User's Manual

BUGSä SCRATCHPAD
For Windows

Contents

1. Introduction

1.1 Description

BUGS SCRATCHPAD is a computer program designed to model many of the subsurface processes in a two-dimensional saturated aquifer. The program models advection and dispersion, sorption and desorption, biotic and abiotic chemical reactions and equilibrium conditions. BUGS SCRATCHPAD does this using an operator-splitting technique coupled with the Linear Integration method to solve the governing equations of each subsurface process..

BUGS SCRATCHPAD runs under Microsoft Windows 3.1, Windows 95 and Windows NT. It provides a straightforward user interface. This interface enables the user to quickly create small simulations for "back of the envelope" calculations; such as estimating initial parameters to be used in a larger simulation. In addition, its cut and paste integration with the Windows clipboard allows for data entry from spreadsheets for larger, more complex groundwater systems.

This user's manual describes how to use BUGS SCRATCHPAD. It assumes the reader has a reasonable understanding of contaminant hydrogeology and its terms; and a working knowledge of Microsoft Windows. For additional information on how BUGS SCRATCHPAD solves the set of governing equations, see the BUGS SCRATCHPAD Technical Reference. For an introduction to contaminant hydrogeology, see *Contaminant Hydrogeology* (Fetter, 1994) or a similar text.

1.2 Organization of this Manual

This manual describes how to use BUGS SCRATCHPAD, to create and run an aquifer simulation and to view results. If the program has not been installed on the computer yet, the user should first read Chapter 2, Installation.

New users should read Chapter 3, Elements of an Aquifer Simulation, first. This chapter explains the program's conceptual framework and modeling perspective. It describes the parts that make up a BUGS SCRATCHPAD aquifer simulation.

For those users desiring a guided tour of BUGS SCRATCHPAD, Chapter 13, Examples and Lessons, is provided. This chapter guides the user through a simple one dimensional aquifer simulation (as well as other more complicated simulations.) All the necessary tasks are included in the lessons, no prior knowledge of BUGS SCRATCHPAD is needed. However, it is recommended to at least read Chapter 3 first.

Chapters 4 through 8 discuss the operational details of BUGS SCRATCHPAD. this includes file operations, entering and editing reactions, running a simulation, and viewing output.

For a quick summary of commands available or a description of the menu hierarchy, see Chapter 10, Menus. This chapter contains a brief description of each menu item and its action.

2. Installation

In order to install and run the BUGS SCRATCHPAD, the computer must be an IBM compatible 386 or higher computer. There must be at least 2.5 Mbytes of free disk space for installation of the program. This excludes the space required for simulation files. BUGS SCRATCHPAD uses Microsoft Windows operating system environment.

To install BUGS SCRATCHPAD, follow these procedures:

- Start Microsoft Windows if not already running.

- Quit any running applications in Windows
  (Setup may interfere with these programs)

- Insert Disk 1 of the BUGS install disks into drive A: or B:

- From the Program Manager Select Run from the File Menu
  or Run from the Taskbar Start Menu for Windows 95 or NT.

- Type "a:\setup" at the prompt (or the location of the setup program.)

- Follow the instructions provided by the setup program.
  (For Windows 3.1 installations, choosing an install directory
  other than the provided default requires extra steps described below)

BUGS SCRATCHPAD should now be installed and ready to run.

Windows 3.1 Installation Note: The setup program provides a default application directory for installation. If a directory other than this default is chosen, the "BCOMP.PIF" file must be modified. The application and working directory in BCOMP.PIF must be changed to reflect the non-default application directory. This file can be edited with the PIF editor provided by Windows 3.1™. (BCOMP.PIF resides in the application directory.) This does not apply if the Windows 95 or Windows NT installation is chosen.

3. Elements of an Aquifer Simulation

 BUGS SCRATCHPAD uses three principal components to represent an aquifer system. They are the aquifer, parameters, and reactions. The aquifer refers to the discretized representation of the aquifer; its size and shape, and mesh properties. Parameters refer to the value of properties at a node such as the value of hydraulic head or hydraulic conductivity. Parameters can also refer to the concentration of various solutes or sorbed species at a given node. Reactions are means by which values of components change, such as desorption of a sorbed phase to a solute phase, first order decay, or reduction in hydraulic conductivity due to biomass growth.

In addition to these three principal building blocks, other components aid the organization of data and simplify editing. They can be thought of as container objects, such as the Reaction System, which refers to a collection of reactions. Also, one can define a name which refers to a point in the aquifer, known as an Alias.

3.1 The Aquifer

Although, an aquifer is usually a continuous body with the porosity conductivity varying as such; it is necessary to represent an aquifer in discreet terms for BUGS to understand it. BUGS divides the aquifer into discrete elements or cells. It assumes the material properties and concentrations are assumed to be constant throughout each element, but are allowed to differ between separate elements. In this way the program represents a non-homogeneous aquifer as a collection of different homogeneous regions.

BUGS can simulate one and two dimensional aquifers. The coordinate system is limited to the Cartesian coordinate system. Elements are rectangles and are node centered. Node centered means the element is defined by a node which is located at the center of the element. Figure 3.1 depicts a "5 X 4" aquifer mesh.

