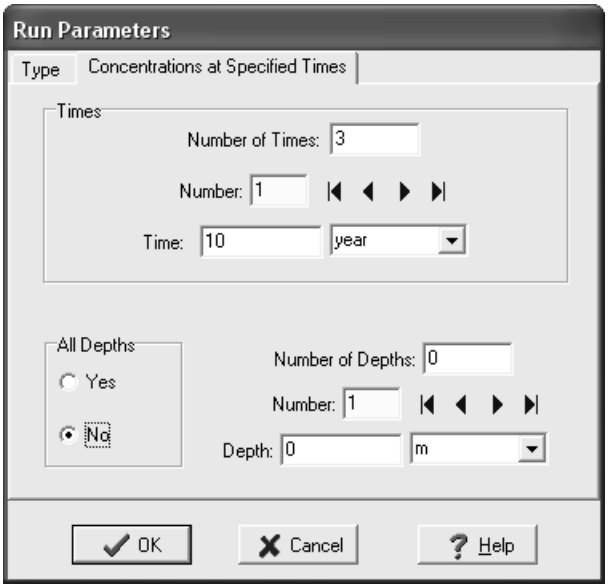
Time Units: The output units for the times can be selected using the combo-box. All of the units selected for the input data will then be converted to units consistent with these units and the output file generated will display these units.

Depth Units: The output units for the depths can be selected using the combo-box. All of the units selected for the input data will then be converted to units consistent with these units and the output file generated will display these units.

Concentration Units: The output units for the concentrations can be selected using the combo-box. All of the units selected for the input data will then be converted to units consistent with these units and the output file generated will display these units.

Concentrations at Specified Times

If the output type is Concentrations at Specified Times the tab below will appear. This option allows the user to calculate contaminant concentrations at selected depths and times. In addition, the flux (total mass/unit area) into the soil and into the base will also be calculated at the selected times.



The following parameters can be specified on this tab.

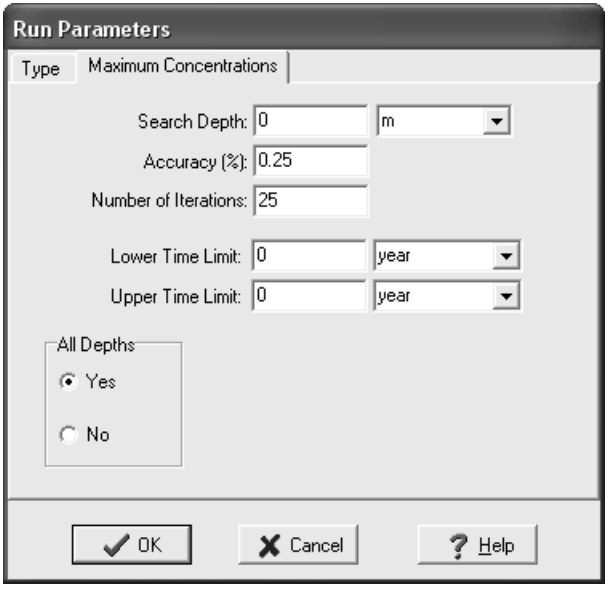
Times: The number of times at which to calculate the concentration of contaminant. The times should be entered in ascending order. The user can use the Next and Previous buttons to switch between times.

All Depths: This allows the user to select whether to calculate the concentrations at all depths (Yes), or at selected depths (No). If the user chooses all depths the concentrations will be calculated at the boundary between all sublayers. If the user wishes to calculate at selected depths then the user will be asked to specify the Number of Depths. After specifying the number of depths the user will be asked to specify the depths to calculate the concentrations.

Maximum Concentrations

If the top boundary condition is Finite Mass, then the contaminant concentration at any depth will reach a maximum value at a determinable time. After reaching this maximum value the concentration will decrease if the contaminant source is finite (i.e., the Reference Height of Leachate is finite), or the concentration will remain at the maximum value if the contaminant source is infinite (i.e., Constant Concentration top boundary condition). See Example 4.

When the output type is maximum concentrations then the Maximum Concentration tab below will appear.



The following parameters can be specified on this tab.

Search Depth: This is the depth for which to search for the maximum concentration, any depth between 0 and the maximum thickness of the deposit above the base boundary. The default depth is the depth of the base boundary. In searching for the maximum concentration the depth used will be the depth closest to the nearest sublayer interface. It is recommended that the user be sure to have a sublayer interface at the depth requested, or specify a large number of sublayers for the layer.

Accuracy: This is the accuracy to which the maximum base concentration is to be calculated, typically a value of 0.1% is used.

Number of Iterations: This is the maximum number of iterations to try to obtain the maximum base concentration to the required accuracy, typically a value of 25 is used. If the lower and upper time limits are well selected, convergence to an accuracy of 0.1% can usually be obtained within 10 iterations.

Upper and Lower Time Limits: The user needs to specify lower and upper time limits in which the maximum is expected to occur. If the lower and upper time limits do not bracket the time of the maximum, the program will usually adjust the time limits to include the time of the maximum. However, if both the specified limits are at times when there is negligible concentrations at the depth being considered, then the program may not be able to find a meaningful maximum.

If the top boundary condition is Constant Concentration and the lower time limit is close to or above the time of the maximum, the program will adjust the lower time limit until it is lower than the time of the maximum. When the top boundary condition is Constant concentration, the user is advised to check the results by using different values for the lower and upper time limits.

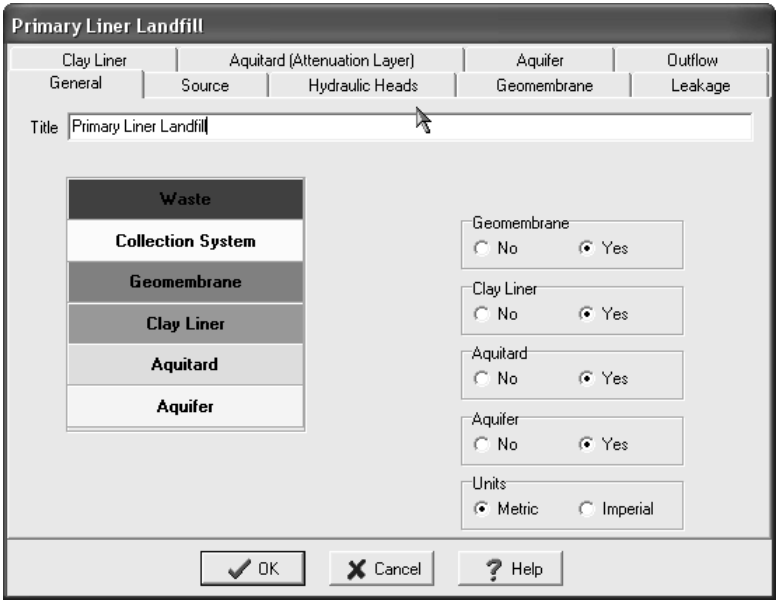
All Depths: This allows the user to select whether to calculate the concentrations at all depths (Yes), or at selected depths (No). If the user chooses all depths the concentrations will be calculated at the boundary between all sublayers. If the user wishes to calculate at selected depths then the user will be asked to specify the Number of Depths. After specifying the number of depths the user will be asked to specify the depths to calculate the concentrations.

Editing a Primary Liner Landfill Model

The Primary Liner (Subtitle D) Landfill option is used to quickly enter a landfill that may contain a leachate collection system, primary composite liner, aquitard, and aquifer. In this option the primary composite liner can be composed of a geomembrane and a primary liner. If the geomembrane is present the leakage through the geomembrane can be calculated using either equations by Rowe et. al., 2004; equations by Giroud et. al., 1992; or by specifying and equivalent hydraulic conductivity for the geomembrane.

Editing Primary Liner Landfill Data

To edit the data for a Primary Liner Landfill model select the Model Parameters menu item from the Data Entry menu. The Primary Liner Landfill form below will be displayed.



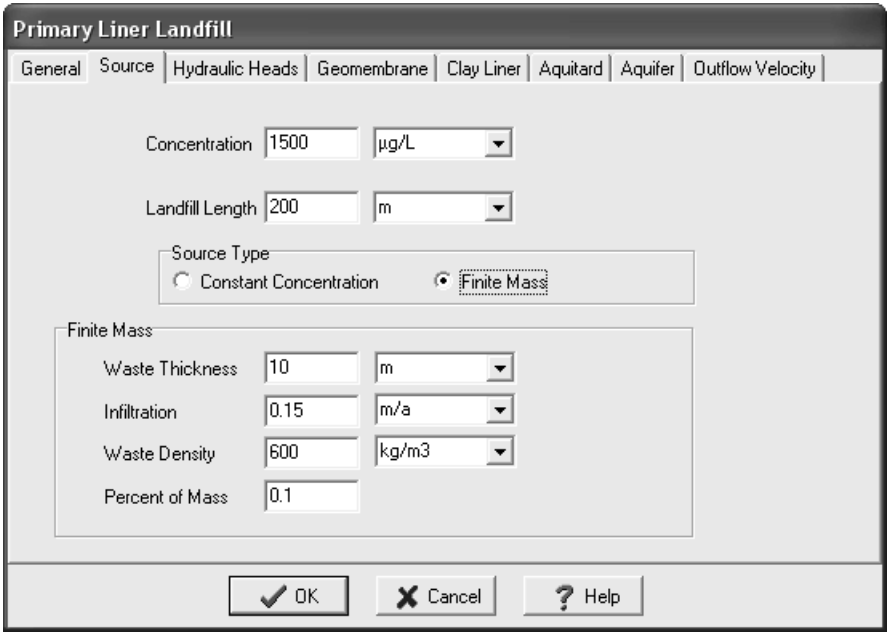
This form has several tabs for editing the general data, source, hydraulic heads, geomembrane, clay liner, aquitard, aquifer, and outflow velocity. Each of these tabs is described in the sections below.

General Tab

This tab, shown above, is for editing the title and selecting what layers are present in the model. The model may contain a geomembrane, clay liner, aquitard, or aquifer. In addition, the units to store the data needs to be specified as metric or Imperial.

Source Tab

This tab, shown below, is used to specify the data for the source of contaminants to be used as the top boundary condition.



The following data can be edited on this tab.

Concentration: Either the constant concentration or initial concentration depending on the source type.

Landfill Length: The length of the landfill in the direction of groundwater flow.

Source Type: Either Constant Concentration or Finite Mass. This option is used to specify the top boundary condition.

If the source type is Finite Mass the following data can also be edited:

Waste Thickness: This is the vertical thickness of the waste, and is used to calculate the mass of contaminant per unit area of waste.

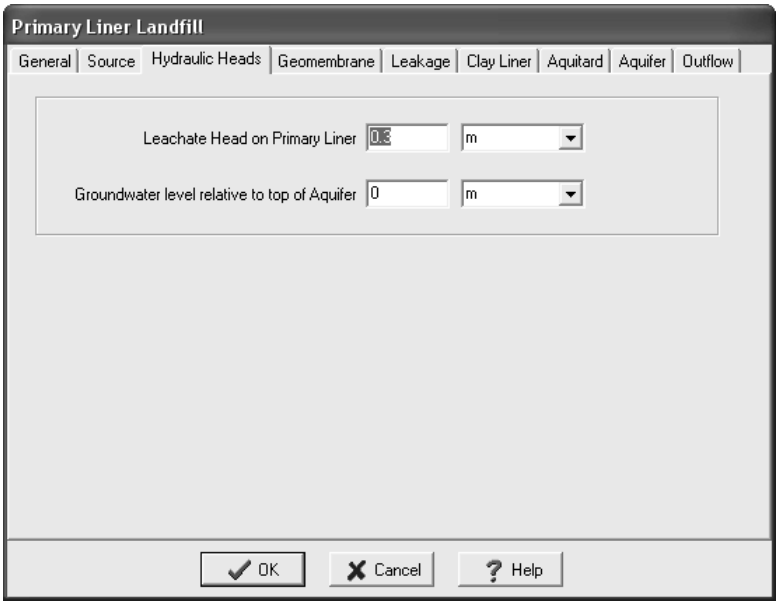
Waste Density: This is the apparent density of the waste (i.e. mass of waste per unit volume of the landfill).

Infiltration: The average infiltration through the landfill cover.

Percentage of Mass: The available (leachable) mass of contaminant in the waste per unit mass of waste (eg. mass of chloride in waste/total mass of waste).

Hydraulic Heads Tab

To calculate the Darcy velocity through the liners the hydraulic heads must be specified in this tab shown below.



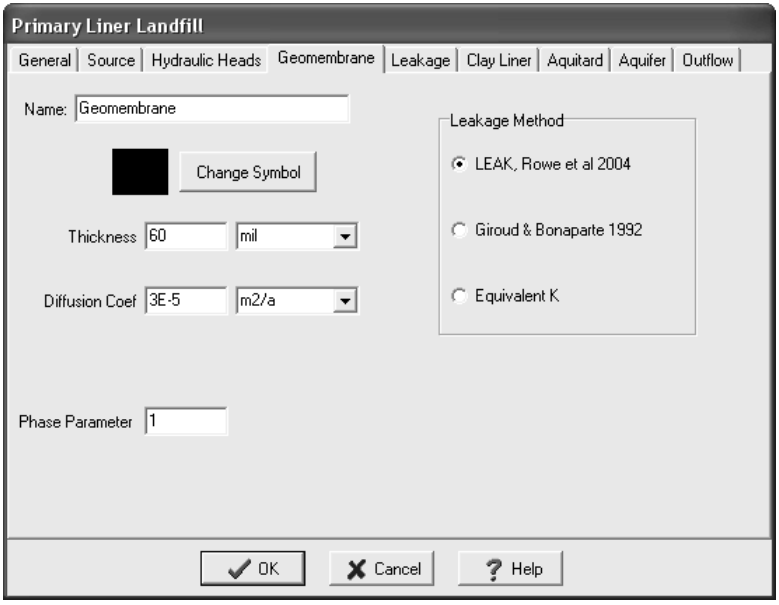
The following data can be edited on this tab:

Leachate Head on Primary Liner: The leachate head above the primary liner.

Groundwater level relative to top of aquifer: The groundwater level relative to the top of the aquifer, or if no aquifer is present the hydraulic gradient in the liner.

Geomembrane Tab

If a geomembrane is present this tab, show below, is used to edit the data for the geomembrane.



The following data can be edited on this tab:

Name: This is the name of the geomembrane layer. It is used only for drawing.

Symbol: This is the symbol used to draw the geomembrane. To change the symbol click on the Change Symbol button. A Change Symbol form will be displayed where you can change the bitmap library, bitmap, foreground color, background color, and fill size for the symbol.

Thickness: This is the thickness of the geomembrane.

Diffusion Coefficient: This is the diffusion coefficient of the geomembrane. See Rowe et al (2004) for a discussion of this parameter and a table of typical values.

Leakage Method: This is used to select the method for calculating the leakage through the geomembrane. It can be calculated using the equations by Rowe et. al., 2004 for either a circular hole in a geomembrane in direct contact with the foundation (similar assumptions to Giroud but allowing one to consider more variables) or for a wrinkle (or series of wrinkles) with holes (the most realistic situation for many applications); Giroud & Bonaparte, 1992; or specifying an equivalent hydraulic conductivity.

Phase Parameter: This is a dimensionless phase parameter, 'KH' or 'Sgf', as discussed in Chapter 2. The default is one; this represents no phase change. See Rowe et al (2004) for a discussion of this parameter and a table of typical values for common contaminants and HDPE geomembranes.

Equivalent K: If the method used to calculate the leakage through the geomembrane is Equivalent K, then this parameter will be displayed. This is the equivalent hydraulic conductivity of the geomembrane. If you are unsure what the value of this is, it is recommended to use a leakage rate landfill. Note: that the use of an equivalent K is a device for convenience of calculation and in no way represents the true leakage mechanisms. We recommend that you use the leakage equations. See Rowe et al (2004) for a discussion of leakage equations.

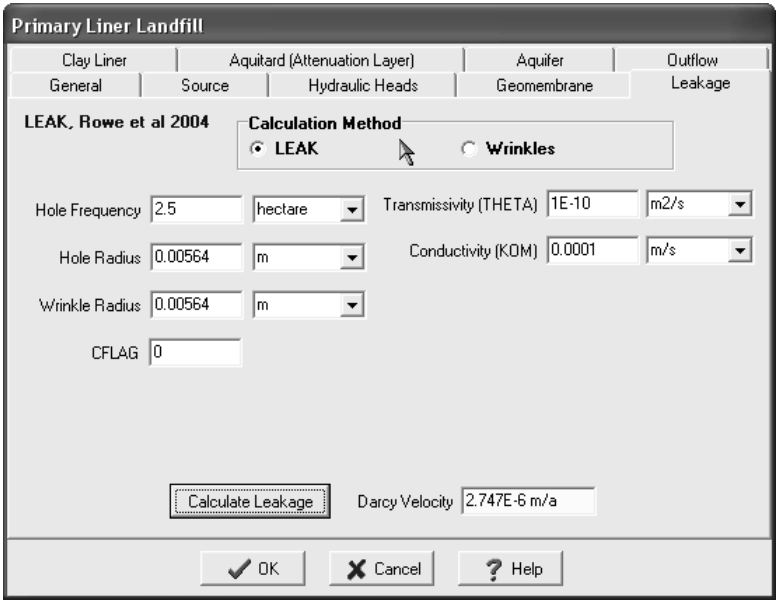
Rowe Leakage Tab

If the Leakage Type specified on the Geomembrane tab is Rowe et. al., 2004 one of the Rowe Leakage tabs below will be displayed. The tab displayed will depend upon the Calculation Method selected.

Calculation Method: The method used to calculate the leakage can be either:

LEAK - a circular hole in a geomembrane in direct contact with the foundation (similar assumptions to Giroud but allowing one to consider more variables) or

Wrinkles - for a wrinkle (or series of wrinkles) with holes (the most realistic situation for many applications).



LEAK

If the Calculation Method is selected as LEAK the tab above will be displayed. The following parameters can be specified:

Hole Frequency: This is the number of holes in the geomembrane per hectare or acre. The default is 2.5 holes per hectare. See Rowe et al (2004, Chapter 13) for a discussion of the number of holes per hectare.

Hole Radius: This is the average radius of the holes in the geomembrane. The default is 0.00564 m.

Wrinkle Radius: This is the optional average radius of the wrinkles in the geomembrane. The default is 0.00564 m. A "circular hole" can be either a wrinkle or a hole (both involve fluid in direct contact with the underlying clay liner. The only differences are (a) the wrinkle is bigger and (b) if it is a wrinkle then you also need a hole in the wrinkle and leakage through that hole can be controlled by benoulli's equation).

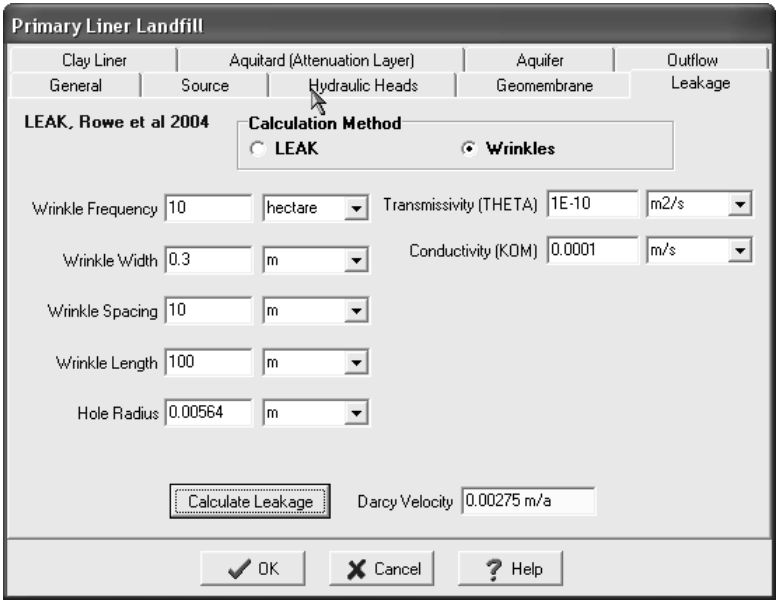
CFLAG: This is either 1 or 0 depending upon the boundary. CFLAG is 1 when head in the underlying aquifer is greater than zero, and is 0 when the head is greater than the thickness of the soil layer above the first aquifer.