Node (1,4)   Node (5,4)

Node (1,1)
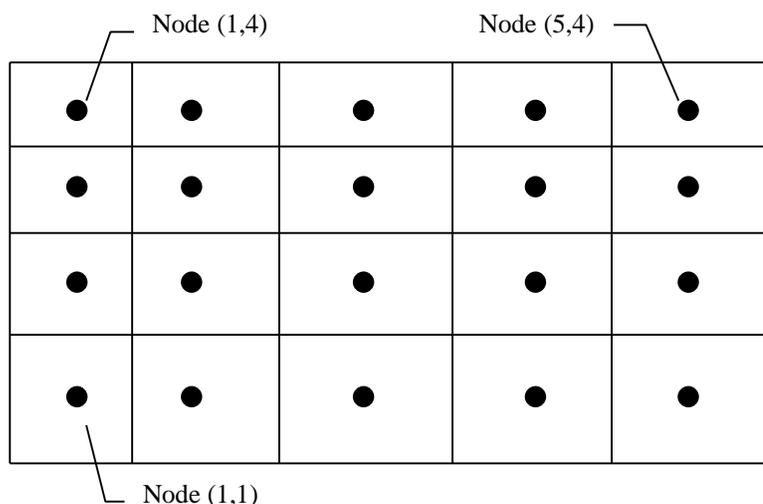
Figure 3.1 Illustration of a 5 x 4 Aquifer Mesh

Element boundaries reside halfway between nodes. Width of boundary elements equal the distance between the boundary node and its neighbor. If a node lies on an aquifer boundary, it is assumed to be a no-flow, no-flux boundary unless otherwise modified by the user.

The amount of data required to properly represent an aquifer at minimum is the number of nodes in both the X and Y dimensions, and their coordinates.

3.2 Parameters

BUGS Scratchpad recognizes three types of parameters; system, mobile, and immobile parameters. It requires the system parameters to represent the most basic of aquifer systems. System parameters include hydraulic head, hydraulic conductivity, and material porosity. They are defined at every node in the aquifer and can not be deleted or added by the user. However, a user can alter initial values and relationships though reactions.

Parameters that are added and deleted by the user are mobile and immobile parameters (collectively referred to as user parameters). Mobile parameters are, as the name implies, mobile. These parameters have advection and dispersion properties. They are usually solutes in the fluid (usually water) that saturates the aquifer. Transport processes and reactions change mobile species concentration at nodes. Immobile species concentrations are only changed by reaction processes.

The minimum amount of data required to represent most parameters is the initial value at each node. This can be done by specifying a default concentration, or by explicitly specifying it at every node. In addition to the initial value, mobile parameters require the definition of dispersivity and diffusion coefficients.

3.3 Reactions

Reactions are a very important part of a aquifer system. They manipulate values of parameters as a function of time and other parameters. (Mobile parameters are also manipulated relative to space and time as a function of their advection-dispersion properties.) There are two types of reactions, equilibrium and kinetic.

Equilibrium reactions are instantaneous while kinetic reactions are rate limited. Each reaction requires two types of data; rate data (for kinetic), rule data (for equilibrium) and Stoichiometry data. For example consider the equilibrium reaction:

$$2 = \frac{A}{B} \tag{3.1}$$

Equation (3.1) states the ratio of parameter *A* to Parameter *B* must always be two. Setting this rule alone is insufficient. It is necessary to tell BUGS how these two parameters relate to each other so the adjustment can take place (and the mass balance preserved). An example of the stoichiometry corresponding to equation (3.2) is:

$$A \leftrightarrow 2B \tag{3.2}$$
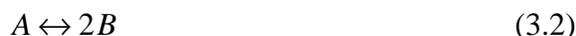
With the stoichiometry relationship, BUGS will know how much of *A* appears when *B* disappears, or the opposite. This is similar for kinetic reactions. Consider the Reaction:

$$A \xrightarrow{\quad rate \quad} 2B \tag{3.3}$$

$$rate = 2A \tag{3.4}$$

Equation (3.3) proceeds forward at the rate specified by equation (3.4).

BUGS SCRATCHPAD recognizes many different types of Equilibrium and Kinetic Reactions, including: Equilibrium, Ordered, Monod, Competitive Inhibition, Linear Isotherm, Fedulich Isotherm, and Langmuir Isotherm. Also, a rule curve reaction is included for special cases. Specific information on each reaction can be found later in this document.

It should be noted that BUGS SCRATCHPAD does not use any particular set of units in its simulation. Units are assumed to be "consistent". The user has to make the conversions from mass to moles if necessary.

3.4 Reaction Systems

Reaction systems are simply a means of specifying a certain group of reactions which occur at a specific node. Each node in the aquifer has a reaction system assigned to it. In this way, reactions can be allowed to occur at certain nodes (such as a well) and not others.

3.5 Alias

Aliases are an alternate way to specify a node. It can be thought of as giving a node a name. Aliases are not necessary, just a convenience for navigating through large aquifers.

4. File Operations

Before the discussion of file operations, it is necessary to give a brief overview of the files used by BUGS. The following table shows the extensions associated with a BUGS project:

Table 4.1 Files used by Bugs

Extension	Description
.bgs	BUGS Database File. It contains all the information associated with constructing an aquifer simulation. Typically this is the only file the user will interact with.
.bgi	Simulation routine input File. It contains a numerical representation of the aquifer. BUGS creates it prior to calling the simulation routine. (ASCII Format)
.bgo	Simulation Routine Output file. These file contain the value profiles of parameters in the aquifer as a function of time. It is written by the simulation routine. (Binary Format)
.bgt	Simulation time file. It contains a list of the simulation time periods written to disk. It is written by the simulation routine. (Binary Format)

Typically only *.bgs files will be seen by the user. BUGS automatically handles the others.

BUGS can only open one project at a time. To create a new project, simply select New from the File menu. To save a BUGS file to disk, chose the Save command from the File menu. If a new project has not been previously saved to disk, the user will be prompted for a filename. A project can be also saved with a new file name by using the Save As command from the File menu. For more information on the File menu, see the section on menus later in this document.

5. About Grid and Form Views

BUGS provides two formats for entering and editing data, "Form" and "Grid" views. A "Form" view of a window usually displays information for one item at a time. This can be quite useful, however it does limit the user to viewing a small part of the system at a time. For one who is most comfortable working in a spreadsheet-type environment, BUGS provides a "Grid" view. The grid view typically shows lists of items in the window. It should be noted that sometimes it would not be logical to show certain information on a grid, and the same for the form view. Some information may only be accessible through a certain view, such as a list of node coordinates.

It is easy to switch between views of a window. If the user wishes to see the form view, they can either click on the button on the tool bar or select Form from the View menu. If the user desires to see the grid view, they can select the button on the tool bar or select Grid from the View menu. If the desired views available, it is because the current information cannot be displayed in that type of view.

6. Editing an Aquifer System

BUGS is a flexible program that allows the user many options in editing. This section is organized by desired task to be accomplished. For a sequential look at available commands, see Chapter 9, Communicating with Other Programs.

6.1 Setting Simulation Times

To edit the starting and editing times of a simulation, select Aquifer Properties from the Window Menu, then select the form view of the window by selecting the [button icon] button from the tool bar or selecting Form from the View menu. This will bring up the Aquifer Properties window as shown in Figure 6.1.
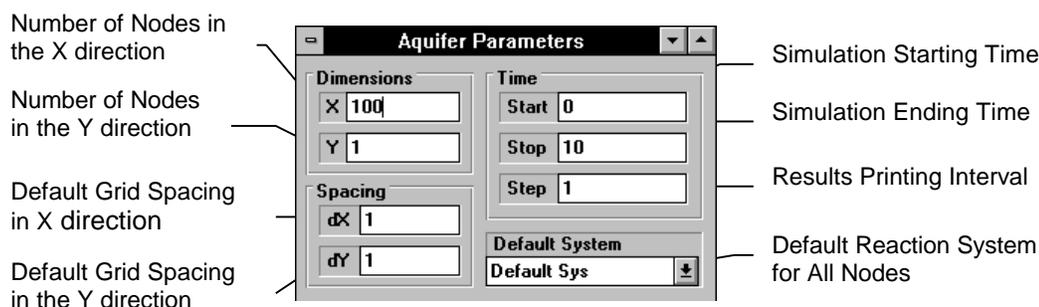

Figure 6.1 Aquifer Properties Window in Form View

The values of interest to be changed are the starting time, ending time, and printing time. Starting and ending times have no limits except for the ending time which must be greater than the starting time. The printing time is the time increment in which the simulation routine writes parameter profiles to intermediate files. A smaller print time will give a higher resolution in output with respect to time, at the cost of increased disk space usage. From this window the user can also edit the aquifer shape and size.

6.2 Aquifer Size and Discretization

In the aquifer properties window (Form View, See Figure 6.1) the user can change the number of nodes in the X and Y directions. The default node spacing can also be changed. It should be noted that the default grid spacing is only used when the aquifer is growing, or in other words, the user specifies a larger number of nodes. Also, the aquifer properties window gives the user a chance to specify the default reaction system.

The form view of the Aquifer Properties window does not allow the user to customize the grid spacing of the aquifer mesh. In order to do this, it is necessary to view the Aquifer Properties Grid.

6.3 *Customizing the Aquifer Mesh*

To edit aquifer node grid spacing, select Aquifer Properties from the Window menu.

Then select the Grid View button ⊞ on the tool bar or select Grid from the View Menu. The active window should now appear as in Figure 6.2
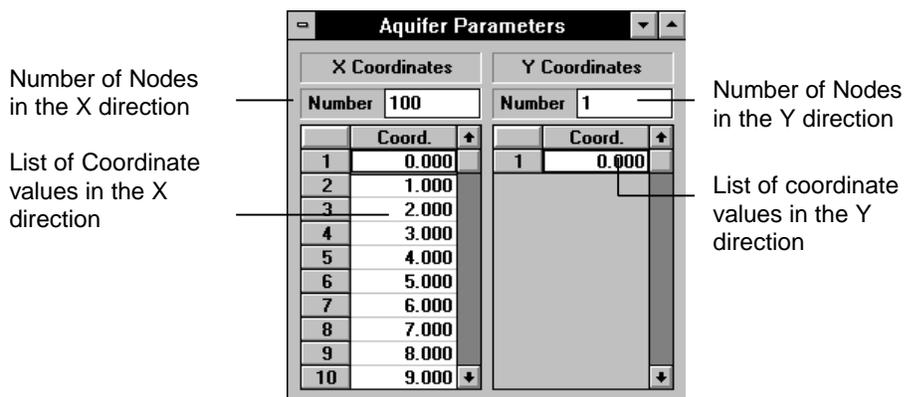

Figure 6.2 Aquifer Properties Window in Grid View

From Here, the user can edit the placement of various nodes in the X and Y directions. The editing tables support the windows copy and paste functions. It should be noted that it is necessary for the node coordinates to be in increasing order. That is, $x_i < x_{i+1}$. This is necessary for proper simulation, BUGS cannot simulate an overlapping aquifer.