Transmissivity (THETA): A detailed discussion of this is given by Rowe (1998) and the effect of this parameter is examined by Rowe et al (2004). Values used in examples include: $1.6x10^{-8}$ m^2/s for “good contact” between a geomembrane (GM) and compacted clay liner (CCL), $1.x10^{-7}$ m^2/s for “poor contact” between a GM and CCL, and $1.x10^{-10}$ m^2/s for “typical” contact between a GM and geosynthetic clay liner (GCL).

Conductivity (KOM): This is the hydraulic conductivity of the collection system or other material directly above the hole in the geomembrane. The default is $1x10^{-4}$ m/s.

Wrinkles

If the Calculation Method is selected as Wrinkles the tab on the next page will be displayed. It is suggested that you sketch up the proposed idealized wrinkle configuration to make sure that it makes physical sense. It is easier to work in term of hectares and remember that a hectare is 100m by100m square. When modelling Wrinkles one is modelling those wrinkles that have holes. The frequency gives the number of wrinkles with holes per hectare (or acre) while the spacing and length give the typical wrinkle dimensions. For the default 10 (100m long) wrinkles/ha the spacing must by 10m (100m/no of wrinkles=10). For 5 (100m) long wrinkles the spacing would be 20m (100m/no of wrinkles=5). But if the wrinkles were only 20m long one could have 12 of them (three row of 4) with a spacing of 25m (100m/4 wrinkles per row).



The following parameters can be specified on this tab:

Wrinkle Frequency: This is the number of wrinkles per hectare or acre. The default is 10 per hectare.

Wrinkle Width: This is the average width of the wrinkles. The default is 0.3 m.

Wrinkle Spacing: This is the average spacing between the wrinkles. The default is 10 m.

Wrinkle Length: This is the average length of the wrinkles. The default is 100 m.

Wrinkle Hole Radius: This the average radius of the holes in the wrinkles. The default is 0.00564 m. This will limit the leakage that can occur through a given wrinkle.

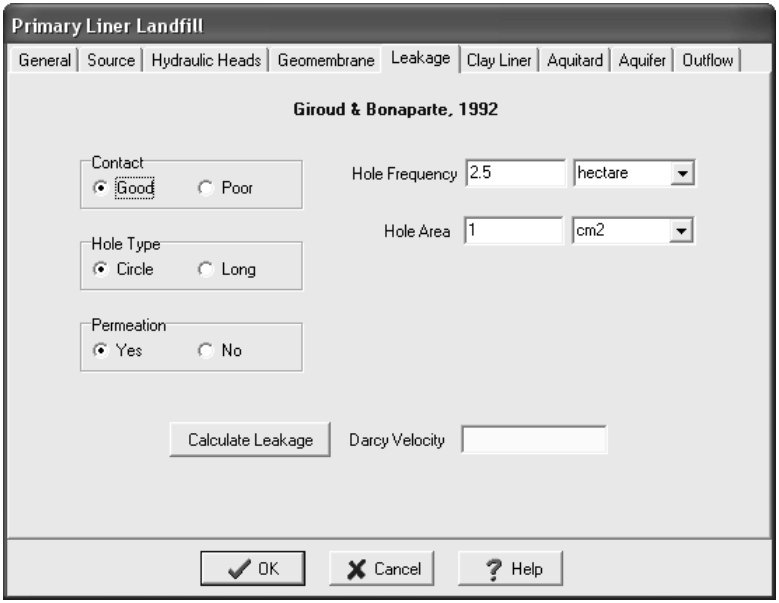
Transmissivity (THETA): This is the same as that used in the LEAK method and is described on the previous page.

Conductivity (KOM): This is the same as that used in the LEAK method and is described on the previous page.

Calculate Leakage: This button can be used to calculate and display the leakage (Darcy velocity) through the geomembrane.

Giroud Leakage Tab

If the Leakage Type specified on the Geomembrane tab is Giroud and Bonaparte., 1992 the Giroud Leakage tab below will be displayed.



The following parameters can be specified on this tab:

Contact: This is the type of contact between the geomembrane and the underlying material (either the clay liner or aquitard).

Hole Type: This is the type of holes in the geomembrane, either circles or long (rectangles).

Permeation: This is whether or not to consider permeation through the geomembrane.

Hole Frequency: This is the number of holes per hectare or acre. The default is 2.5 per hectare.

Hole Area: If the Hole Type is Circle then this parameter will be displayed. It is the average area of the holes in the geomembrane.

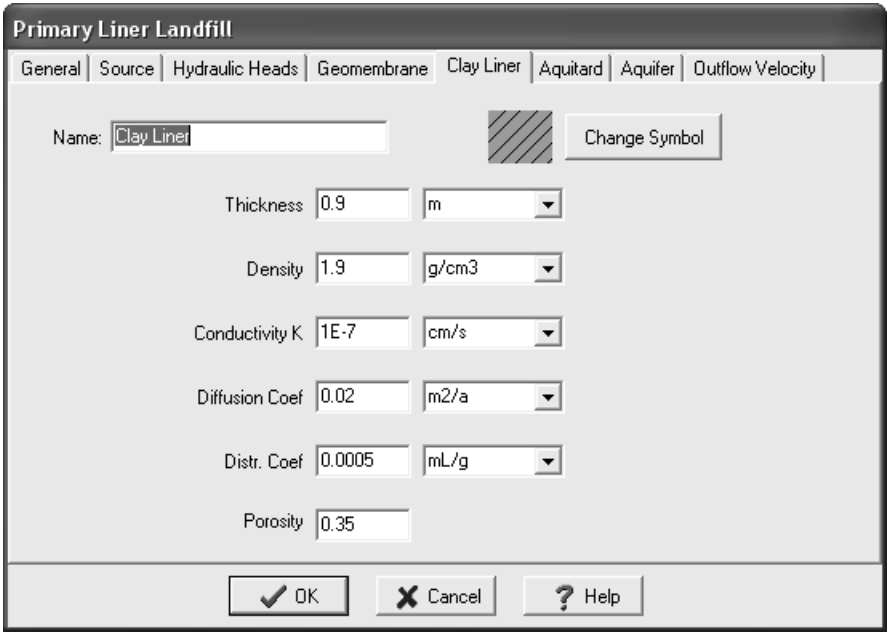
Hole Length: If the Hole Type is Long then this parameter will be displayed. It is the average length of the holes in the geomembrane.

Hole Width: If the Hole Type is Long then this parameter will be displayed. It is the average width of the holes in the geomembrane.

Calculate Leakage: This button can be used to calculate and display the leakage (Darcy velocity) through the geomembrane.

Clay Liner Tab

This tab, shown below, is used to edit the properties of the clay liner if it is present.



The following parameters can be edited on this tab:

Name: This is the name of the clay liner. It is used only for drawing.

Symbol: This is the symbol used to draw the clay liner. To change the symbol click on the Change Symbol button.

Thickness: This is the thickness of the clay liner.

Density: This is the density of the clay liner.

Equivalent K: The is the equivalent hydraulic conductivity of the clay liner. If you are unsure what the value of this is, it is recommended to use a leakage rate landfill.

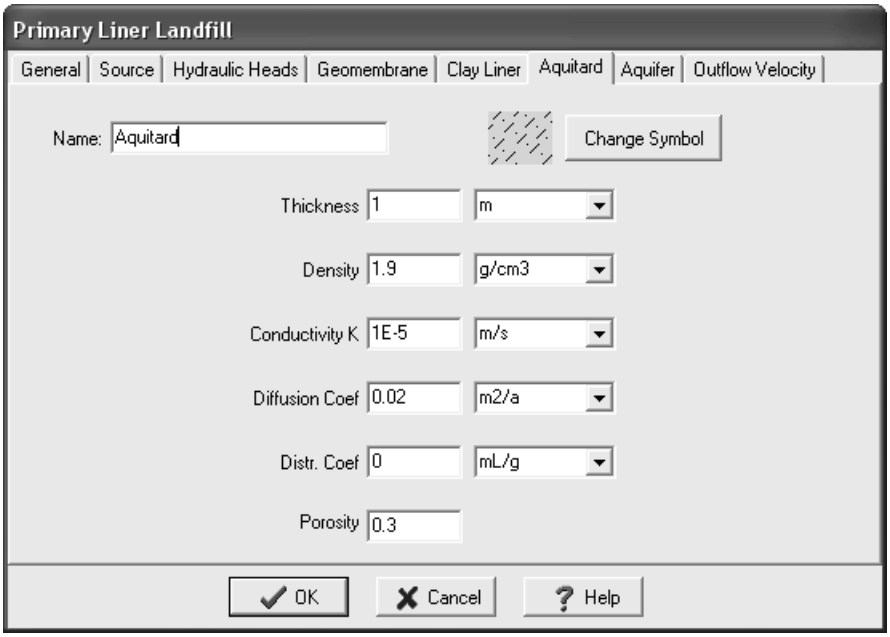
Diffusion Coefficient: This is the coefficient of hydrodynamic dispersion for the clay liner.

Distribution Coefficient: This is the distribution coefficient for the clay liner.

Porosity: The porosity of the clay liner.

Aquitard Tab

This tab is used to edit the properties of the aquitard if it is present. Note that this layer is an attenuation layer beneath the Clay liner. It is typically a layer with a hydraulic conductivity higher than that required for a clay liner ($1x10^{-9}$ m/s) but less than an aquifer.



The following parameters can be edited on this tab:

Name: This is the name of the aquitard. It is used only for drawing.

Symbol: This is the symbol used to draw the aquitard. To change the symbol click on the Change Symbol button.

Thickness: This is the thickness of the aquitard.

Density: This is the dry density of the aquitard.

Equivalent K: The is the equivalent hydraulic conductivity of the aquitard. If you are unsure what the value of this is, it is recommended to use a leakage rate landfill.

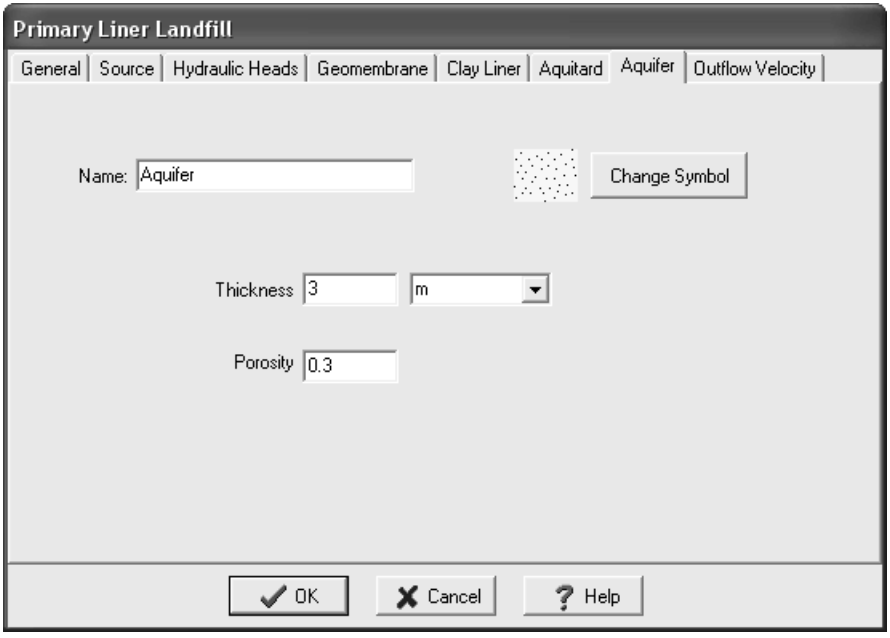
Diffusion Coefficient: This is the coefficient of hydrodynamic dispersion for the aquitard.

Distribution Coefficient: This is the distribution coefficient for the aquitard.

Porosity: The porosity of the aquitard.

Aquifer Tab

The properties of the aquifer can be edited on this tab if present.



The following parameters can be edited on this tab:

Name: This is the name of the aquifer. It is used only for drawing.

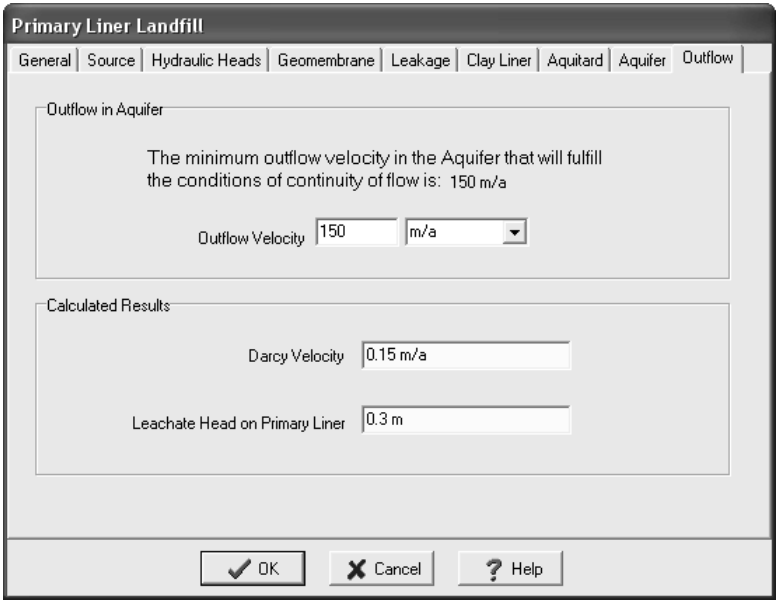
Symbol: This is the symbol used to draw the aquifer. To change the symbol click on the Change Symbol button. A Change Symbol form will be displayed where you can change the bitmap library, bitmap, foreground color, background color, and fill size for the symbol.

Thickness: This is the thickness of the aquifer.

Porosity: The porosity of the aquifer.

Outflow Velocity Tab

After this all of the information on the previous tabs has been entered the minimum horizontal outflow velocity in the aquifer will be calculated. You will then have the option of using this velocity or a higher velocity. In addition the calculated Darcy velocity and leachate head on the primary liner will be displayed.



Editing Run Parameters

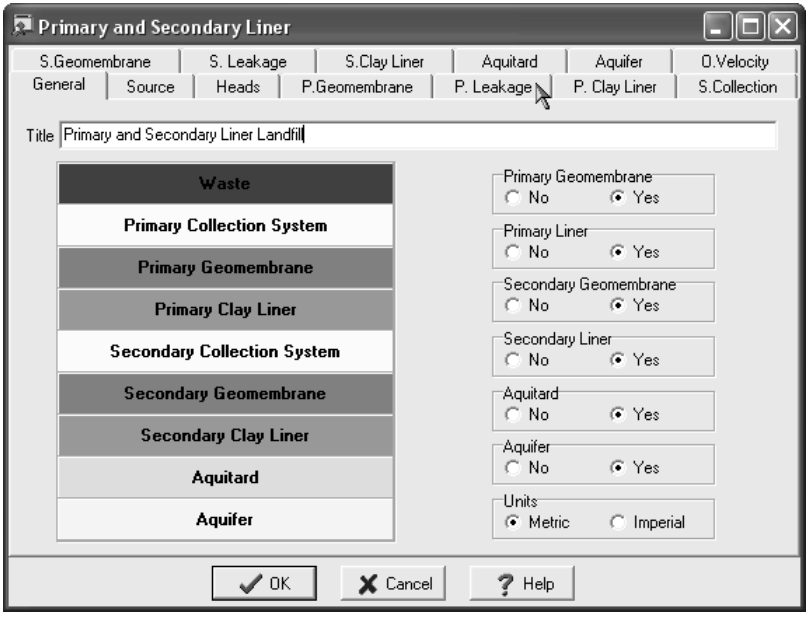
The data editing for the Run Parameters is the same as for a Normal Model and is described in that section above.

Editing a Primary and Secondary Liner Landfill Model

The Primary and Secondary Liner Landfill model is used to quickly enter a landfill that may contain a primary leachate collection system, primary composite liner, secondary leachate collection system, secondary composite liner, aquitard, and aquifer. In this option the composite liners can be composed of a geomembrane and/or compacted clay or GCL.

Editing Primary and Secondary Landfill Data

To edit the data for a Primary and Secondary Liner Landfill model select the Model Parameters menu item from the Data Entry menu. The Primary and Secondary Liner Landfill form below will be displayed.



This form has several tabs for editing the data for the model. Each of these tabs is described in the sections below.

General Tab

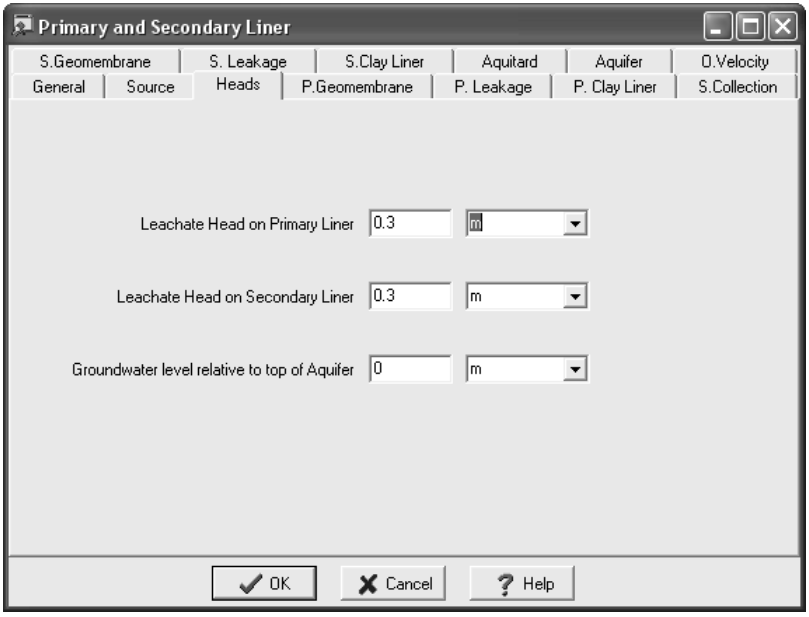
This tab is for editing the title and selecting what layers are present in the model. The model may contain a primary geomembrane, primary clay liner, secondary geomembrane, secondary clay liner, aquitard, or aquifer. A secondary leachate collection system is always assumed to exist in this landfill model. In addition, the units to store the data needs to be specified as metric or Imperial.

Source Tab

This tab is used to specify the data for the source of contaminants. It is the same as the Source tab for Primary Liner Landfills and is described in that section above.

Heads Tab

To calculate the Darcy velocity through the liners the hydraulic heads must be specified in this tab shown below.



The following data can be edited on this tab:

Leachate Head on Primary Liner: The leachate head above the primary liner.

Leachate Head on Secondary Liner: The leachate head above the secondary liner.

Groundwater level relative to top of aquifer: The groundwater level relative to the top of the aquifer, or if no aquifer is present the hydraulic gradient in the liner.

Primary Gemembrane Tab

This tab is used to specify the data for the primary geomembrane. It is the same as the Geomembrane tab for Primary Liner Landfills and is described in that section above.

Primary Leakage Tab

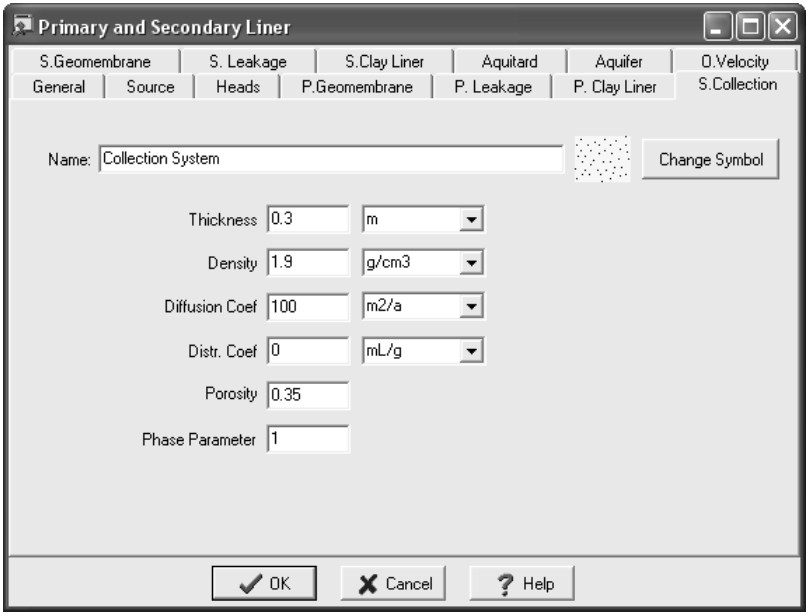
This tab is used to specify the data for the leakage through the primary geomembrane. It is the same as the Leakage tab for Primary Liner Landfills and is described in that section above.

Primary Clay Liner Tab

This tab is used to specify the data for the primary clay liner. It is the same as the Clay Liner tab for Primary Liner Landfills and is described in that section above.

Secondary Collection Tab

This tab, shown below, is used to specify the data for the secondary leachate collection system.



The following parameters can be edited on this tab:

Name: This is the name of the secondary collection system. It is used only for drawing.

Symbol: This is the symbol used to draw the secondary collection system. To change the symbol click on the Change Symbol button. A Change Symbol form will be displayed where you can change the bitmap library, bitmap, foreground color, background color, and fill size for the symbol.

Thickness: This is the thickness of the secondary collection system.

Density: This is the dry density of the secondary collection system.

Diffusion Coefficient: This is the coefficient of hydrodynamic dispersion for the secondary collection system.

Distribution Coefficient: This is the distribution coefficient for the secondary collection system.

Porosity: The porosity of the secondary collection system.

Phase Parameter: This is a dimensionless phase parameter as discussed i n Chapter 2. The default is one, that represents no phase change.

Secondary Gemembrane Tab

This tab is used to specify the data for the secondary geomembrane. It is the same as the Geomembrane tab for Primary Liner Landfills and is described in that section above.

Secondary Leakage Tab

This tab is used to specify the data for the leakage through the secondary geomembrane. It is the same as the Leakage tab for Primary Liner Landfills and is described in that section above.

Secondary Clay Liner Tab

This tab is used to specify the data for the secondary clay liner. It is the same as the Clay Liner tab for Primary Liner Landfills and is described in that section above.

Aquitard Tab

This tab is used to specify the data for the aquitard. It is the same as the Aquitard tab for Primary Liner Landfills and is described in that section above.

Aquifer Tab

This tab is used to specify the data for the aquifer. It is the same as the Aquifer tab for Primary Liner Landfills and is described in that section above.

Outflow Velocity Tab

After this all of the information on the previous tabs has been entered the minimum horizontal outflow velocity in the aquifer will be calculated. You will then have the option of using this velocity or a higher velocity. It is the same as the Outflow Velocity tab for Primary Liner Landfills and is described in that section above.

Editing Run Parameters

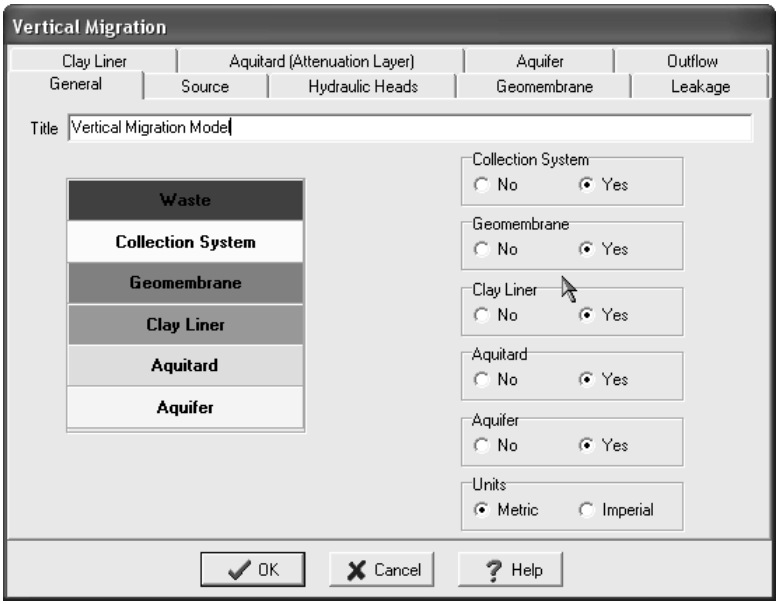
The data editing for the Run Parameters is the same as for a Normal Model and is described in that section above.

Editing a Vertical Migration Model

The Vertical Migration model is used to quickly enter a model for the vertical migration of a contaminant from a waste mass into an aquifer. The model may contain a primary composite liner, aquitard, and aquifer. In this option the primary composite liner can be composed of a geomembrane and a primary liner. If the geomembrane is present the leakage through the geomembrane is calculated using equations by Rowe et. al., 2004.

Editing Vertical Migration Data

To edit the data for a Vertical Migration model select the Model Parameters menu item from the Data Entry menu. The Vertical Migration form below will be displayed.



This form has several tabs for editing the data for the model. Each of these tabs is described in the sections below.

General Tab

This tab is for editing the title and selecting what layers are present in the model. The model may contain a collection system, geomembrane, clay liner, aquitard, or aquifer.

Source Tab

This tab is used to specify the data for the source of contaminants. It is the same as the Source tab for Primary Liner Landfills and is described in that section above.

Hydraulic Heads Tab

This tab is used to specify the hydraulic head data for the model. It is the same as the Heads tab for Primary Liner Landfills and is described in that section above.

Gemembrane Tab

This tab is used to specify the data for the geomembrane. It is the same as the Geomembrane tab for Primary Liner Landfills except that the Leakage Method is assumed to be Rowe et. al, 2004. It is described in that section above.

Leakage Tab

This tab is used to specify the data for the leakage through the geomembrane. It is the same as the Rowe Leakage tab for Primary Liner Landfills and is described in that section above.

Clay Liner Tab

This tab is used to specify the data for the clay liner. It is the same as the Clay Liner tab for Primary Liner Landfills and is described in that section above.

Aquitard Tab

This tab is used to specify the data for the aquitard. It is the same as the Aquitard tab for Primary Liner Landfills and is described in that section above.

Aquifer Tab

This tab is used to specify the data for the aquifer. It is the same as the Aquifer tab for Primary Liner Landfills and is described in that section above.

Outflow Velocity Tab

After this all of the information on the previous tabs has been entered the minimum horizontal outflow velocity in the aquifer will be calculated. You will then have the option of using this velocity or a higher velocity. It is the same as the Outflow Velocity tab for Primary Liner Landfills and is described in that section above.

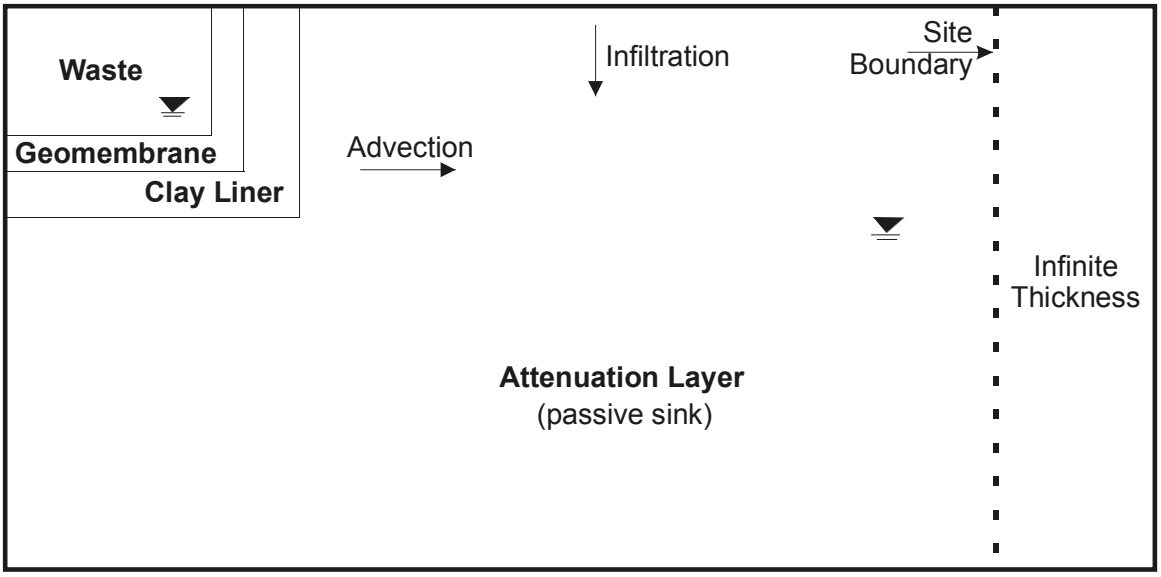
Editing Run Parameters

The data editing for the Run Parameters is the same as for a Normal Model and is described in that section above.

Editing a Horizontal Migration Model

The Horizontal Migration option is used to quickly enter a model for the horizontal migration of a contaminant from a waste mass to the site boundary. The model may contain a primary composite liner and an aquitard. In this option the primary composite liner can be composed of a geomembrane and a primary liner. If the geomembrane is present the leakage through the geomembrane is calculated using equations by Rowe et. al., 2004.

In this model the attenuation layer is modeled as a passive sink, where there is downward flow due to infiltration from precipitation and horizontal flow due to a difference in heads between the waste and the attenuation layer. The infiltration will have the effect of removing contaminant by acting as a passive sink with inflow. To avoid this effect set the infiltration into the attenuation layer to zero. Unless your really understand what you are doing, it is recommended that you set the infiltration to zero.

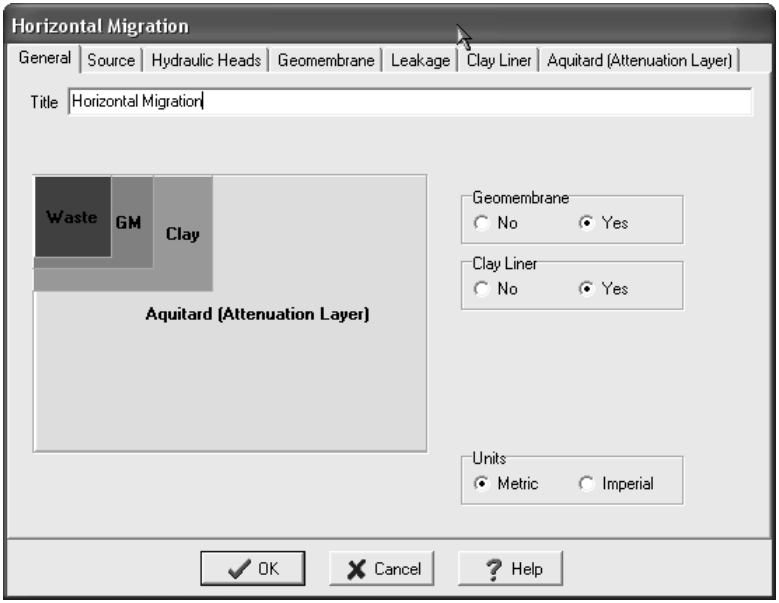


At the site boundary, the attenuation layer is assumed to continue indefinitely and is modelled as an Infinite Thickness boundary.

If a geomembrane is present the horizontal flow is calculated using the leakage through the geomembrane calculated using the equations by Rowe et. al., 2004. And if the geomembrane is not present the horizontal flow is calculated using the average gradient (using the head in the waste and the head in the attenuation layer) and the harmonic mean hydraulic conductivity between the head measurements.

Editing Horizontal Migration Data

To edit the data for a Horizontal Migration model select the Model Parameters menu item from the Data Entry menu. The Horizontal Migration form below will be displayed.



This form has several tabs for editing the data for the model. Each of these tabs is described in the sections below.

General Tab

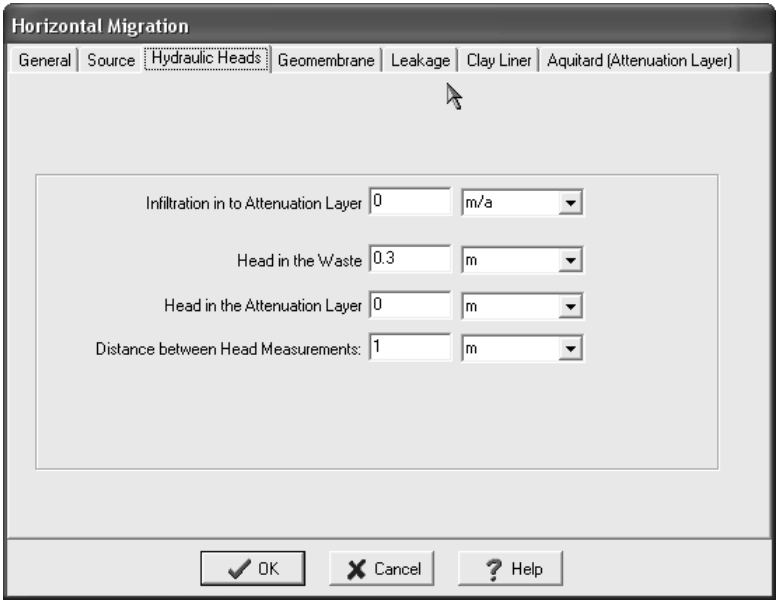
This tab is for editing the title and selecting what layers are present in the model. The model may contain a geomembrane, clay liner, or aquitard.

Source Tab

This tab is used to specify the data for the source of contaminants. It is the same as the Source tab for Primary Liner Landfills and is described in that section above.

Hydraulic Heads Tab

This tab is used to specify the hydraulic heads, infiltration in to the attenuation layer and distance between head measurements.



The following parameters can be specified on this tab:

Infiltration in to Attenuation Layer: This is the downward infiltration due to precipitation in the attenuation layer. The infiltration will have the effect of removing contaminant by acting as a passive sink with inflow. To avoid this effect set the infiltration into the attenuation layer to zero.

Head in the Waste: This is the head in the waste, relative to the same datum (depth) as the head in the attenuation layer.

Head in the Attenuation Layer: This is the head in the attenuation layer at a location outside of the barrier (liner system).

Distance between Head Measurements: This is the horizontal distance between the two head measurements above.

Gemembrane Tab

This tab is used to specify the data for the geomembrane. It is the same as the Geomembrane tab for Primary Liner Landfills and is described in that section above.

Clay Liner Tab

This tab is used to specify the data for the clay liner. It is the same as the Clay Liner tab for Primary Liner Landfills and is described in that section above.

Aquitard Tab

This tab is used to specify the data for the aquitard. It is the same as the Aquitard tab for Primary Liner Landfills and is described in that section above.

Editing Run Parameters

The data editing for the Run Parameters is the same as for a Normal Model and is described in that section above.

Editing Special Features

The Special Features menu lets you add and edit a variety of special features for the model. These features are:

- **Radioactive/Biological Decay**,
- **Initial Concentration Profile**,
- **Non-linear Sorption**,
- **Variable Properties**,
- **Passive Sink**,
- **Maximum Thickness**,
- **Print Mass into Base**,
- **Monte Carlo Simulation**,
- **Sensitivity Analysis.**

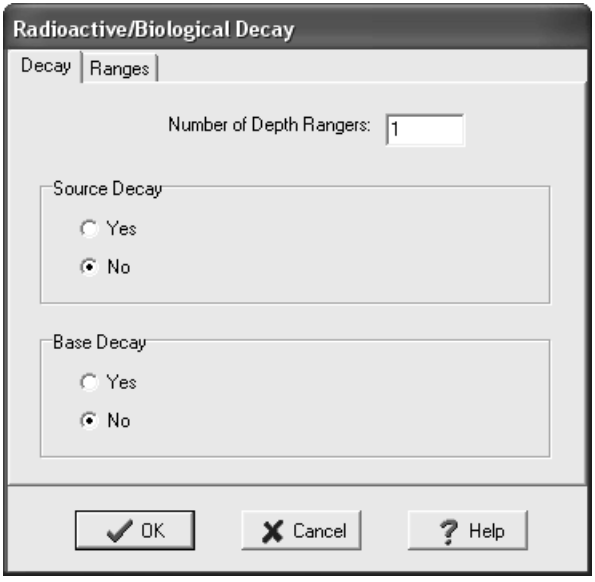
Radioactive/Biological Decay

This feature is used to model radioactive or biological decay of the contaminant species. The decay can take place in the source, the deposit, or the base. First order (exponential) decay is used for both radioactive and biological decay, eg.

$$c(t) = c(0)\ e^{-\lambda * t}$$

where,
c(t) = concentration at time t,
c(0) = initial concentration,
λ = decay constant = .693147/half life.

To add or edit radioactive or biological decay for a model select the Radioactive/Biological Decay menu item from the Special Features menu. The Radioactive/Biological Decay form below will be displayed. This form has two tabs, one for entering the decay settings and the other the depth ranges.



Decay Tab

The following can be edited on the Decay tab shown above.

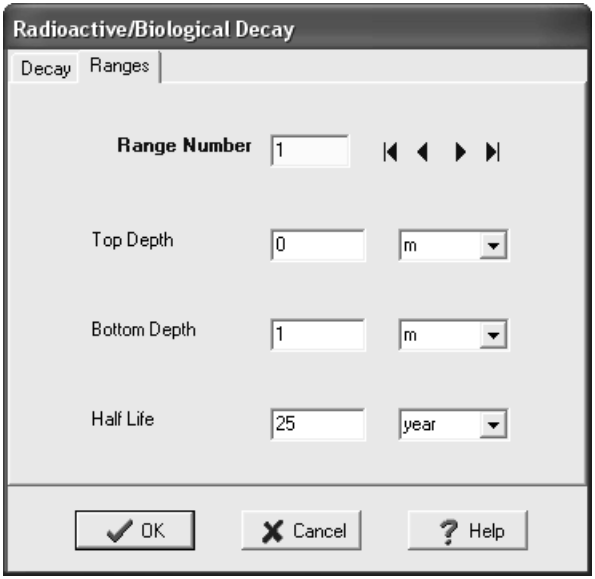
Number of Depth Ranges: This is the number of depth intervals throughout the model where you wish to specify different first order decay constants (eg. radioactive or biological).

Source Decay: This allows the user to select whether first order decay of contaminant will be modelled in the source. If selected the user will be asked to specify the half-life in the source. If not selected the half-life in the source is assumed to be infinite (i.e., no first order decay).

Base Decay: This allows the user to select whether first order decay will be modelled in the base of the deposit (eg. an underlying aquifer). If selected the user will be asked to specify the half-life in the base. If not selected the half-life in the base is assumed to be infinite (i.e., no first order decay).

Ranges Tab

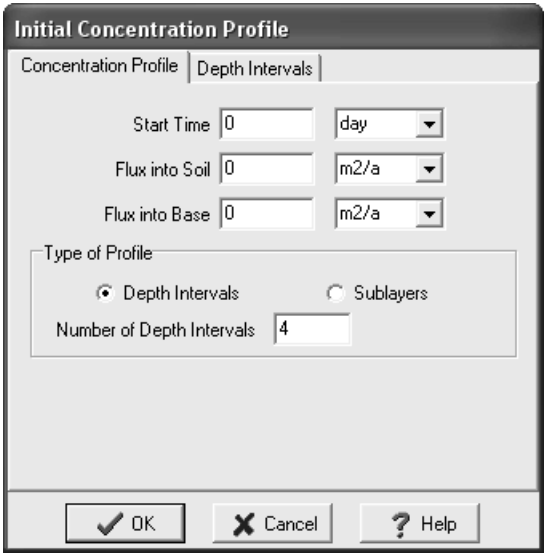
The Ranges tab shown on the next page is used to specify the Top Depth, Bottom Depth and Half-Life for each depth range. The specified half-life will be assigned to all layers between the top and bottom depths specified depths. Any layers which do not have a half-life explicitly specified are assumed to have an infinite half-life (i.e., no decay).