6.4 *Adding and Removing Parameters*

Only two of three types of parameters can be added and deleted; mobile and immobile parameters, or otherwise called user defined parameters. System parameters are required for computing the hydraulic flow field. Although system parameters cannot be added or deleted, their initial values can be changed at the discretion of the user.

To add a parameter to the aquifer system, the Parameters window must be open. To open the window, select Parameters from the Window Menu. If necessary, click the

Form view button ▦ on the tool bar, or select Form from the View menu, to bring up the form view of Parameters.
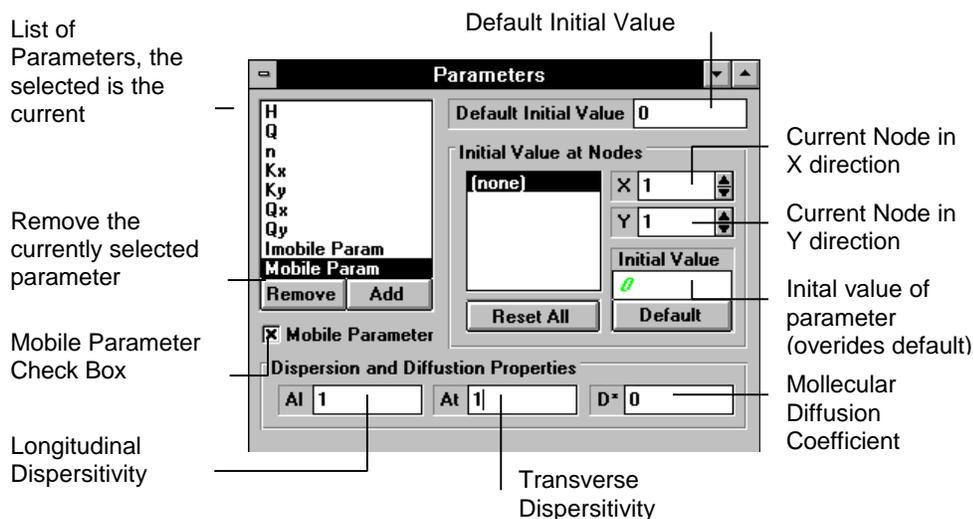
Figure 6.3 Parameters Window in Form View

Figure 6.3 illustrates the Parameters Window. To add a parameter, check on the Add Button. A dialog box will appear requesting the name of the new parameter.
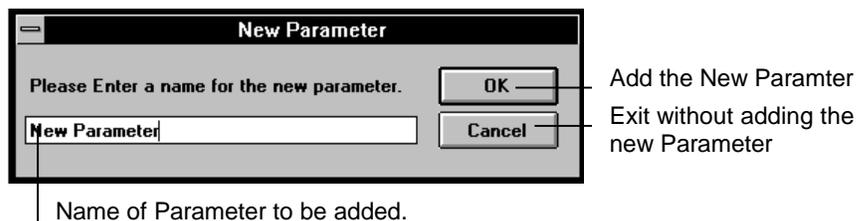

Figure 6.4 Add Parameter Dialog Box

Parameters must have unique names. If the user specifies a name that already exists, a new parameter will not be added to the system.

To delete a parameter from the system, simply select the parameter form the list of names and click on the remove button. One should note this is an irreversible process. It can not be undone. All references to this parameter will be removed. If the remove button is not enabled, it is because the selected parameter is a system parameter, which can not be deleted.

6.5 Specifying Mobile and Immobile Parameters

User defined parameters can be specified to be mobile or immobile. Immobile parameters can represent entities such as a sorbed species or ionic strength of the solution at a node. To specify an immobile parameter from the list of parameter names, activate the Parameters Window in Form View (discussed above), select the desired parameter, and clear the Mobile check box located below the list of parameters.

To specify a user defined parameter as mobile, check the mobile check box. When this option is checked, three edit boxes will appear. These boxes allow the user to edit the longitudinal dispersivity, transverse dispersivity and diffusion coefficient. For a further discussion of these parameters, see the BUGS SCRATCHPAD Technical Manual.

6.6 Specifying Initial Values of Parameters

There are two ways to specify the initial value of a parameter (the value at the beginning simulation time). First, the user can specify the default initial value for the parameter. This default value can be overridden by setting the value at a given aquifer node explicitly. To specify the default initial value of a parameter, the parameters window in form view must be active. (discussed above) the "Co" field corresponds to the default initial value of the parameter at every node unless overridden by the method described below.

There are three ways in which the user can override the default initial values of a parameter. The first way is to use the Form View of the parameters window described above. In the frame called Initial Values (see Figure 6.3 above) the user can specify the node coordinates and initial value of the parameter for the specified node. The second method involves a similar interface contained in the form view of the nodes window (to be discussed later).

The third way to explicitly define initial parameters is to use the grid view of the nodes window. To activate the nodes window in grid view, Select Nodes from the Window menu and click on the ⊞ button on the tool bar or select Grid from the View menu. Figure 6.5 illustrates the window.

Figure 6.5 Nodes Window in Grid View

In this way the user can enter the initial values in a spreadsheet like manner. BUGS supports the windows clipboard cut, copy and paste commands. Thus, initial values can be imported from other programs via the clipboard. For more information on using the clipboard with bus, see Chapter 9, Communicating with Other Programs.

6.7 Editing Reactions

BUGS hosts a large suite of reactions found in many aquifers. Since reactions are the most important part of the BUGS implementation, they are also the most difficult to explain.

Reactions are used in a variety of ways. They are serve as rules defining how mass transfer between parameters occurs. For example, sorption of methane to aquifer solids is an example of a linear isotherm reaction. A more complicated example would be consumption of methane and oxygen by a concentration of methanotrophs producing carbon dioxide using a double Monod relationship. Cometabloism of TCE and intermediate toxicity effects of TCE-Epoxide could affect methane consumption, not to mention biomass growth and decay. One can see how a set of individually simple equations can couple together to produce a highly nonlinear aquifer system. This section describes how simple components combine together to form the complex system that BUGS can understand.

6.8 Opening the Reactions Window

The Reactions Window can only be seen in the form view. To open the Reactions window select Reactions from the Window menu. Figure 6.6 illustrates the initial view of the Reactions Window
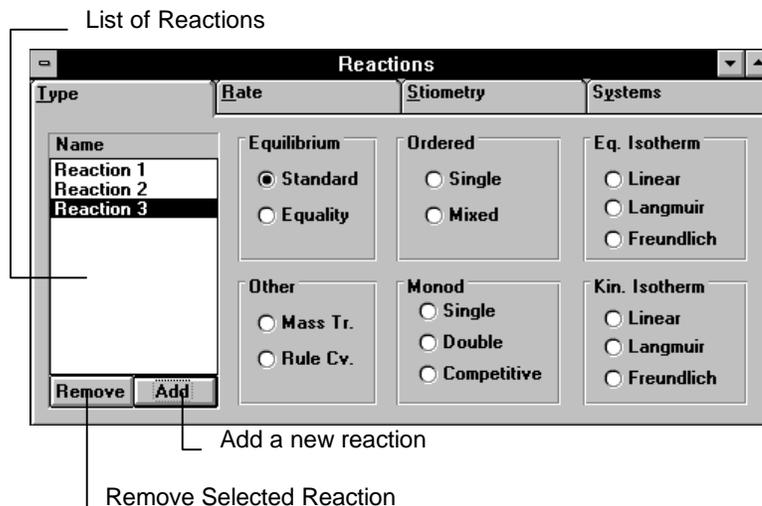

Figure 6.6 Reactions Window

If the aquifer system does not contain any reactions yet, the user will first be prompted to enter a name for the first reactions to be added to the aquifer system.

6.9 Adding and Removing Reactions

To add a reaction to the aquifer system first display the Reactions Window (as discussed above). When the reactions window opens for the first time, there will be no reactions in the aquifer system. The user will be automatically prompted to enter a name for a new reaction. Figure 6.7 shows the add reaction dialog box
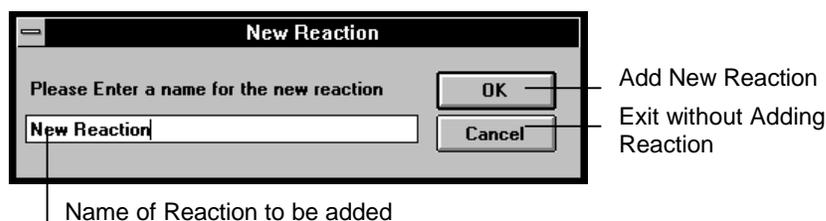

Figure 6.7 Add Reactions Dialog Box

Simply type in the name of the reaction and press ENTER on the keyboard or click the OK button. To add additional reactions, click on the Add button in the reactions window and follow the above procedure again. Reaction names must be unique. If the user specifies a name already used by a reaction, no reaction will be added to the system.

To remove a reaction, select the reaction name to be deleted in the name list box and click the remove button. If only one reaction exists, the remove button will not be enabled. Each Aquifer system usually should have at least one reaction. Removing a reaction is an irreversible process, all references to the reaction will be removed.

6.10 Setting the Reaction Type

With the reactions window open, click on the type tab This will display the various reaction types. Figure 6.8 illustrates the "Type" page for the reactions window.
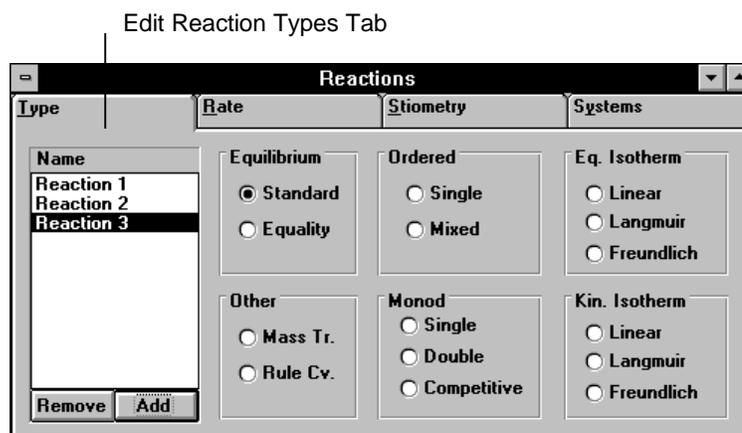

Figure 6.8 Reactions Window for Editing Reaction Type

The user can select a type of reaction by simply selecting the desired option button. A discussion of the various reaction types is explained later in this section