Initial Concentration Profile

This option allows the user to input an initial concentration profile at specified depths and also the initial flux into and out of the deposit. A situation where this may be appropriate, is if there is an initial background concentration in a sample, and one is modelling outward diffusion from the sample in a laboratory experiment (eg. see Barone et. al. 1990).

To edit this feature select the Initial Concentration Profile menu item from the Special Features menu. The Initial Concentration form below will be displayed. This form has two tabs, one for the profile parameters and one for the depth data.



Note: If any of the layers have fractures, this option cannot be used.

Warning: If using this option it is a good idea to specify a thin layer between zones where there are significant differences between initial concentration (eg. between the soil and a top or bottom reservoir in a diffusion test - see Example 8).

Concentration Profile Tab

The following information can be edited on this tab:

Start Time: This is the time for the start of the initial concentration profile, it is usually zero.

Flux into Soil: This is the flux of contaminant into the soil at the top boundary up to the start time (usually zero for a start time of zero).

Flux into Base: This is the flux of contaminant out of the soil into the base up to the start time (usually zero for a start time of zero).

Type of Profile: The initial concentration profile can be specified over depth intervals, or for every sublayer. For example, if there were only two different zones with different initial concentrations, then it would be best to specify the profile over these depth intervals. However, if the deposit had a continuously changing initial concentration profile with depth, then it would be better to specify the concentration for each sublayer (the number of sublayers is specified in the entry of the layer data).

If the profile type is Depth Intervals then the second tab will be for entering the Depth Intervals or if the profile type is Sublayers then the second tab will be for entering the Sublayer values.

In addition if the Print Mass into the base Special Feature is selected, the user will be asked for:

Mass into the Soil: This is the mass of contaminant into the soil at the top boundary up to the start time (usually zero for a start time of zero).

Mass into the Base: This is the mass of contaminant out of the soil into the base up to the start time (usually zero for a start time of zero).

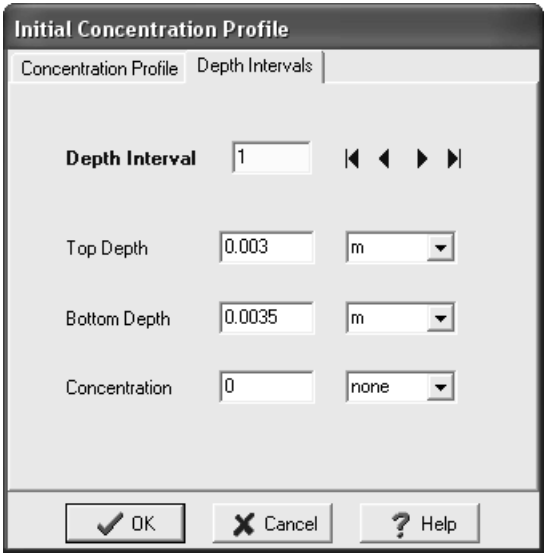
Depth Intervals Tab

If the profile type is Depth Intervals the Depth Intervals tab on the next page will appear. The following data can be edited on this tab, shown on the next page.

Top Depth: This is the top depth for the interval.

Bottom Depth: This is the bottom depth for the interval.

Concentration: This is the initial concentration for the interval.



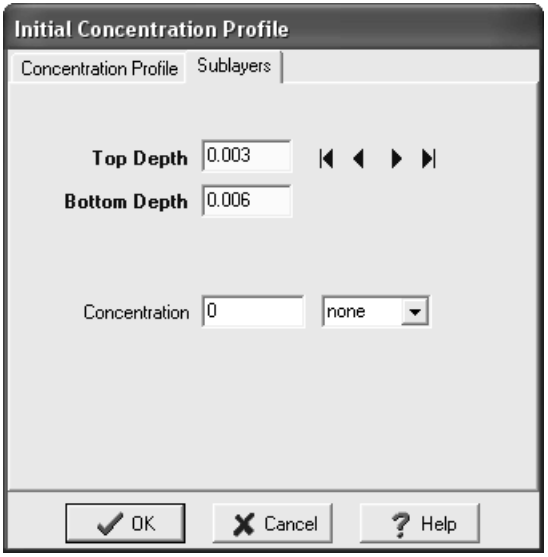
The First, Previous, Next, and Last buttons beside the Depth Interval can be used to navigate between depth intervals.

Sublayers Tab

If the profile type is Sublayers the Sublayers tab on the next page will appear. The following data can be edited on this tab, shown on the next page.

Concentration: This is the initial concentration for the sublayer.

The First, Previous, Next, and Last buttons beside the Depth Interval can be used to navigate between sublayer.


Initial Concentration Profile
Concentration Profile
Sublayers
Top Depth
0.003
Bottom Depth
0.006
Concentration
0
none
OK
Cancel
Help

Non-Linear Sorption

In addition to linear sorption, there are two types of non-linear sorption can be modeled. These are Freundlich or Langmuir.

Freundlich Non-Linear Sorption

Freundlich Non-Linear Sorption is represented by the relationship:

$$S = K_f \; c^E$$

where,
S = mass of solute sorbed per unit mass of soil,
K_f = empirically determined parameter,
E = empirically determined exponent.

The parameters K_f and E are best determined by performing batch tests on samples. When non-linear sorption is used, the program splits the deposit into sublayers and uses an iterative technique to determine an equivalent linear distribution coefficient (K) value of each layer. Since this is an empirical equation, particular care is required ensuring correct units, especially when E is not unity. Large errors can result from the use of mixed units or errors in converting from one set of units to another. This is done by:

(a) calculating the concentration at the top and bottom of each sublayer based on an estimated linear K value for each sublayer.

(b) determining a new secant K for each sublayer.

$$K = K_f \; c'^{E-1}$$

where,
c' = the average of the previous estimates of the concentration at the top and bottom of the sublayer.

(c) repeating steps (a) and (b) using the new estimate of K for each sublayer until the process converges.

The number of sublayers should be experimented with to ensure that the results obtained are sufficiently accurate.

Langmuir Non-Linear Sorption

Langmuir Non-Linear Sorption is represented by the relationship:

$$S = (S_m\ b\ \ c) / (1 + b\ \ c)$$

where,

S_m = solid phase concentration corresponding to all available sorption sites being occupied,

b = parameter representing the rate of sorption,

S = mass of solute sorbed per unit mass of soil,

c = concentration of solute.

The parameters S_m and b are best determined by performing batch tests on samples of the deposit.

When non-linear sorption is used, the program splits the deposit into sublayers and uses an iterative technique to determine an equivalent linear distribution coefficient (K) value of each layer. This is done by:

(a) calculating the concentration at the top and bottom of each sublayer based on an estimated linear K value for each sublayer.

(b) determining a new secant K for each sublayer:

$$K = (S_m\ \ b) / (1 + b\ \ c')$$

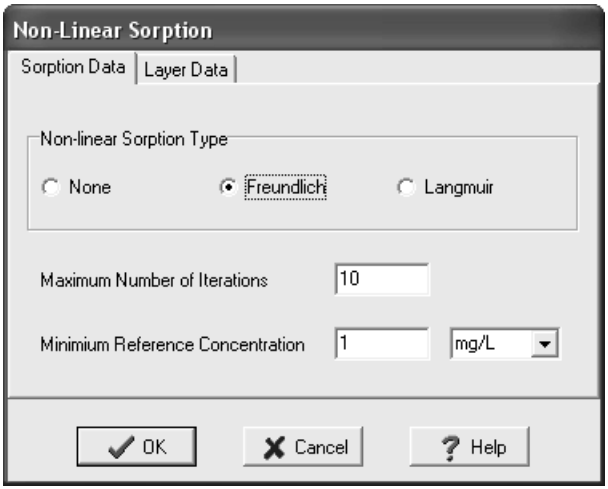
where,

c' = the average of the previous estimates of the concentration at the top and bottom of the sublayer.

(c) repeating steps (a) and (b) using the new estimate of K for each sublayer until the process converges.

The number of sublayers should be experimented with to ensure that the results obtained are sufficiently accurate.

To add or edit non-linear sorption select the Non-Linear Sorption menu item from the Special Features menu. The Non-Linear Sorption form below will be displayed. This form has two tabs one for selecting the type of sorption and the other for entering the sorption parameters for each layer.



The following parameters can be edited on this tab:

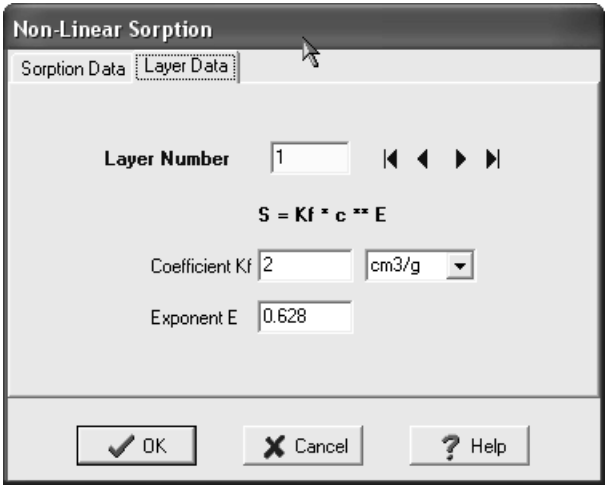
Non-Linear Sorption Type: This can be either None, Freundlich, or Langmuir. The layer parameters entered on the second tab will depend on the type of non-linear sorption.

Maximum Number of Iterations: The iterative procedure used to determine K, repeats until either the maximum change in concentration between iterations is less than 0.1% or the maximum number of iterations is reached.

Minimum Reference Concentration: This is the minimum value that will be used when calculating the secant (linear) distribution coefficient, K. If the average concentration in the sublayer is less than this value, then the Reference value is used.

Layer Data Tab

The data entered on the Layer Data tab will depend on the type of non-linear sorption specified. If the type of non-linear sorption is Freundlich the tab will appear as shown on the next page.

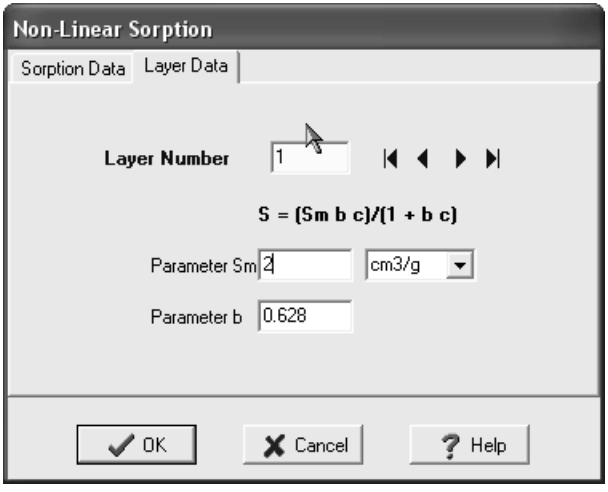


The following parameters can be edited on this tab:

Coefficient Kf: This is an empirically determined parameter for the layer.

Exponent E: This is an empirically determined parameter for the layer.

If the type of non-linear sorption is Langmuir the tab will appear as shown below.



The following parameters can be edited on this tab:

Parameter Sm: This is an empirically determined parameter for the layer.

Parameter b: This is an empirically determined parameter for the layer.

The First, Previous, Next, and Last buttons beside the Depth Interval can be used to navigate between layers..

Time Varying Properties

The program is normally capable of determining the concentrations any time without determining them at previous times. However, if there is a complex source concentration history or a change in velocities or layer properties with time then it is necessary to sequentially follow this history.

For example, the program can model a working landfill which experiences progressive failure of the leachate collection system and resulting buildup in the leachate mound (i.e., an increase in Darcy velocity) over a period of years [Rowe and Fraser, 1993a, 1993b].

This option allows the user to vary the source concentration, reference height of leachate, volume of leachate collected, rate of concentration increase, Darcy velocity, outflow velocity, dispersivity, layer properties, and decay rate with time.

The Variable Properties option implements a “time-marching” scheme, where the program stops and restarts the solution every time parameters are changed. In the basic mode of operation the accuracy of the solution is independent of the number of sublayers. **However, if the Variable Properties option is used then the accuracy of this procedure depends on the number of sublayers used in the model, and the user should experiment with the number of sublayers to ensure that the results obtained are sufficiently accurate** (see Examples 10, 11, and 15).

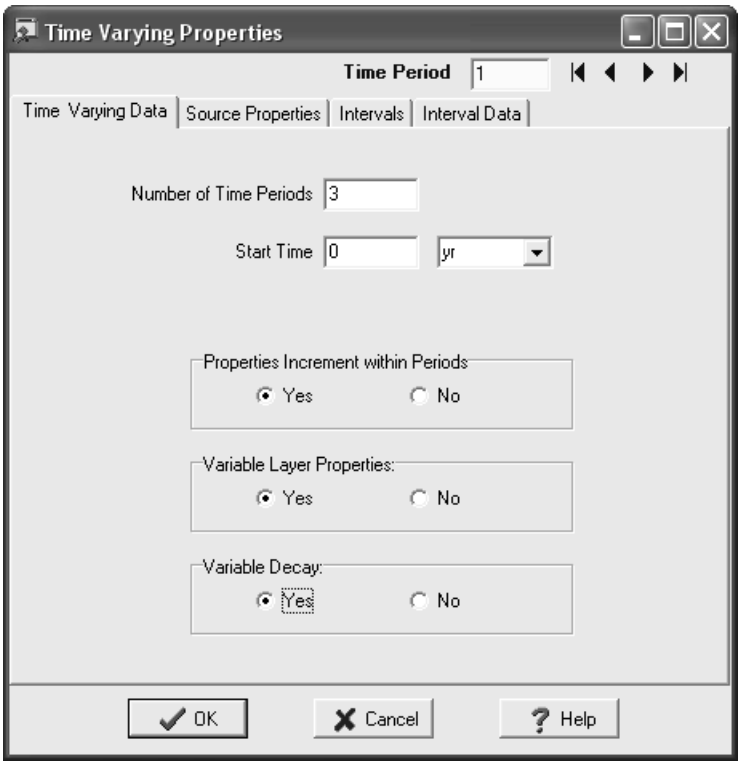
WARNING: This option should only be used by someone with the hydrogeologic and engineering background necessary to appreciate the subtleties associated with the physical situation and the steps necessary for appropriate modelling of the physical situation.

THIS OPTION SHOULD NOT BE USED FOR A PROJECT OF IMPORTANCE WITHOUT THE GUIDANCE OF THE PROGRAM DEVELOPERS.

To edit the variable properties for a model select the Variable Properties menu item from the Special Features menu. The Time Varying Properties form on the next page will be displayed.

This form will have between two and four tabs, depending upon the options selected on the first tab. If either Variable Layer or Variable Decay Properties is selected then the form will have four tabs. The two additional tabs will be for specifying the depth intervals for the Variable Layer and/or Variable Decay Properties.

At the top of the form the current Time Period is indicated and there are buttons to move to the first, previous, next, and last time period.



Time Varying Data Tab

The Time Varying Data tab shown above is used to specify the following:

Number of Time Periods: This is the number of time groups for which the user wishes to specify different properties.

Start Time: This is the start time of the first group, and is the time at which calculations begin (usually zero).

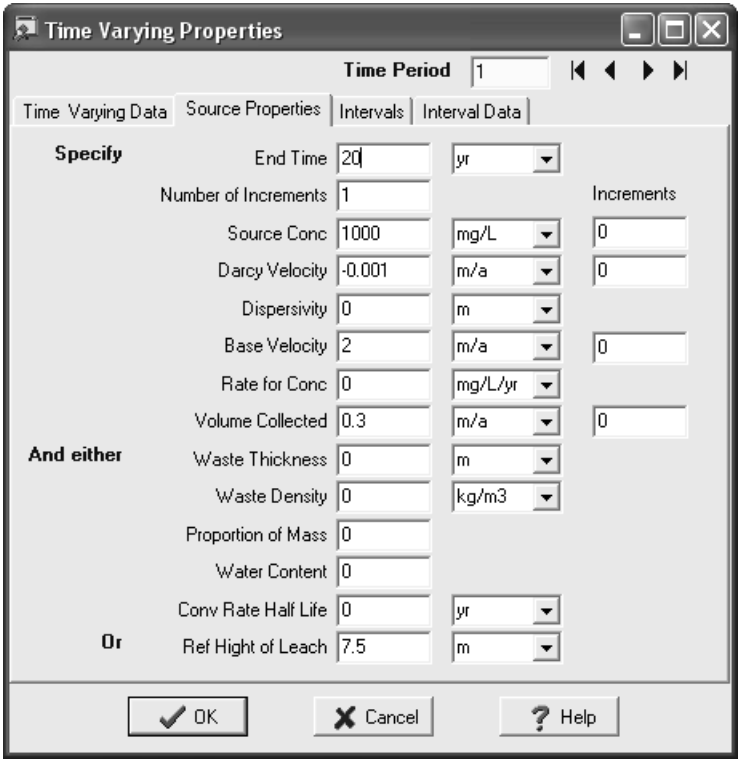
Properties Increment within Periods: This allows the user to choose whether the properties increment within time groups or are constant within time groups.If the properties increment within groups, the user can specify the number of increments and the increment size of the properties. For example, if the Darcy velocity increased linearly from .01 m/a to .11 m/a between 10 and 20 years, the user could specify 10 increments and a Darcy velocity increment of .01.

If however, the properties remain constant between time groups the user need only specify the values of the properties. For example, if the Darcy velocity was .01 m/a between 0 and 10 years and then .02 m/a between 11 and 30 years, the user could specify two groups the first from 0 to 10 years with a Darcy velocity of .01 m/a and the second from 11 to 30 years with a Darcy velocity of .02 m/a.

Variable Layer Properties: This option can be used to vary both source and layer properties with time. The model is divided into a number of depth intervals, and in each interval the user can specify the Diffusion Coefficient (or Coefficient of Hydrodynamic Dispersion), Porosity, Density, and Distribution Coefficient. If this option is selected two additional tabs will appear for the interval data.

Variable Decay: This option is used to vary the radioactive or biological decay with time. The source, base, and depth interval decay rates can be varied. If this option is selected two additional tabs will appear for the decay rates and interval data.

Source Properties Tab



The following can be edited on the Source Properties tab shown on the previous page.

End Time: This is the end time of the group, and will be the start time of the next group.

Number of Increments: This is the number of increments to use in sub-dividing the time period. The concentrations will be calculated for the times at the end of each increment, if there is only one increment specified for the group the time will be calculated at the end time. For example, if the group started at 0 years and ended at 20 years and the number of increments was 4, concentrations would be calculated at 5, 10, 15, and 20 years.

Source Concentration: This is the source concentration at the beginning of the time period. The calculated concentration from the end of the last period will be used if the user specifies a negative value for the source concentration. For the first time period the source concentration does not decrease until the end of the time period. To model a landfill with a depleting source, the concentration should be set for the first time period and then -1 should be used for the following time periods.

Note: The actual source concentration will vary with time due to the migration of contaminant into the soil and the collection of leachate. This is automatically handled by the program.

Source Concentration Increment: This is the increment size by which to increase the source concentration for each increment in the group. This field will only be shown if the Properties Increment within Periods option has been selected on the previous tab. If no additional mass is being added to the source then this should be zero.

Darcy Velocity: This is the Darcy velocity at the beginning of this time period. If an increment in Darcy velocity is specified, it will be added to this velocity to get the velocity at the start of the next increment.