6.11 Setting the Stoichiometry of a Reaction

As mentioned earlier, most reactions require the user to explicitly define reaction stoichiometry. With the Reactions window open in Form View, select the Stoichiometry tab. Figure 6.9 depicts the corresponding window
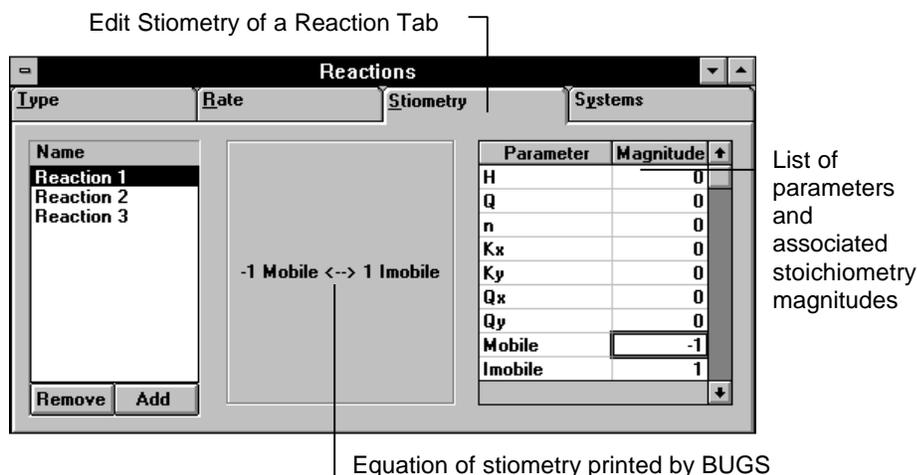

Figure 6.9 Reactions window for Editing Reaction Stoichiometry

To specify the magnitude for a parameter in a Stoichiometry reaction, enter the magnitude in the grid next to the desired parameter. Negative values will place the parameter on the left side of the arrow while positive numbers are placed on the right. The Stoichiometry reaction as understood by BUGS is echoed in the Stoichiometry box. It is important to specify the order correctly with kinetic reactions. The reaction will proceed to the right by the rate specified in the rate data (to be discussed later). For Equilibrium reactions the order of reaction is not important, just the mass balance.

6.12 Specifying a Reaction System for a Reaction

Before a reaction can be used by BUGS, it needs to be included in a reaction system. The Reaction System in turn is specified at a node. This is the way in which BUGS assigns which reactions occur at each node.

With the Reactions Window open in Form View, select the Reaction Systems Tab Figure 6.10 illustrates the corresponding screen.

Link and Unlink Reactions and Reaction Systems Tab
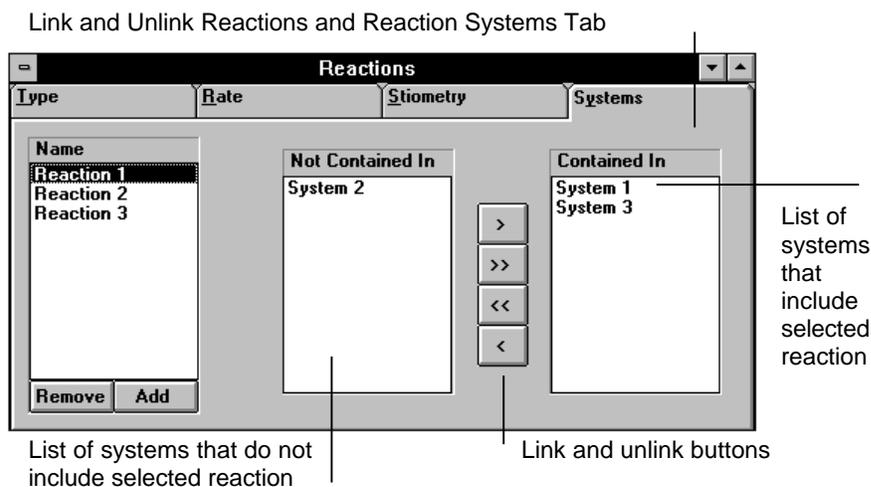
Figure 6.10 Reactions Window for Choosing Reaction Systems

This screen allows the user to select which reaction systems include this particular reaction. It can be seen from Figure 6.10 that reaction 1 is included in Reaction Systems 1 and 3, but not 2. Reaction Systems 1 and 3 include Reaction 1. To link Reaction with a Reaction System, select the reaction in the Not Contained In list and click the ⟩ button (or simply double click the system). To remove the link, select the system in the Contained In list and click the ⟨ (or double click on the system). To unlink all systems click the ⟨⟨ button and to link all systems click the ⟩⟩ button.

6.13 Specifying Reaction Rate Data

To edit the rate or rule data for a reaction, the user must bring up the rate data editing page for the reaction. This is the same regardless of the reaction type. First the Form View Reactions Window must be active. Then select the rate data tab. BUGS supports many different types of reactions. Each reaction appears in a different screen. This section illustrates how to enter rate or rule data for each type of a Reaction.

6.13.1 Equilibrium Equation

Equilibrium Constant

Parameter	Power
H	0
Q	0
n	0
Kx	0
Ky	0
Qx	0
Qy	0
Solute	-1
Sorbed	1
X	0

Ke = 1

1 = [Solute]^-1 (Sorbed)^1

Echo of Equation   Powers of Parameters

Figure 6.11 Equilibrium Reaction

The equilibrium reaction adjusts the values of parameters given in the Stoichiometry relationship (if possible) such that the ratios of their values match the equilibrium constant.

6.13.2 Equality Equation

Dependent Parameter

Depndt. O2

Coeffient. 10

Constant Coefficient

O2 = 10 + 1 CH4

Parameter	Coeff.
n	0
Kx	0
Ky	0
Qx	0
Qy	0
Solute	0
Sorbed	0
X	0
O2	0
CH4	1

Echo of Equation   Parameter Coefficients

Figure 6.12 Equality Reaction

The equality reaction simply sets the dependent parameter to the value specified by the linear combination of parameters and constant.

### 6.13.3 Single Order Reaction Equation
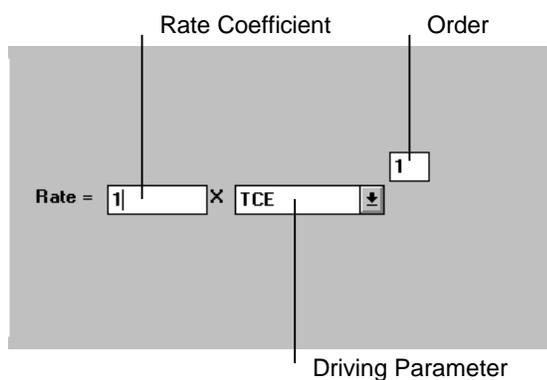
Figure 6.13 Single Order Reaction

The single order reaction only uses data from one parameter to determine the rate of reaction.

### 6.13.4 Mixed Ordered Reaction Equation
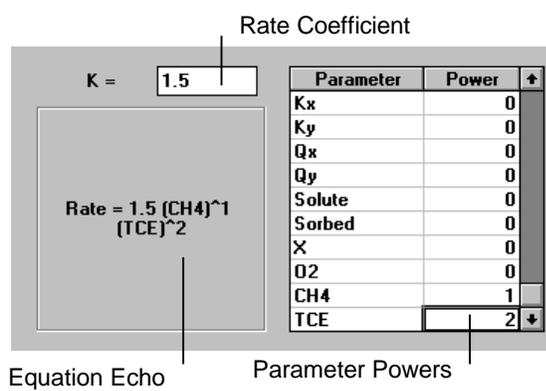
Figure 6.14 Mixed Ordered Reaction

The mixed order reaction uses values of multiple parameters to determine the rate of the reaction.

### 6.13.5 Linear Equilibrium Isotherm

Sorbed Species   Solute Species

Solute ▼ = 1.0 × Solute ▼

Porportionality Constant
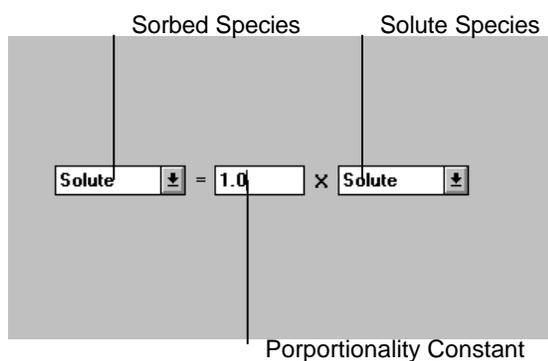
Figure 6.15 Linear Equilibrium Isotherm

The linear equilibrium sorption isotherm adjusts parameters using the relationship defined in the Stoichiometry to set the left hand side of the equation equal to the right hand side.

6.13.6 Langmuir Equilibrium Isotherm

Sorbed Species   Solute Species

Sorbed ▼ = 1 × Solute ▼ / (1.5 + Solute)

Porportionality Constant   Porportionality Constant
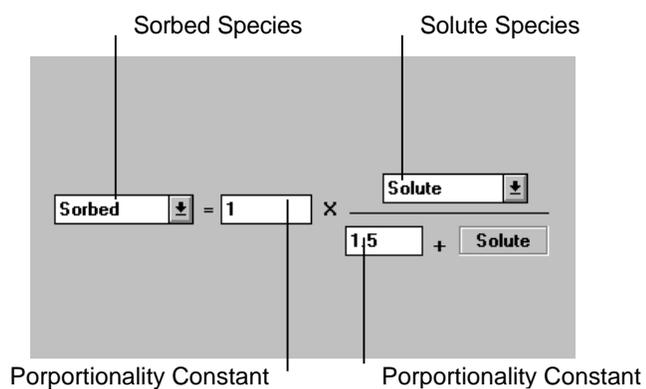
Figure 6.16 Langmuir Equilibrium Isotherm

The Langmuir Equilibrium sorption isotherm adjusts parameters using the relationship defined in the Stoichiometry to set the left hand side of the equation equal to the right hand side.

6.13.7 Fredulich Equilibrium Isotherm
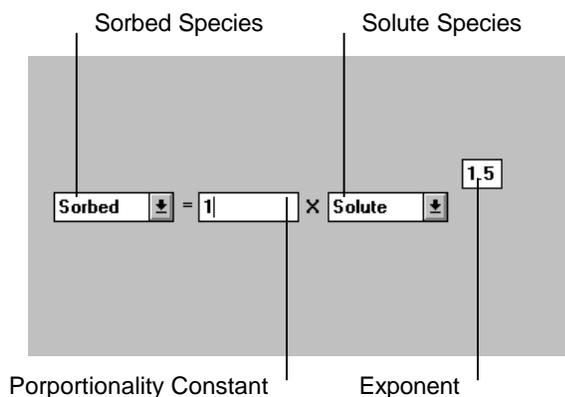
Figure 6.17 Fredulich Equilibrium Isotherm

The Fredulich Equilibrium sorption isotherm adjusts parameters using the relationship defined in the Stoichiometry to set the left hand side of the equation equal to the right hand side.