Note: When using both the Variable Properties option and the Passive Sink option together, the Darcy velocity used is the product of the Darcy velocity specified in both of the options. For clarity, it is recommended the user specify the Darcy velocity on the Variable Properties option as 1, and vary the Passive Sink Darcy velocity.

Darcy Velocity Increment: This is the increment size by which to increase the Darcy velocity for each increment in the group. This field will only be shown if the Properties Increment within Periods option has been selected on the previous tab.

Dispersivity: This is the dispersivity for the model. When the Variable Properties option is used the dispersivity () and diffusion coefficient (D_{md}) can be specified independently.

Base Velocity: If the bottom boundary condition is fixed outflow, the user can specify the base horizontal Darcy velocity at the down-gradient edge of the landfill for the beginning of the time period.

Base Velocity Increment: This is the increment size by which to increase the base velocity for each increment in the group. This field will only be shown if the Properties Increment within Periods option has been selected on the previous tab.

Rate for Conc. If the top boundary condition is finite mass, the user can specify the rate at which the source concentration changes per year. For the case where there is no additional mass added or removed from the landfill this value should be set at zero.

Volume Collected: When the top boundary condition is finite mass, the user needs to specify the Volume of Leachate Collected for the beginning of the time period.

Volume Collected Increment: This is the increment by which to increase the volume of leachate collected during each time increment. If the infiltration through the cover of the landfill is constant, the increment in the volume of leachate collected should be equal and of opposite sign to the increment in the Darcy velocity.

If the top boundary condition is finite mass, the user can specify either:

- **Thickness of Waste**,
- **Waste Density**,
- **Proportion of Mass**,
- **Volumetric Water Content** of the waste,
- **Conversion Rate Half-Life** of the contaminant.

or:

- **Reference Height of Leachate**,

Thickness of Waste: This is the vertical thickness of the waste for the time period, and is used to calculate the mass of contaminant per unit area of waste.

Waste Density: This is the apparent density of the waste for the time period (i.e. mass of waste per unit volume of the landfill).

Proportion of Mass: The available (leachable) mass of contaminant in the waste per unit mass of waste for the time period (eg. mass of chloride in waste/total mass of waste).

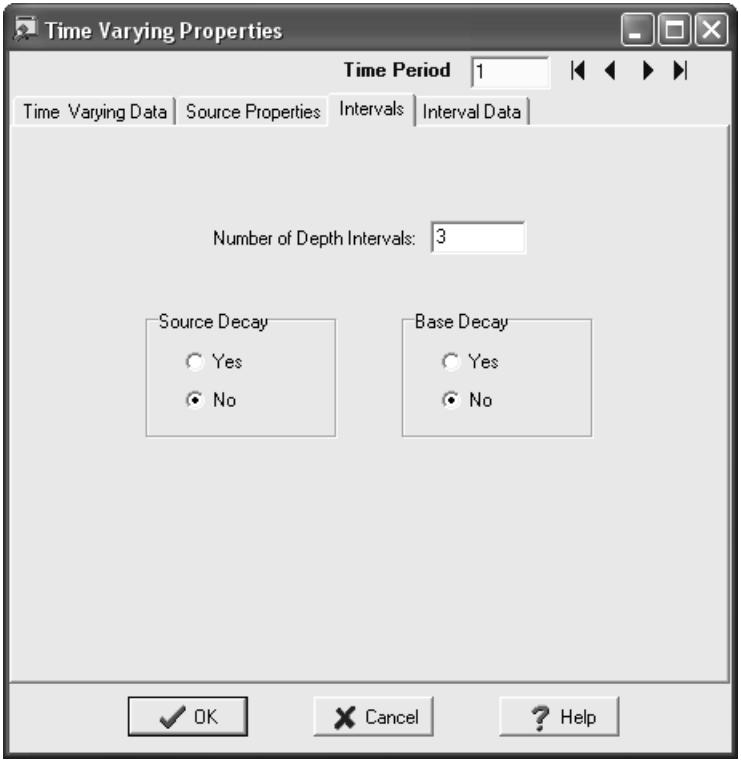
Volumetric Water Content: This is the volumetric water content of the waste for the time period.

Conversion Rate Half-Life: The generation coefficient is calculated based on the conversion rate half-life K, such that = ln 2 / K. A value of = 0 implies no generation of concentration with time. In the program = 0 is obtained by specifying K = 0 (this is the default case).

Reference Height of Leachate: The reference height of leachate represents the volume of leachate that would contain the total leachable mass of the contaminant of interest at the initial source concentration. Thus, the reference height (H_r) is equal to the mass of contaminant (M) per unit area divided by the initial source concentration (c_o) (i.e. $H_r = M/c_o$).

Intervals Tab

If either of the Variable Layer or Variable Decay options has been selected the Intervals tab below will be displayed.



The following data can be edited on this tab.

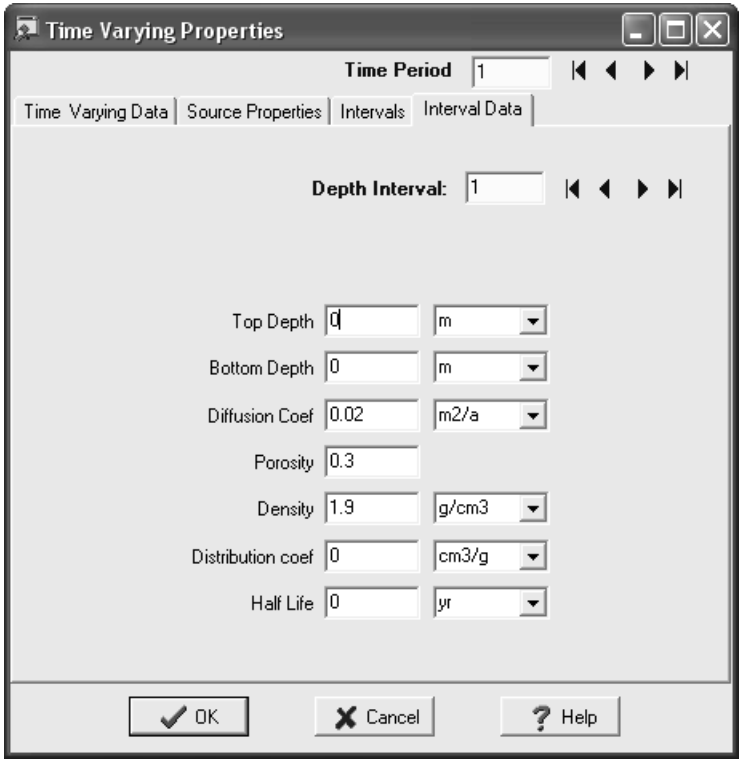
Number of Depth Intervals: This is the number of depth intervals for the varying layer or decay properties. The set of depth intervals should cover the entire thickness of the model. If both layer and decay properties vary, then the depth intervals must be the same for both properties.

Source Decay: If the Variable Decay option has been selected on the Time Varying Data tab, the Source Decay can be specified. This allows the user to select whether first order decay of contaminant will be modelled in the source for this time period. If selected the user will be asked to specify the half-life in the source. If not selected the half-life in the source is assumed to be infinite (i.e., no first order decay).

Base Decay: If the Variable Decay option has been selected on the Time Varying Data tab, the Source Decay can be specified. This allows the user to select whether first order decay will be modelled in the base of the deposit for this time period (eg. an underlying aquifer). If selected the user will be asked to specify the half-life in the base. If not selected the half-life in the base is assumed to be infinite (i.e., no first order decay).

Interval Data Tab

If either of the Variable Layer or Variable Decay options has been selected the Interval Data tab below will be displayed.



At the top of the tab the current Depth Interval is indicated and there are buttons to move to the first, previous, next, and last depth interval.

The following data can be edited on this tab:

Top Depth: This is the top depth of the depth interval and time period. The set of depth intervals should cover the entire thickness of the model.

Bottom Depth: This is the bottom depth of the depth interval and time period. The set of depth intervals should cover the entire thickness of the model.

Diffusion Coefficient: This is the diffusion coefficient for the depth interval and time period. This field will only be shown if the Variable Layer option has been selected on the Time Varying Data tab.

Porosity: This is the porosity for the depth interval and time period. It must be greater than 0 and less than or equal to 1. If the interval is being used to represent a geomembrane the porosity should be set to 1. This field will only be shown if the Variable Layer option has been selected on the Time Varying Data tab.

Density: The dry density of the depth interval and time period. This field will only be shown if the Variable Layer option has been selected on the Time Varying Data tab.

Distribution Coefficient: This is the distribution coefficient for the depth interval and time period. In the basic mode (ie. where Langmuir Non-linear sorption and Freundlich Non-linear sorption have not been selected) the sorption-desorption of a conservative species of contaminant is assumed to be linear. This field will only be shown if the Variable Layer option has been selected on the Time Varying Data tab.

Half-Life: This is the half-life for the depth interval and time period. This field will only be shown if the Variable Decay option has been selected on the Time Varying Data tab.

Passive Sink

This option allows the user to incorporate one or more passive sinks or a phase change with depth into a model. A passive sink is a depth interval in which there is a horizontal velocity which will have the effect of removing contaminant from beneath the landfill. Typically, a passive sink is used to represent intermediate aquifers or secondary leachate collection systems [Rowe and Fraser, 1993].

In the Passive Sink feature the model is divided into a number of depth intervals, and in each interval the user can specify the Darcy velocity, rate of removal, rate of inflow, and phase parameter. The set of depth intervals should cover the entire thickness of the model, between the top and bottom boundary. If a fixed outflow bottom boundary is used, the depth interval should stop at the top of the base aquifer (i.e., it should not include the base aquifer).

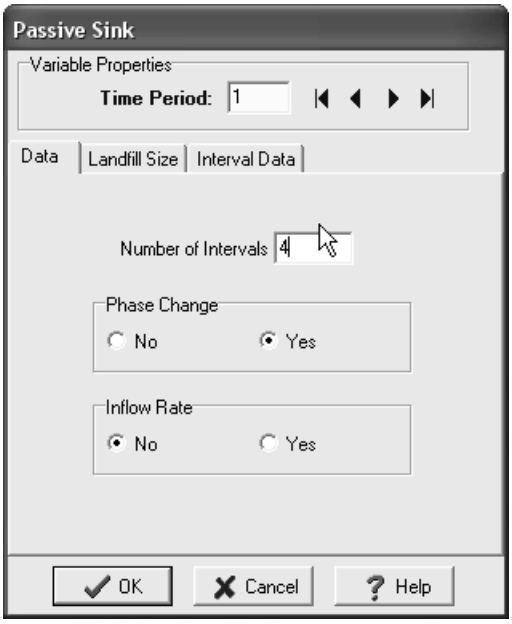
Note: When using both the Variable Properties option and the Passive Sink option, the Darcy velocity used is the product of the Darcy velocity specified in both of the options. For clarity, it is generally recommended the user specify the Darcy velocity on the Variable Properties option as 1, and vary the Sink Darcy velocity with time.

WARNING: This option should only be used by someone with the hydrogeologic and engineering background necessary to appreciate the subtleties associated with the physical situation and the steps necessary for appropriate modelling of the physical situation.

THIS OPTION SHOULD NOT BE USED FOR AN IMPORTANT PROJECT WITHOUT THE GUIDANCE OF THE PROGRAM DEVELOPERS.

To use this feature, select the Passive Sink option from the Special Features menu. The Passive Sink form on the next page will be displayed. This form has either two or three tabs, one for the sink data, one for the interval data, and if the bottom boundary condition is not Fixed Outflow one for the landfill size.

If the Variable Properties feature has also been selected then the Passive Sink properties will need to be specified for each time period. In this situation,, at the top of the form the current Time Period is indicated and there are buttons to move to the first, previous, next, and last time period. If the Variable Properties feature is not selected the time period information will not be displayed.



Data Tab

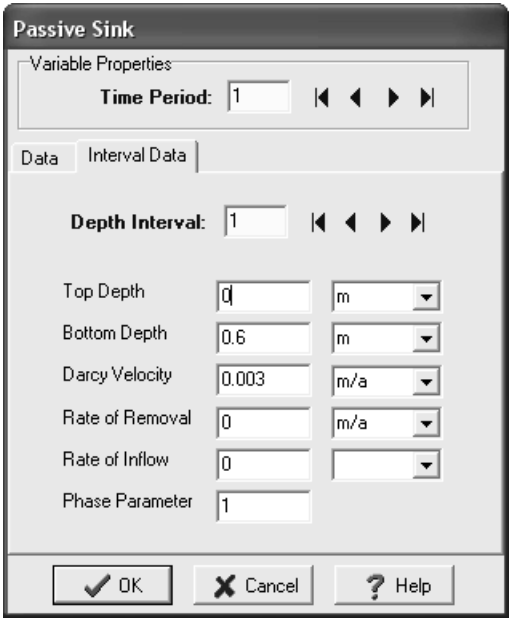
The following parameters can be edited on this tab (shown above):

Number of Intervals: This is the number of depth intervals for the passive sink and phase change properties. The set of depth intervals should cover the entire thickness of the model. If both passive sink and phase change properties are being specified, then the depth intervals must be the same for both properties. If the Time Varying Properties feature has also been selected, this will be the number of intervals for the selected time period.

Phase Change: This option is used to incorporate a phase change with depth. If the Time Varying Properties feature has also been selected, this will be the phase change option for the selected time period.

Inflow Rate: This option is used to specify the inflow rate with depth. If the Time Varying Properties feature has also been selected, this will be the inflow rate option for the selected time period.

Interval Data Tab



The following data can be entered on the Interval Data tab shown above:

Top Depth: This is the top depth of the depth interval. The set of depth intervals should cover the entire thickness of the model. If the Time Varying Properties feature has also been selected, this will be the top depth for the selected interval and time period.

Bottom Depth: This is the bottom depth of the depth interval. The set of depth intervals should cover the entire thickness of the model. If the Time Varying Properties feature has also been selected, this will be the bottom depth for the selected interval and time period.

Darcy Velocity: This is the Darcy Velocity for the depth interval. A negative value indicates an upward flow or flow in towards the source. If the Time Varying Properties feature has also been selected, this will be the Darcy velocity for the selected interval and time period.

Note: When using both the Variable Properties option and the Passive Sink option, the Darcy velocity used is the product of the Darcy velocity specified in both of the options. For clarity, it is recommended the user specify the Darcy velocity on the Variable Properties option as 1, and vary the Sink Darcy velocity.

Rate of Removal: This is the rate of removal of contaminant by the passive sink. If the Time Varying Properties feature has also been selected, this will be the Rate of Removal for the selected interval and time period. According to the principle of continuity of flow the rate of removal should be equal to:

$$Rr = (v_{a1} - v_{a2})\ L / h$$

where,

R_r = Rate of removal or outflow velocity (flow per unit area per unit time),

v_{a1} = Darcy velocity above the interval,

v_{a2} = Darcy velocity below the interval,

L = Landfill length,

h = thickness of the layer from which fluid is being removed.

An example would be a 600 m (L) long landfill with a 0.3 m thick (h) secondary leachate collection system. The Darcy velocity above the secondary leachate collection system is 0.01 m/a (v_{a1}), and below is 0.003 m/a (v_{a2}). The rate of removal is then:

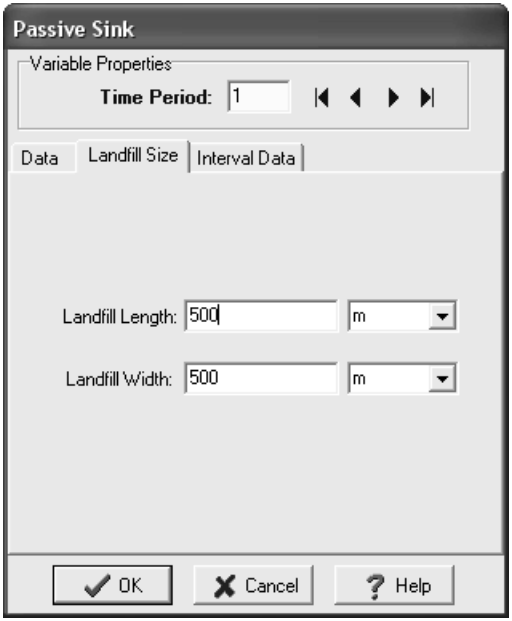
$$R_r = (0.01 - 0.003) * 600 / 0.3 = 14\ m^3/a/m^2 = 14\ m/a$$

Rate of Inflow: If the Inflow Rate option has been selected on the previous tab, the Rate of Inflow field will be shown. This is the rate of inflow into the passive sink. If the Time Varying Properties feature has also been selected, this will be the Rate of Inflow for the selected interval and time period.

Phase Parameter: If the Phase Change option has been selected on the previous tab, the Phase Parameter field will be shown. This is a dimensionless phase parameter as discussed i n Chapter 2. If the Time Varying Properties feature has also been selected, this will be the Phase Parameter for the selected interval and time period.

Landfill Size Tab

If the bottom boundary condition is not Fixed Outflow the Landfill Size tab (on the next page) will be shown. This tab is used to enter the length and width of the landfill. The landfill size is required for the passive sink calculating, even if the bottom boundary is not Fixed Outflow.

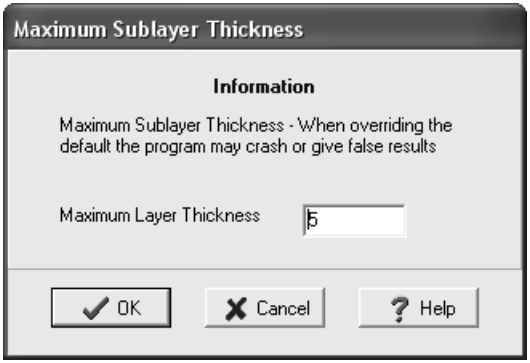

Passive Sink
Variable Properties
Time Period: 1
Data
Landfill Size
Interval Data
Landfill Length: 500
m
Landfill Width: 500
m
OK
Cancel
Help

Maximum Sublayer Thickness

This option allows the user to override the default maximum sublayer thickness of 5 units. The maximum sublayer thickness is set at 5 to avoid possible exponential overflow in the program, which can occur sometimes if the sublayers are too large.

If the maximum sublayer thickness is not changed then the number of sublayers is automatically increased if required to keep their thickness to less than 5. For example, if the layer thickness was 50m with 5 sublayers (giving a sublayer thickness of 10), the program will automatically adjust the number of sublayers to 10.

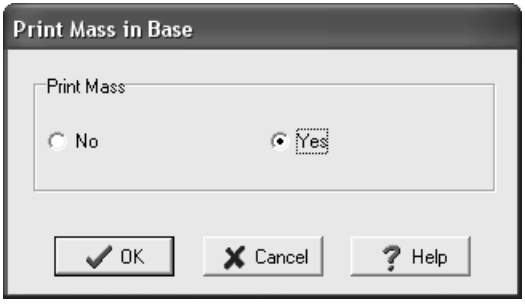
To select this option select the Maximum Sublayer Thickness menu item from the Special Features menu. The Maximum Sublayer Thickness form below will be displayed.



WARNING: When overriding this maximum sublayer thickness the user takes the risk that the program could crash or give false results.

Print Mass into Base

This option will print the total mass into the soil and the base, it is not normally used. To use this option select the Print Mass into Base menu item from the Special Features menu. The Print Mass into Base form below will be displayed.

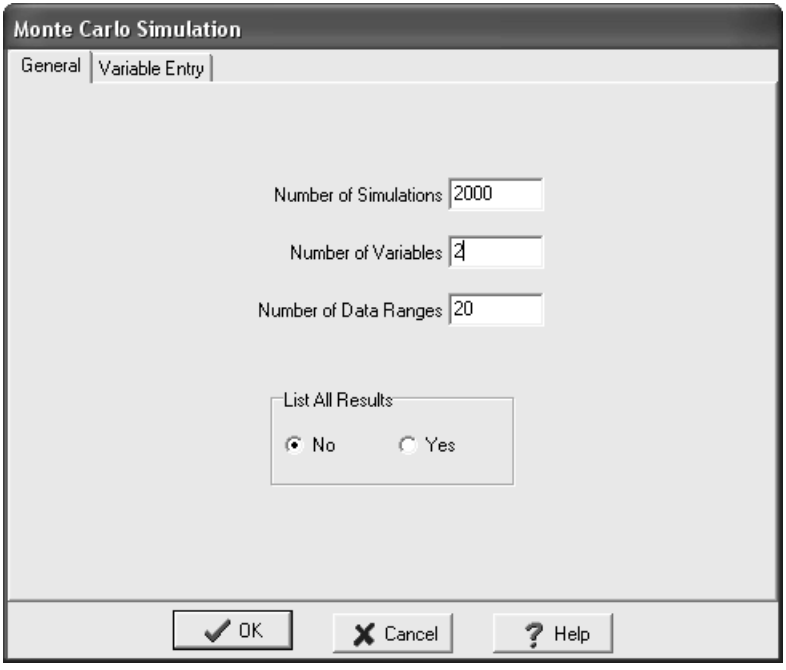


Monte Carlo Simulation

In the description of a soil deposit and a contaminant source (eg. a landfill) the values of all the input data are not always known with certainty. For example, the length of time that the primary leachate collection system will function before becoming clogged [Rowe and Fraser, 1993a, 1993b]. However, if the probability distribution can be estimated for the variable then Monte Carlo simulation can be used to predict the expected contaminant concentrations.

This feature supports the use of Monte Carlo simulation, to evaluate the effects of uncertainty in the values of some of the input data. The input data are described using probability distributions, from which data values are randomly chosen for each simulation pass. Numerous simulations are performed, and the results describe the probability distribution of the function being simulated, in this program the probability distribution is that of the peak concentration at various depths. Once the distributions of peak concentrations are determined, the user can make statistical predictions of the peak concentration; such as, the probability of the peak concentration exceeding a specific value.

To use this feature select the Monte Carlo Simulation menu item from the Special Features menu. The Monte Carlo Simulation form below will be displayed. This form has two tabs, one for the general data and one for the variable data.



General Tab

The following data can be entered on the General tab shown on the previous page.

Number of Simulations: This is the number of simulation analysis (realizations) to make, during each simulation the probability distributions of each variable are randomly sampled and the concentrations calculated. To obtain sufficiently reliable results at least 500 simulations are recommended, and for some cases between 1000 to 10000 simulations (realizations) may be required. The user should experiment with this parameter to determine the sensitivity of the results to the number of simulations. This is a computationally intensive feature, and the user should be aware that it may take anywhere from a few minutes to hours to complete with computation time depending on the speed of the computer, the number of simulations to be performed, the number of layers, and the Talbot integration parameter 'N'.

Number of Variables: This is the number of variables the user would like to incorporate into the simulation. Each **variable** represents one data item in the input data, and is described using a probability distribution. There can be up to 5 variables. The types of variables that can be changed are initial source concentration, Darcy velocity, layer thickness, layer diffusion coefficient, layer distribution coefficient, or Variable Properties end time.

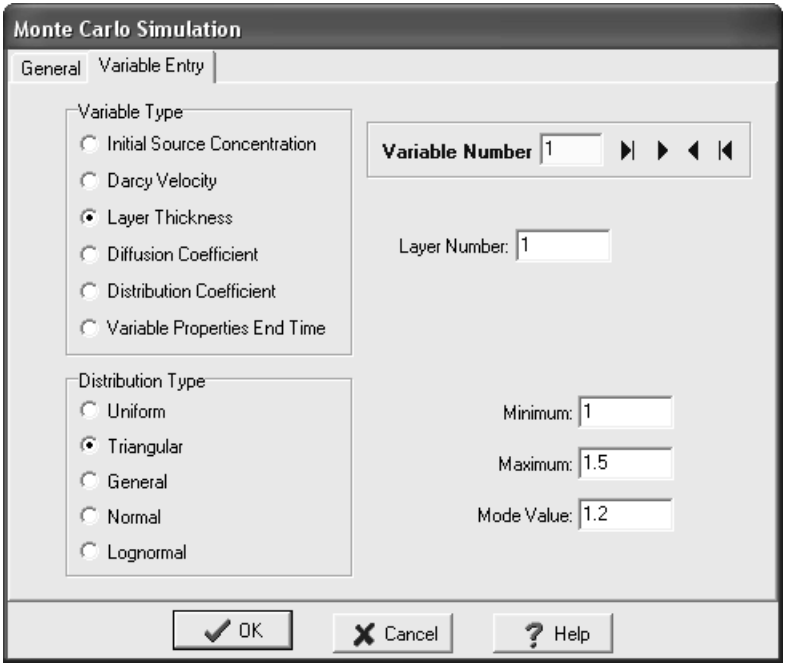
Number of Data Ranges: This is the number of data ranges to divide the probability distributions into in the output of the results of the simulation. A maximum of 20 ranges may be specified. This parameter does not affect the accuracy of the results and is for display purposes only.

List All Results: By selecting the 'Yes' response to this option, the user can obtain a list of all the simulation results. By selecting 'No' as a response, the user limits the output to a summary of the results. Listing all the results will include the results of every simulation pass in the output, the output file that is obtained may be extremely large. This option can be used to list all the results for a limited number of simulations (e.g. 10), to obtain a better idea of how the program is functioning, prior to running it for all the simulations.

Variable Entry Tab

The Variable Entry tab (shown on the next page) is used to describe each variable for the Monte Carlo simulation. The data that can be edited on this tab will depend upon the Variable Type and Distribution Type.

At the top of the tab the current Variable Number is shown and there are buttons to move to the first, previous, next and last variable.



Variable Type: This is the type of data for which the user wishes to enter a probability distribution. There are 6 types of data that can be used:

Initial Source Concentration: This is the Initial Source Concentration of the top boundary, and can only be used if the top boundary condition is NOT zero flux.

Darcy Velocity: This is the Darcy Velocity of the model.

Layer Thickness: This allows the user to specify a distribution for the thickness of a layer. The user will be asked to specify the layer for which to vary the thickness.

Diffusion Coefficient: This is the Diffusion Coefficient of a layer, the user will be asked to specify the layer for which to vary the Diffusion Coefficient.

Distribution Coefficient: This is the Distribution Coefficient of a layer, the user will be asked to specify the layer for which to vary the Distribution Coefficient. If the layer selected is fractured the distribution coefficient along the fracture will be varied.

Variable Properties End Time: This is the End Time of a Variable Properties Time Group, the user will be asked to specify the Time Group for which to vary End Time. When varying the end time of a time group the program will shift the end times of subsequent time groups to maintain their relative position, and will try to keep the end times of any previous time groups the same. This variable type will not show up if the Variable Properties feature has not been previously selected.

Distribution Type: A distribution must be entered for each variable, the distribution types can be different for different variables. There are five types of probability distributions that can be entered:

Uniform Distribution: This is used to specify a uniform probability distribution, in which there is the equal probability that a data point has any value between a specified minimum and maximum. The probability distribution curve would be a horizontal straight line. The user will need to specify the Minimum and Maximum data values.

Triangular Distribution: This is used to specify a triangular probability distribution function, where the probability is a maximum for a given value (mode) then linearly drops off on each side of this value. The probability distribution curve would be a triangle. The user will need to specify the Minimum, Mode, and Maximum data values.

General Distribution: This is used to specify a set of data and probability pairs that will be linearly interpolated. The probability distribution curve would be a continuous function, which is approximated by a set of straight line segments. The set of values must cover the entire data range, and the probability values do not have to sum to 1. The user will first be asked to specify the number of data value and probability pairs. Then, for the number of pairs entered previously the user will need to specify the data value and probability value.

Normal Distribution: This is used to specify a normal distribution for the variable. The distribution is symmetrical in shape similar to a bell, and is sometimes called a Gaussian distribution. To define the distribution the user needs to specify the mean and standard deviation.

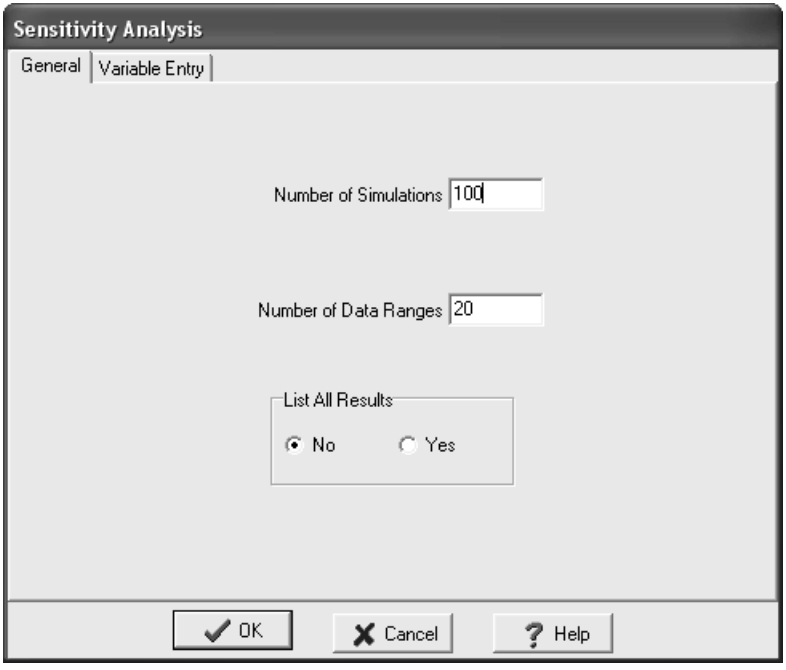
Lognormal Distribution: A lognormal distribution can be specified for the variable with this option. This distribution is similar to the normal distribution except that it is based on the logarithm of the random variable (eg. Darcy velocity or layer thickness). The user will need to specify the mean of the log of the variable and the standard deviation of the log of the variable.

Sensitivity Analysis

In the description of a soil deposit and a contaminant source (eg. a landfill) the values of all the input data are not always known with certainty. For example, the length of time that the primary leachate collection system will function before becoming clogged [Rowe and Fraser, 1993a, 1993b]. However, if the minimum and maximum values of the parameter can be estimated then Sensitivity Analysis can be used to predict the expected range of contaminant concentrations.

This feature is vary simular to Monte Carlo simulation; except, that when performing a Sensitivity Analysis only one variable may be evaluated at a time.

To use this feature select the Sensitivity Analysis menu item from the Special Features menu. The Sensitivity Analysis form below will be displayed. This form has two tabs, one for the general data and one for the variable data.



General Tab

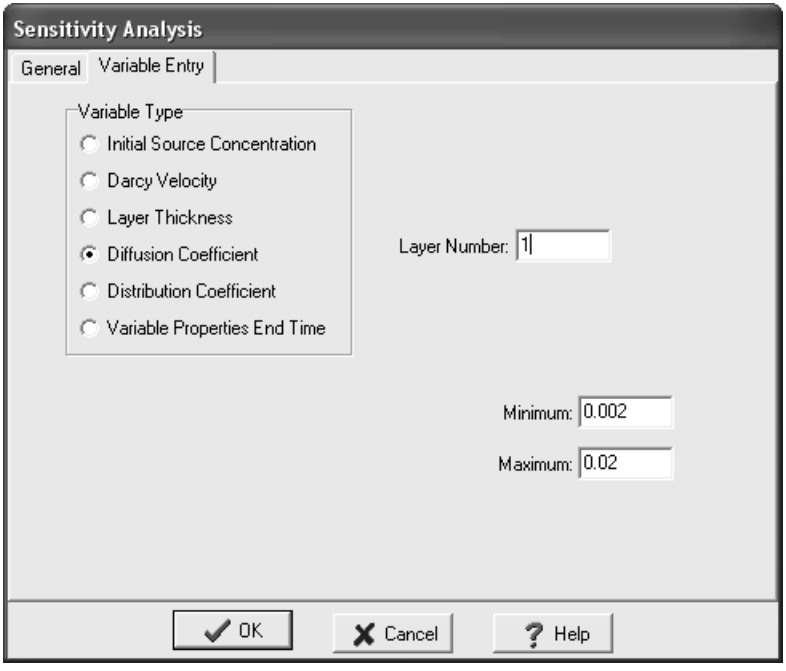
The following data can be entered on the General tab shown on the previous page.

Number of Simulations: This is the number of simulation analysis (realizations) to make. During the simulations the value of the variable will be interpolated linearly from the minimum to the maximum specified value. For example, if the number of simulations is 100 and the minimum value is 10 and the maximum value is 20, the variable will be incremented by 0.1 between simulations.

Number of Data Ranges: This is the number of data ranges to divide the output results into for the simulations. A maximum of 20 ranges may be specified. This parameter does not affect the accuracy of the results and is for display purposes only.

List All Results: By selecting the 'Yes' response to this option, the user can obtain a list of all the simulation results. By selecting 'No' as a response, the user limits the output to a summary of the results. Listing all the results will include the results of every simulation pass in the output, the output file that is obtained may be extremely large.

Variable Entry Tab



The Variable Entry tab on the previous page is used to describe the variable for the Sensitivity Analysis. The following data can be edited on this tab:

Variable Type: This is the type of data for which the user wishes to conduct the sensitivity analysis. There are 6 types of data that can be used:

Initial Source Concentration: This is the Initial Source Concentration of the top boundary, and can only be used if the top boundary condition is NOT zero flux.

Darcy Velocity: This is the Darcy Velocity of the model.

Layer Thickness: This allows the user to specify a distribution for the thickness of a layer. The user will be asked to specify the layer for which to vary the thickness.

Diffusion Coefficient: This is the Diffusion Coefficient of a layer, the user will be asked to specify the layer for which to vary the Diffusion Coefficient.

Distribution Coefficient: This is the Distribution Coefficient of a layer, the user will be asked to specify the layer for which to vary the Distribution Coefficient. If the layer selected is fractured the distribution coefficient along the fracture will be varied.

Variable Properties End Time: This is the End Time of a Variable Properties Time Group, the user will be asked to specify the Time Group for which to vary End Time. When varying the end time of a time group the program will shift the end times of subsequent time groups to maintain their relative position, and will try to keep the end times of any previous time groups the same. This variable type will not show up if the Variable Properties feature has not been previously selected.

Minimum Value: This is the minimum value for the variable. During the simulations the value of the variable will be interpolated linearly from the minimum to the maximum value.

Maximum Value: This is the maximum value of the variable. During the simulations the value of the variable will be interpolated linearly from the minimum to the maximum value.

Saving a Model

After a model has been created or edited it can be saved by either selecting the Save Model menu item from the Models submenu of the File menu or by clicking on the Save button on the Model toolbar.

The model can also be saved under a different name by using the Save As menu item from the Models submenu or the SaveAs button on the Model toolbar. The Save Model As form shown below will be displayed. Enter the new model title and then click on the Ok button to save the model under a new name.

Running a Model


After the data for the model has been entered, to calculate the concentrations with time and depth the model needs to be run. To run a model either select the Run menu item from the Execute menu or click on the Run button on the Model toolbar. The concentrations for the model will then be calculated and the results displayed on the output window.

Displaying Model Output

After a model has been run, the calculated concentrations can be displayed a number of ways. If they model did not use the Monte Carlo or Sensitivity Analysis special features these are:

 Concentration versus Depth Graph

 Concentration versus Time Graph

 Time versus Depth Graph

 Flux versus Time Graph

 Text Listing,.

If the model used the Monte Carlo or Sensitivity Analysis features they are:

 Distribution of the Maximum Concentration

 Distribution of the Time of the Maximum Concentration

 Distribution of the Variable Values

 Text Listing

The initial display after the model has been run is set in the Preferences for the program. However, this display can be changed by clicking on the appropriate button on the Output toolbar or by selecting the display type from the Output menu.

All of the graphs use the buttons on the Output toolbar to control their display and printing. These buttons are explained in detail in the Graphing Output section below.

The text listing has a different Output toolbar, that can be used to format, edit, save, and print the text listing. These functions are explained in detail in the Listing Output section below.

In addition, the model output can also be exported to a wide variety of formats; such as, database files, text files, html, Word, Excel, etc. This feature is described in the Exporting Output section below.

Graphing Output

Model output can be graphed in several different ways depending on wether the model used the Monte Carlo or Sensitivity Analysis special features. The majority of the functions on the model output toolbar behave the same for all of the graphs.

This display can be changed by clicking on the appropriate button on the Output toolbar or by selecting the display type from the Output menu. When one of these four graphs is used to display the model output, the Output toolbar will appear as shown below

The buttons on this toolbar can be used for the following:

The **Normal** button returns the graph editing to normal mode and deactivates the panning and rotation of the graph.

The **Rotation** button puts the graph into rotation mode, where the mouse can be used to rotate the graph up and down or left and right. To rotate the graph press and hold down the left mouse button.

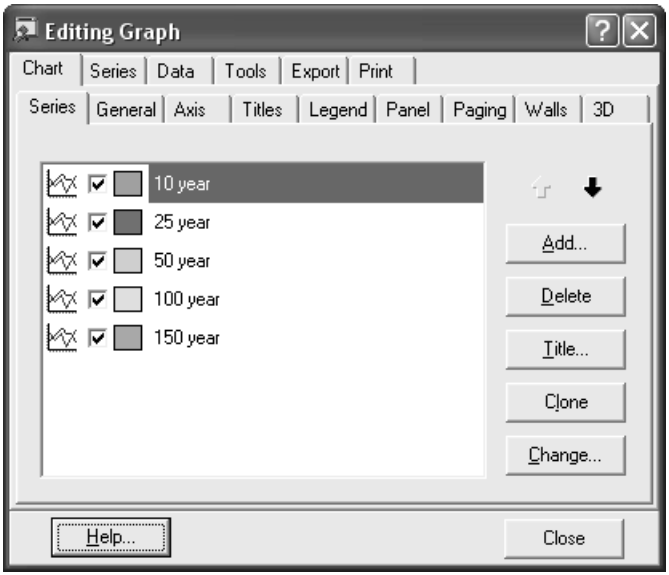
The **Pan** button puts the graph into pan mode, where the mouse can be used to move the graph up and down or left and right. To move the graph press and hold down the left mouse button.

The **Zoom** button puts the graph into zoom mode, where the mouse can be used to zoom in or out of the graph. To zoom in press and hold down the left mouse button while moving the mouse towards the top of the screen. To zoom out press and hold down the left mouse button while moving the mouse towards the bottom of the screen.

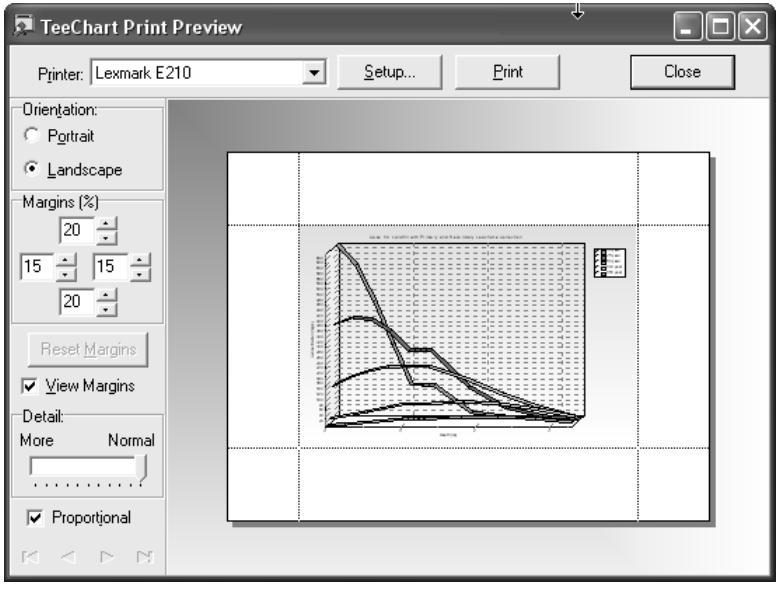
The **3D Depth** button is used to adjust the depth of the graph in 3D perspective mode. To adjust the depth, press and hold the left mouse button.

The **3D** button is used to toggle the graph in and out of 3D mode.

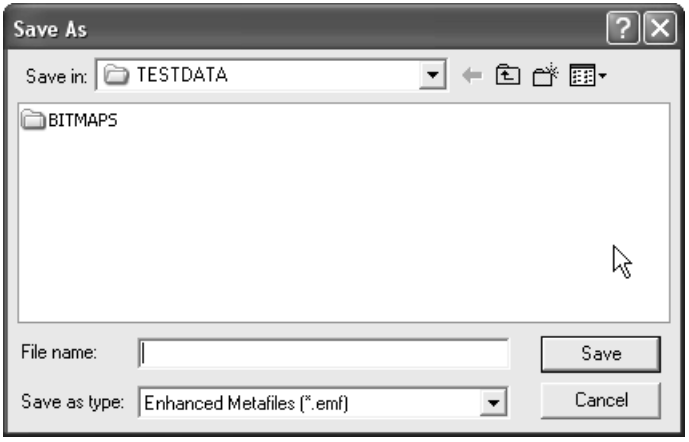
The **Edit** button is used to edit the format of the graph. When this button is pressed the Editing Graph form on the next page is displayed.For more information on how to use this form press the Help button.



The **Print** button is used to print the output. When the button is pressed the Print Preview form below is displayed. To send the output to the printer, press the Print button on the form.



The **Save** button will save the output to either a bitmap or metafile. When the button is pressed the Save As form below is displayed.



The **Concentration vs Depth** button switches the display of the output to a graph of concentration versus depth. If the Monte Carlo or Sensitivity Analysis special features are used this button will display a graph of the **Distribution of the Maximum Concentration**.

The **Concentration vs Time** button switches the display of the output to a graph of concentration versus time. If the Monte Carlo or Sensitivity Analysis special features are used this button will display a graph of the **Distribution of the Time of the Maximum Concentration**.

The **Time vs Depth** button switches the display of the output to a graph of time versus depth. If the Monte Carlo or Sensitivity Analysis special features are used this button will display a graph of the **Distribution of the Variable Values**.

The **Flux vs Time** button switched the display of the output to a graph of flux versus time.

The **Listing** button switched the display of the output to a text listing.

Listing Output

In addition to the above graphs, the model output can be displayed as a text listing by clicking on the Listing button or selecting it from the Output menu. The display will then change to a listing and the Output toolbar will appear as shown below.

The buttons on this toolbar can be used for the following:

The **Font Type** box can be used to change the font type of the selected text.

The **Font Size** box can be used to change the size of the selected text.

The **Font Color** box can be used to change the color of the selected text.

The **Font Background Color** box can be used to change the background color of the selected text.

The **Background Color** box can be used to change the background color.

The **Bold** button is used to toggle bold text on or off.

The **Italic** button is used to toggle italic text on or off.

The **Underline** button is used to toggle underline text on or off.

The **Superscript** button is used to toggle superscript text on or off.

The **Subscript** button is used to toggle subscript text on or off.

The **Left Justify** button is used to left justify the selected text.

The **Center Justify** button is used to left justify the selected text.

The **Full Justify** button is used to full justify the selected text.

The **Right Justify** button is used to right justify the selected text.

The **Save** button is used to save the output listing to a file.

The **Print** button is used to print the output listing


The **Print Setup** button is used to set printer options.


The **Undo** button is used to undo the previous command.


The **Select All** button is used to select all of the text in the listing.


The **Cut** button is used to cut the selected text to the clipboard.


The **Copy** button is used to copy the selected text to the clipboard.


The **Paste** button is used to paste the text from the clipboard to the listing.


The **Find** button is used to find specified text in the listing.


The **Replace** button is used to replace specified text in the listing.


The **Concentration vs Depth** button switches the display of the output to a graph of concentration versus depth.


The **Concentration vs Time** button switches the display of the output to a graph of concentration versus time.


The **Time vs Depth** button switches the display of the output to a graph of time versus depth.


The **Flux vs Time** button switched the display of the output to a graph of flux versus time.


The **Listing** button switched the display of the output to a text listing.

Exporting Output

The output from the model can be exported to one of 19 different file formats in either Time vs Concentration or Depth vs Concentration format. To export the output select either Time vs Concentration or Depth vs Concentration from the Export submenu from the Output menu. The Export Output wizard will be displayed. The wizard takes you through an 8-step process in which you can select the file type and other formatting options.

Time vs Concentration

This option will output the data in the format below; where T1 refers to time 1, C11 refers to the concentration at time 1 and depth 1; C12 refers to the concentration at time 1 and depth 2, etc.

T1 C11 C12 C13 C14 ....
T2 C21 C22 C23 C24 ....
....

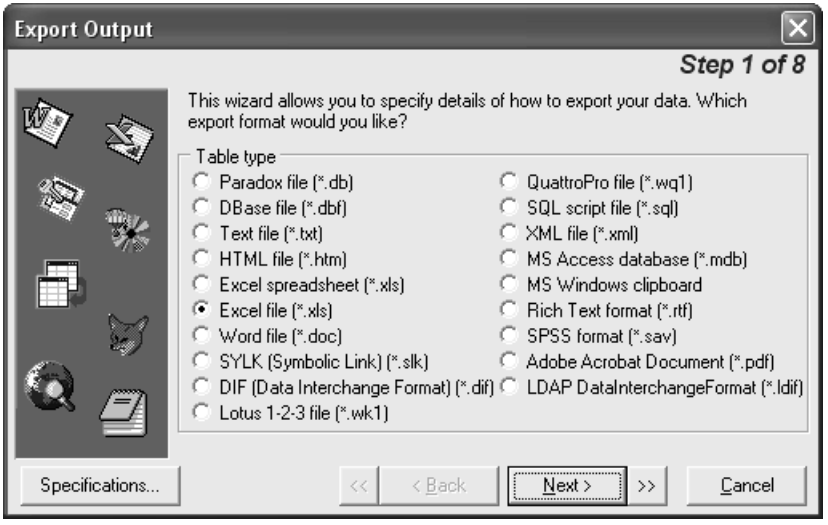
Depth vs Concentration

This option will output the data in the format below; where T1 refers to time 1, D1 refers to depth 1. C11 refers to the concentration at time 1 and depth 1; C12 refers to the concentration at time 1 and depth 2, etc.

T1 D1 C11
T1 D2 C12
....
T2 D1 C21
T2 D2 C22
....

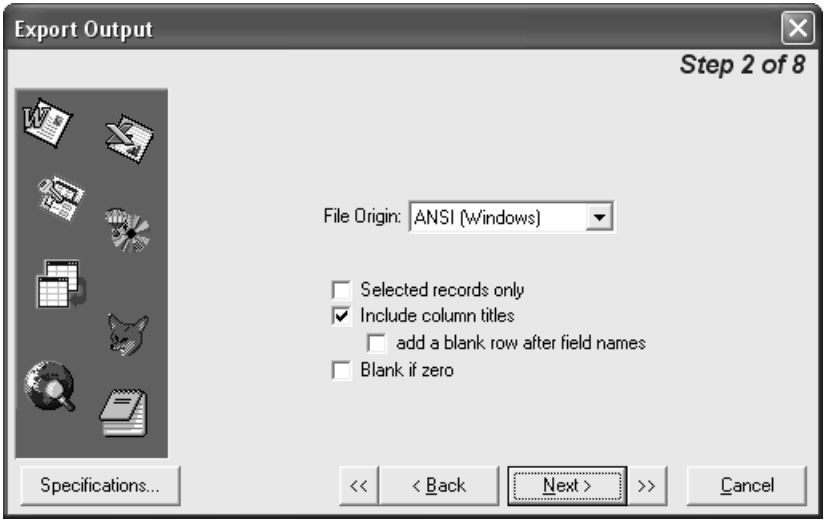
Step 1

Select the file type to export the report to.



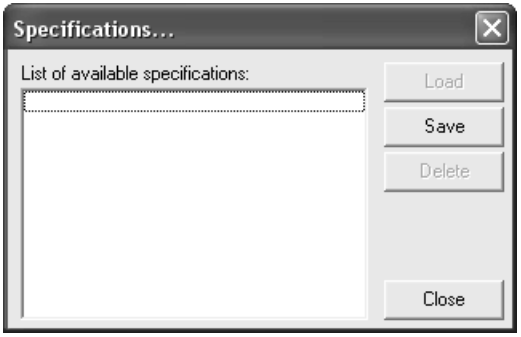
Step 2

Chooses the File origin from either windows or ms-dos. It also allows you to choose to include the column titles, and insert a blank row after the column titles.



Step 3

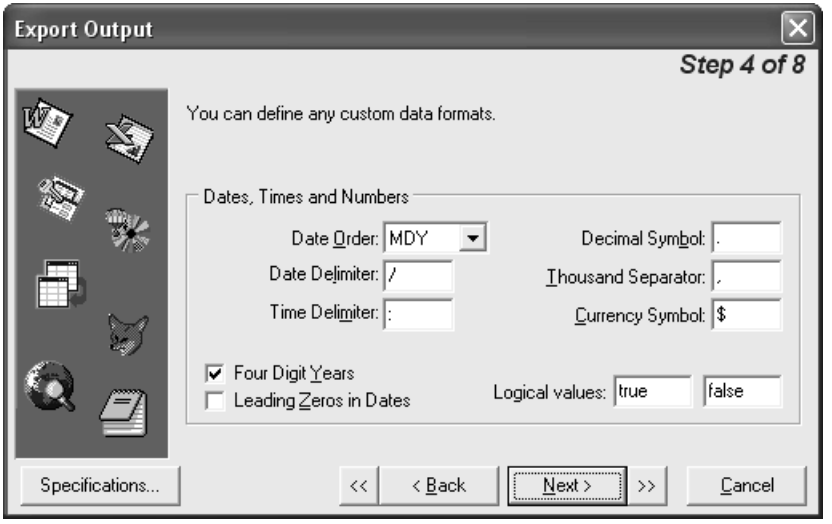
Clicking the **Specifications** button allows the user to load a previous export specification scheme or it also allows the user to save the current export specification scheme.



The user may also Delete previous schemes which are no longer useful to them.

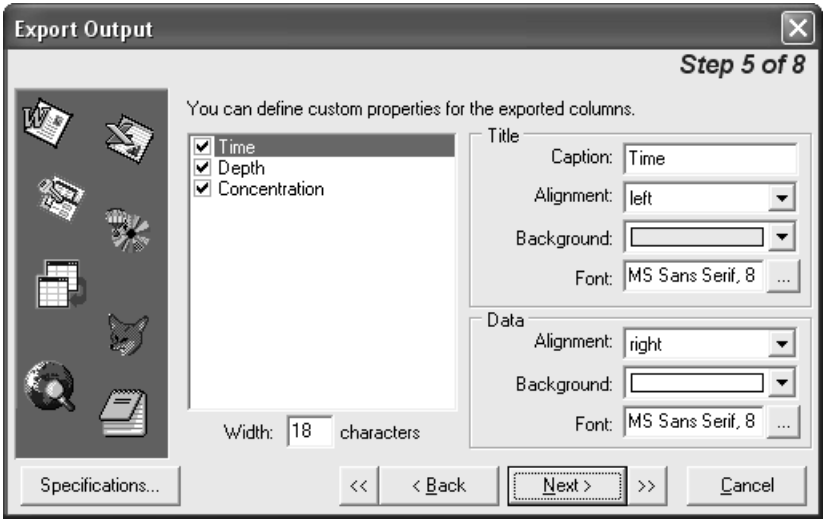
Step 4

In step 4, you choose the dates, times and numbers formats.



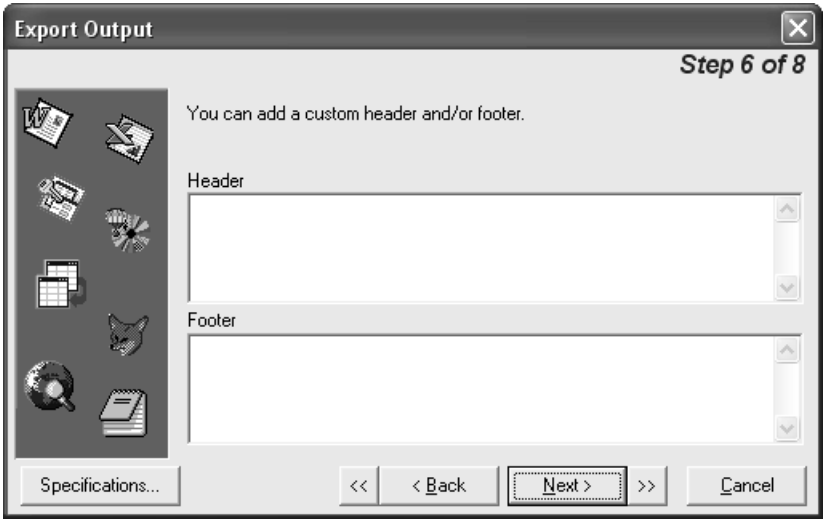
Step 5

In step 5, you choose which columns to export. In addition, you can define custom properties for each exported column.



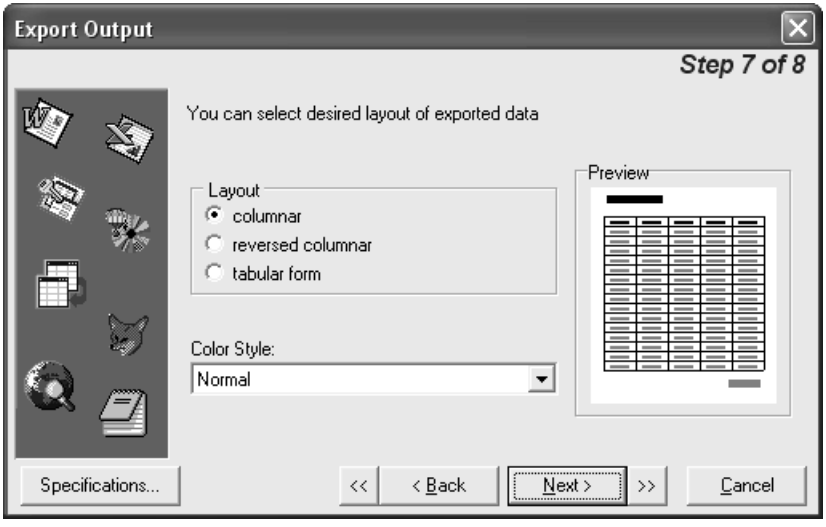
Step 6

In step 6, you choose whether to add a header and footer section to the output file.



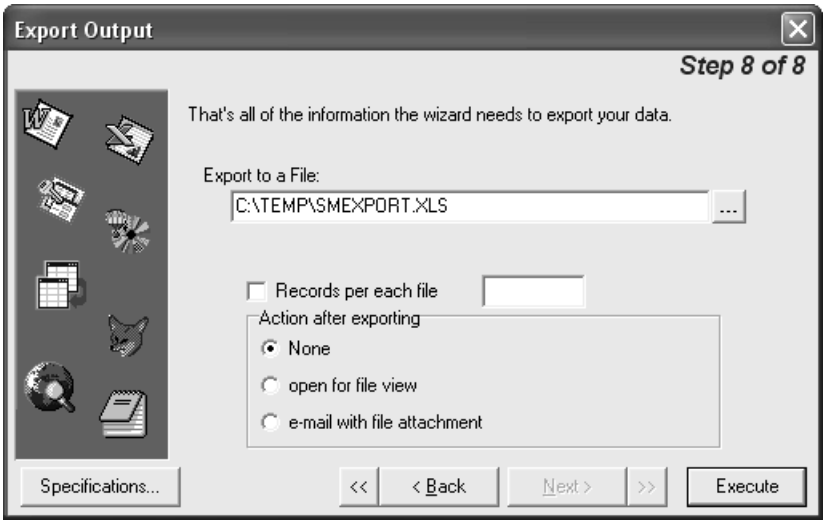
Step 7

In step 7, you choose the desired layout of the exported data. The user can also select between 12 different color styles.



Step 8

In step 8, you choose a file name to export the data to. You can also select the number of records to include in the exported file.



In addition, you can choose one of three options to occur after the exporting has completed.

* None -- do nothing
* Open File for View
* Email with file attachment.

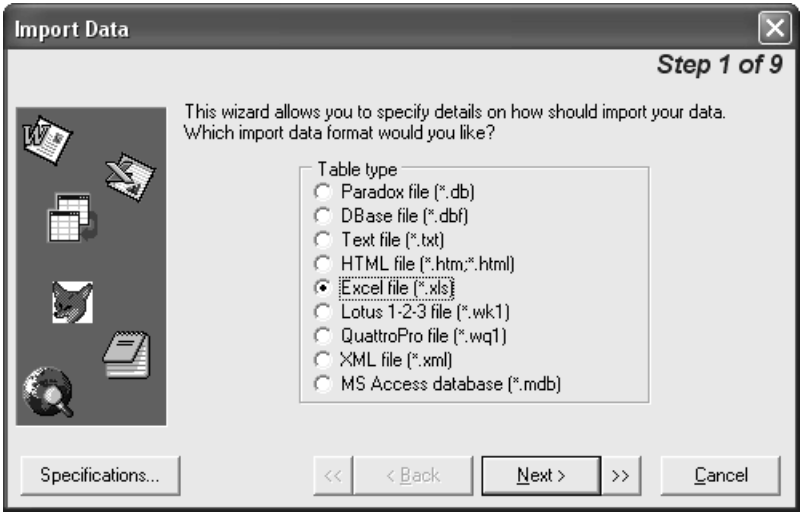
Click **Execute** to export the data to the specified file type and complete the exporting process.

Importing Output Data

In addition to the calculated results of the model, imported output data can also be displayed on the concentration vs depth and concentration vs time graphs. This imported data can be from other models, experimental results, or theoretical results. The imported data can be extracted from a file, other models in the project, or created and entered directly. After the imported data has been entered in can be edited or deleted.

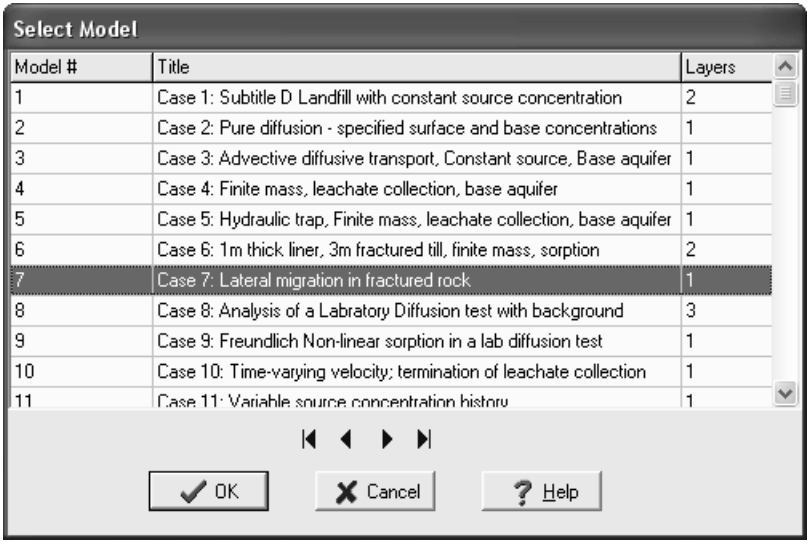
Importing from a File

To import the data from a file select the Import from File menu item from the Import Data submenu or the Output menu. The imported data can be in one of 9 different file formats. The Import Data wizard will be displayed. The wizard takes you through an 9-step process, similar to the Export Wizard described above, in which you can select the file type, file name, data fields, and other formatting options.

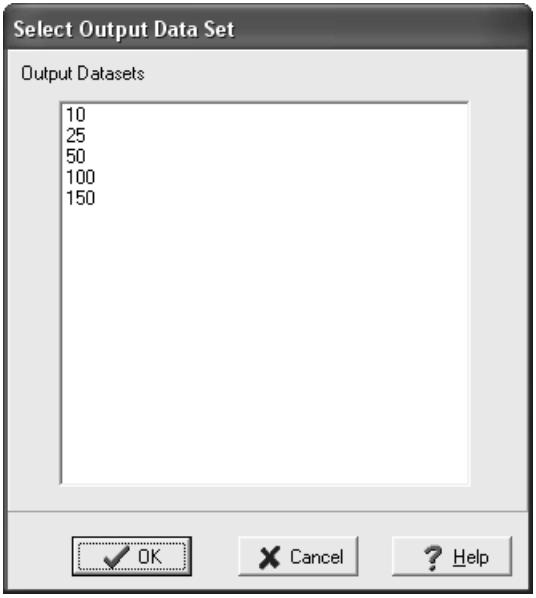


Importing from a Model

Output data from a different model in the project can be imported to compare the results of two different models. To import this data select the Import from Model menu item from the Imported Data submenu of the Output menu. The Select Model form on the next page will then appear.



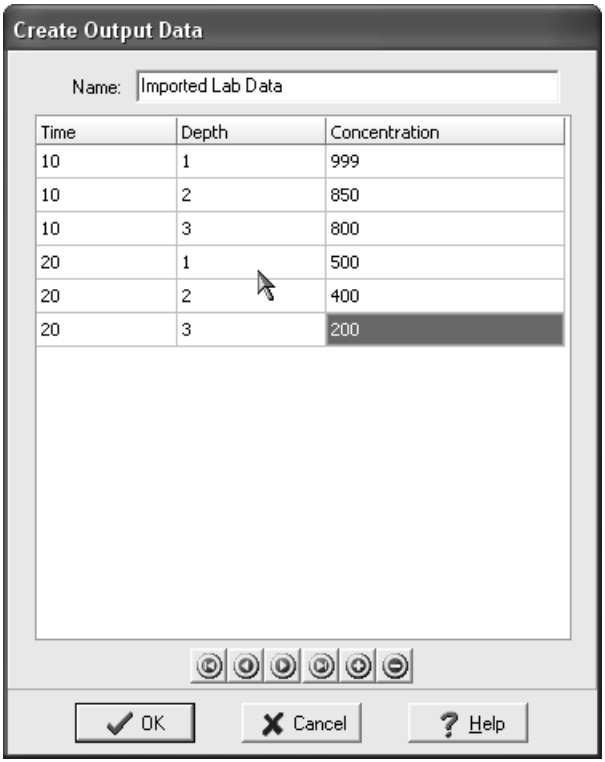
Select the model you wish to use from the form and then click on the Ok button. The Select Output dataset form below will be displayed. This form lists all of the output times for the selected model. Select the output time that you wish to import and then click on the Ok button.



After the model has been selected, the Dataset Name form below will be displayed. Enter the name for the imported dataset and then press the Ok button. The output graph will then be updated with the imported data.

Creating New Data

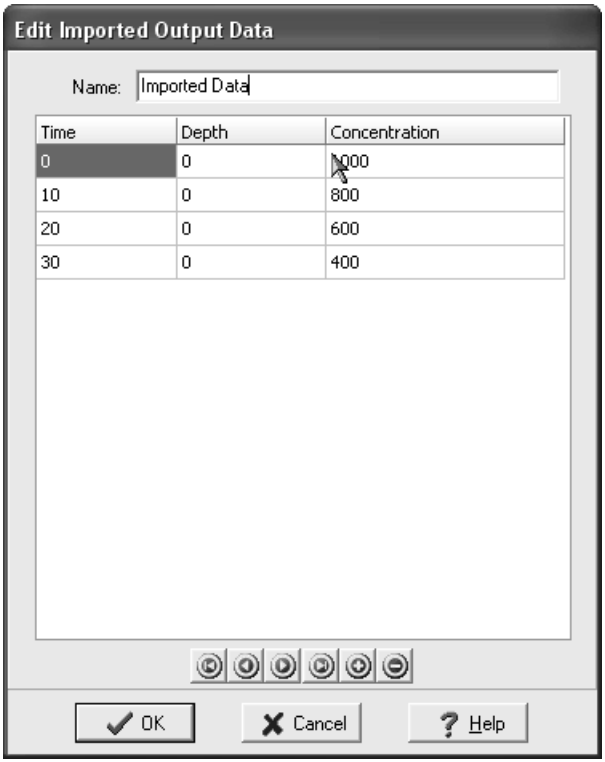
Data can also be imported by creating a dataset and entering the data. To create new data select the Create New Data menu item from the Imported Data submenu of the Output menu. The Create Output Data form below will then be displayed.



Enter the name of the dataset and the times, depths, and concentrations of the data. Normally, only one time will be entered with multiple depths and concentrations. To add or delete rows, select the row with the mouse and then press the Insert or Delete keys or use the buttons at the bottom of the form. The buttons at the bottom of the form can be used to move to the first point, move to the previous point, move to the next point, move to the last point, add a point, or delete a point. After the data has been entered click on the Ok button. The graph will then be updated with the new data.

Editing Imported Data

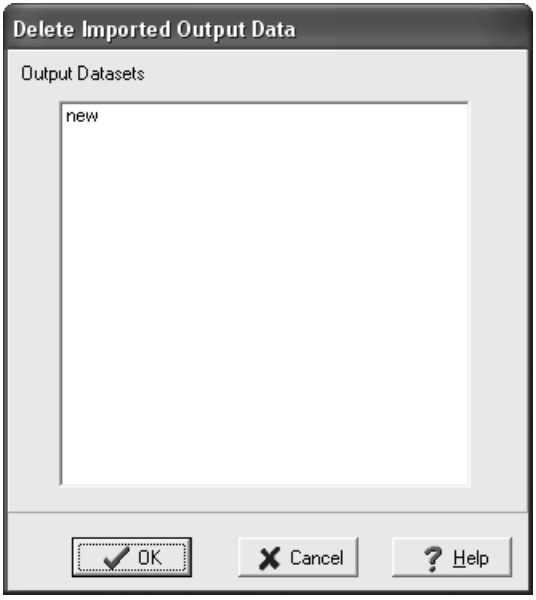
After the data has been imported it can be edited by selecting the Edit Data menu item from the Imported Data submenu of the Output menu. The Edit Imported Output Data form below will be displayed.



On this form you can edit the dataset name, times, depths, and concentrations. The buttons at the bottom of the form can be used to move to the first point, move to the previous point, move to the next point, move to the last point, add a point, or delete a point. After the data has been entered click on the Ok button. The graph will then be updated with the new data.

Deleting Imported Data

Imported output data can be deleted when you no longer want it to be displayed on the graphs. To delete the data select the Delete Data menu item from the Imported Data submenu of the Output menu. The Delete Imported Output Data form below will be displayed.



Select the dataset to be deleted from the form and then press the Ok button. The imported data will then be deleted from the graph.

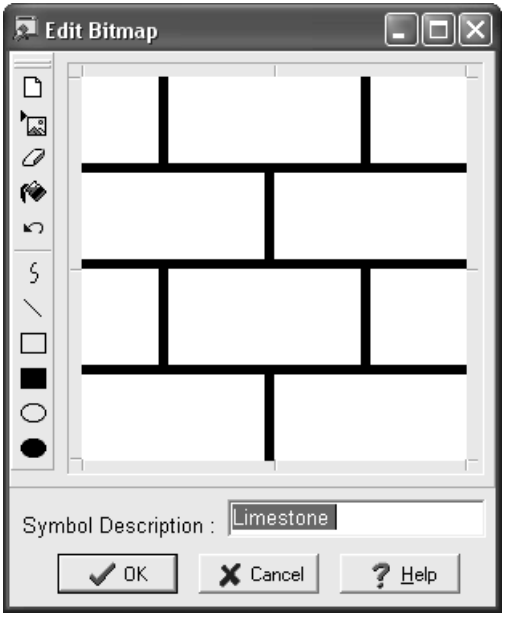
Printing a Model

The model shown on the left of the screen can be printed by clicking on the Print button on the Model toolbar.

Deleting a Model

A model can be deleted from the project by selecting the Delete Model menu item from the Models sub-menu or the File menu. The Delete Model form will be displayed. Select the model to delete and then press the Ok button.

5. Symbol Libraries



5. Symbol Libraries

Libraries are used to store lithologic bitmaps that can be used for the strata symbols. Each library contains 18 bitmap symbols. POLLUTEv7 comes with several previously defined libraries. In addition, any number of new libraries can be created, making the number of lithologic symbols available unlimited.

All of the symbol library descriptions are stored in the main database and all of the bitmaps are stored in the bitmap directory.

This chapter describes how to:

1. Create a new library
2. Edit a library
3. Save a library
4. Close a library
5. Delete a library

Creating a New Symbol Library

Since libraries are stored in the main database, they can be created and edited at any time (no project has to be open). To create a library select the New Library menu item of the Symbol Libraries submenu of the File menu. The Create New Lithologic Library form below will be displayed.

The following information can be entered on this form:

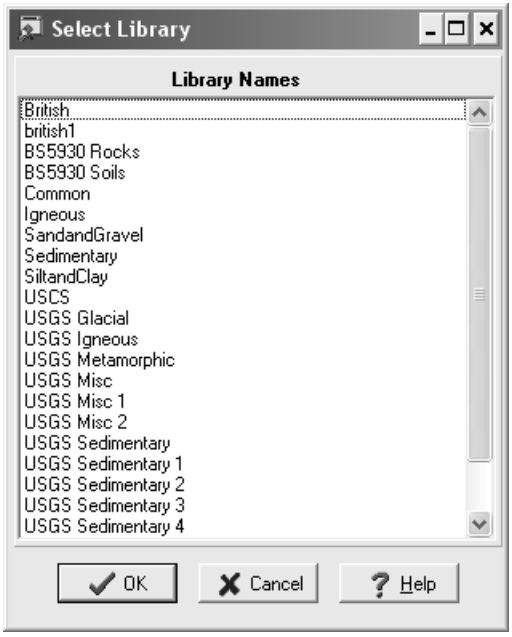
Unique Library ID: This is a unique id or name for the library (up to 100 characters). The Library ID cannot include any of the characters "/ \ # | * ( )".

Name: This is the name of the library (up to 255 characters).

After the above information has been entered a blank library will be created and displayed. This library will contain 18 blank symbols and descriptions, that can be edited and saved as discussed below.

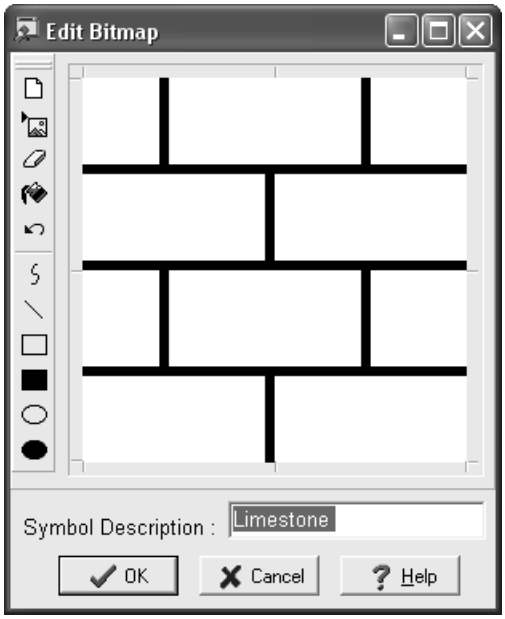
Opening a Symbol Library

To open an existing library select the Open Library menu item of the Symbol Libraries submenu. The Open Library form below will be displayed. Select the library to open and then press the Ok button.



Editing a Symbol Library

Each library can contain 18 lithologic symbols. Lithologic symbols are used to represent soils and rocks. The lithologic symbols and descriptions in the library can be changed by clicking on one of the lithologic symbols in the library. The Symbol Descriptions form below will then be displayed.

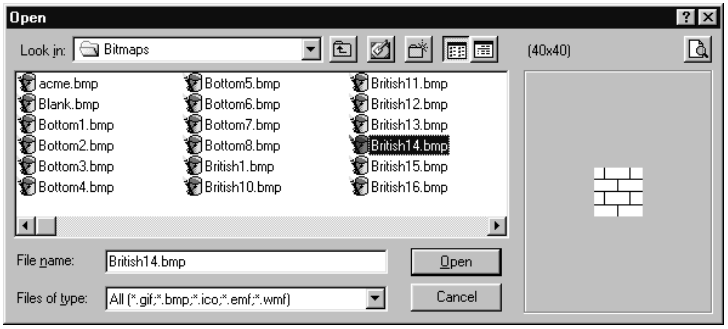


The Edit Bitmap form is used to create and edit the symbols and description. At the left side of the tab there is a toolbar used to edit the symbol.

The buttons on the toolbar perform the following actions:

The **Clear** button is used to erase the current symbol and provide a blank page.

The **Import Picture** button is used to import a bitmap picture from a file into the current symbol. When this button is pressed, the Open bitmap form below will be displayed. Select the bitmap file to import and then press the Open button.



The **Erase** button is used to delete parts of the symbol. When this button is pressed the cursor will change to an eraser. To erase a part of the symbol, hold the left mouse button down and move the cursor over the area to be erased.

The **Fill** button is used to fill regions of symbols. When this button is pressed the cursor will change to a paint can. To fill an area click inside the region.

The **Undo** button is used to undo the previous edit operation.

The **Curve** button is used to draw a curved line on the symbol. When pressed the cursor will change to a pencil. To draw a curve, hold down the left mouse button and move the mouse. When finished drawing the line, release the mouse button.

The **Line** button is used to draw a straight line on the symbol. When pressed the cursor will change to a pencil. To draw a line, press and hold down the left mouse button at the start of the line. Move the mouse to the end of the line and release the mouse button.

The **Rectangle** button is used to draw a hollow rectangle on the symbol. When pressed the cursor will change to a cross. To draw a rectangle, press and hold down the left mouse button at the upper left corner of the rectangle. Move the mouse to the lower right corner of the rectangle and release the mouse button.


The **Filled Rectangle** button is used to draw a filled rectangle on the symbol. When pressed the cursor will change to a cross. To draw a rectangle, press and hold down the left mouse button at the upper left corner of the rectangle. Move the mouse to the lower right corner of the rectangle and release the mouse button.


The **Ellipse** button is used to draw a hollow ellipse on the symbol. When pressed the cursor will change to a cross. To draw an ellipse, press and hold down the left mouse button at the upper left corner of the ellipse. Move the mouse to the lower right corner of the ellipse and release the mouse button.


The **Filled Ellipse** button is used to draw a filled ellipse on the symbol. When pressed the cursor will change to a cross. To draw an ellipse, press and hold down the left mouse button at the upper left corner of the ellipse. Move the mouse to the lower right corner of the ellipse and release the mouse button.

Saving a Symbol Library

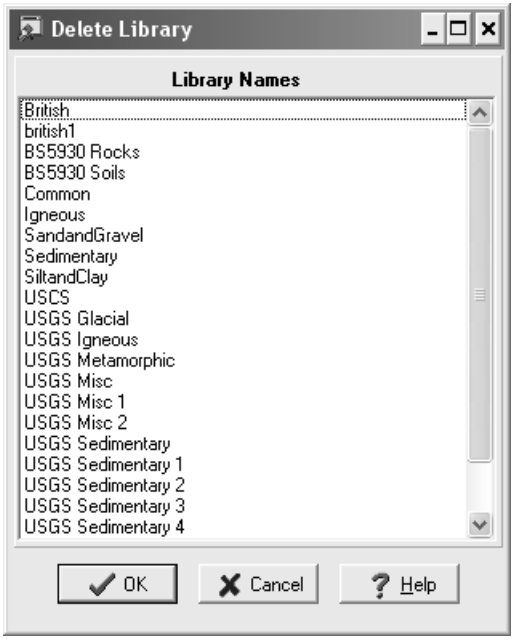
To save a library after it has been edited select the Save Library menu item of the Symbol Libraries submenu.

Closing a Symbol Library

To close a library select the Close Library menu item of the Symbol Libraries submenu.

Deleting a Symbol Library

To delete a library, select the Delete Library menu item from the Libraries submenu of the File Menu. The Delete Libraries form below will be displayed.



A single library can be selected by clicking on it and pressing the Open button. A range of libraries can be selected by clicking on the beginning of the range, and then holding down the Shift key while clicking on the end of the range. Multiple libraries can be selected, by holding down the CTRL key while clicking on the libraries.

6. Help

6. Help

POLLUTEv7 uses the latest type of help system for Microsoft Windows called HTML Help. This help system uses a similar style of display as Internet Explorer.

The Help System can be used to find information on-line rather than by using this manual. Both sources will provide the same information, but are organized somewhat differently. Help will appear in a separate window with its own menu bar and controls as shown below.

This chapter describes how to:

1. Display help

2. Use help

3. Get technical support

4. Upgrade POLLUTEv7

These tasks can be performed using menu commands on the Help menu shown on the previous page. The Transfer Registration menu item is explained in Chapter 1 Getting Started.

Displaying Help

There are several ways to access the Help System, these are:

- Press the Help button. To display the help contents at any time press the help button on the Toolbar.
- Click a Help button in a form. For more information on using a particular form click the Help button.
- Choose a command from the Help menu. The Help menu offers several options:

  - Contents displays the same Help Contents that appear when you press F1 with no commands highlighted.

  - Search displays the Search dialog box and a list of keywords you can use to find topics.

  - About POLLUTEv7 gives information about the program, including the 3-digit version number required by technical support.

Using Help

You can move back and forth between topics or search through the entire help system for the topic you want. Topics that are underlined can be displayed by clicking on them, and topics that have dotted underlines can have their definition displayed by clicking on them.

The tabs on the Help form are used for the following:

- **Contents** displays the complete Table of Contents of the Help System.
- **Index** is used to look for help topics listed by keyword.
-•**Search** can be used to search for a specific help topic by one or more keywords.

The buttons at the top of the Help form are used for the following:

- **Hide** is used to hide the tabs on the left side of the form.
- **Back** displays the previous help topic, if any.
- **Print** is used to print the current help topic.
- **Options** is used to change the preferences for the Help system.

Getting Technical Support

GAEA offers a variety of services to help you with your questions and problems. You will be automatically registered when you obtain an unlock code for the program. Free technical support to registered users includes assistance in the use of the software and in getting any bugs you may find in the software fixed.

To expedite support services, we prefer electronic communications, through email or the Internet. These communications minimize the possibility for any mistakes, and allow us to better track your request. You can email technical support by selecting the Email Technical Support menu item from the Help menu. This menu item will create an email message using your default email program.

To connect to GAEA's Internet site, select the GAEA's Web Site menu item from the Help menu.

Below are the various methods to contact technical support:

Service	**Contact Method**
Web Site	http:\\www.gaea.ca
E-mail	support@gaea.ca
Phone	(905) 666-7527
FAX	(905) 666-3744
Mail	GAEA Technologies Ltd. 87 Garden Street Whitby, Ontario Canada L1N 9E7

After receiving your communication, GAEA will respond promptly with either the solution to the problem or a schedule for solving the problem.

Before Contacting GAEA

Before contacting technical support, we suggest you try the following to help us resolve your problem.

- Determine if the problem is specific to the cross-section you are creating. Does it occur with other templates or other cross-section?
- Does the problem occur every time or intermittently?
- If you have another PC, does the problem occur on it?

Information to Provide

When contacting GAEA, please include or have the following information available.

- The 3-digit version of the POLLUTEv7 program you are using. This can be obtained from the About form on the Help menu.
- A description of the problem to help us duplicate the problem. Including any error messages.
- Copies of the project database containing the model.
- The type and model of your PC.
- The Windows version you are using.

Appendix A. References

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