6.13.8 Linear Kinetic Isotherm
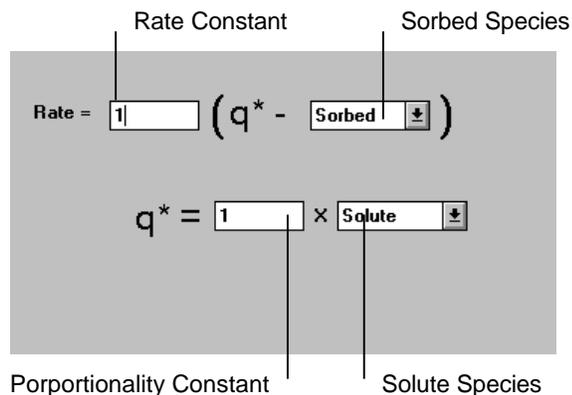
Figure 6.18 Linear Kinetic Isotherm

The linear kinetic isotherm computes a target sorbed phase concentration with the linear isotherm relationship. A mass transfer equation is then used to determine the rate of reaction.

6.13.9 Langmuir Kinetic Isotherm

Figure 6.19 Langmuir Kinetic Isotherm

The Langmuir Kinetic isotherm uses the Langmuir isotherm relationship to compute a target sorbed phase concentration. A mass transfer equation is then used to determine the rate of reaction.

6.13.10 Fredulich Kinetic Isotherm

Figure 6.20 Fredulich Kinetic Isotherm

The Fredulich Kinetic isotherm uses the Fredulich isotherm relationship to compute a target sorbed phase concentration. A mass transfer equation is then used to determine the rate of reaction.

6.13.11 Single Monod Equation
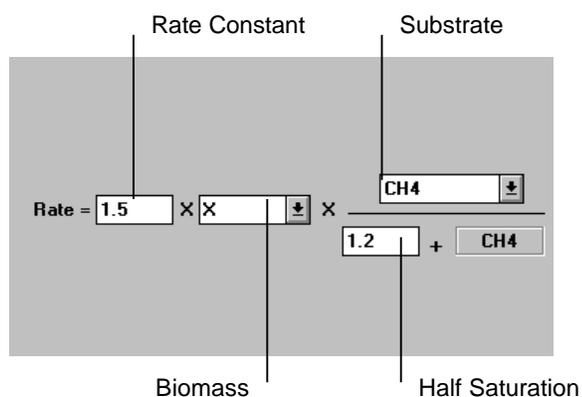
Figure 6.21 Single Monod Reaction

The Single Monod equation relies on values from two parameters to determine the rate of reaction. However, the biomass portion can be ignored by setting to "unity".

6.13.12 Double Monod Equation
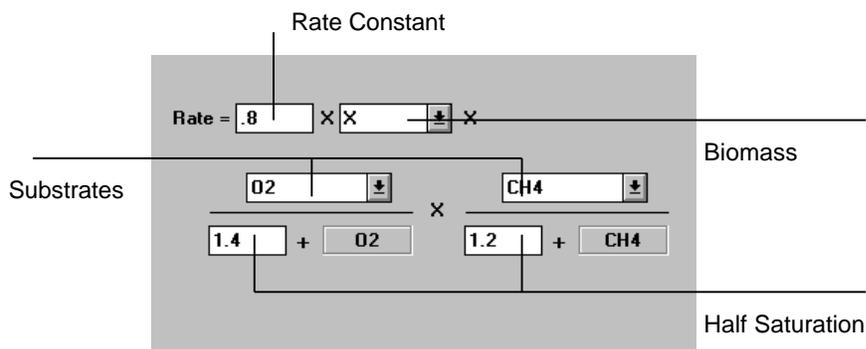
Figure 6.22 Double Monod Reaction

The Double Monod equation relies on three parameters to compute the rate of reaction, two substrate and one biomass. If the biomass component is not needed, it can be set to "unity".

6.13.13 Competitive Inhibition Equation
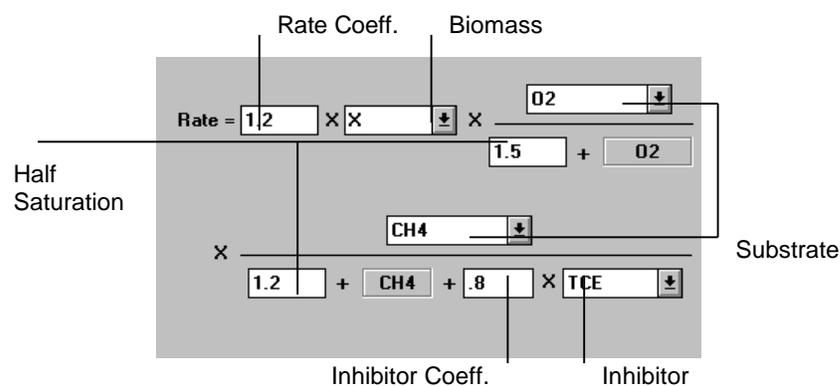
Figure 6.23 Competitive Inhibition Reaction

The Competitive Inhibition equation includes a term for a competitive parameter in one of the substrate terms of a double monod relationship. If the biomass term is not needed, it can be set to unity.

6.13.14 Mass Transfer Equation
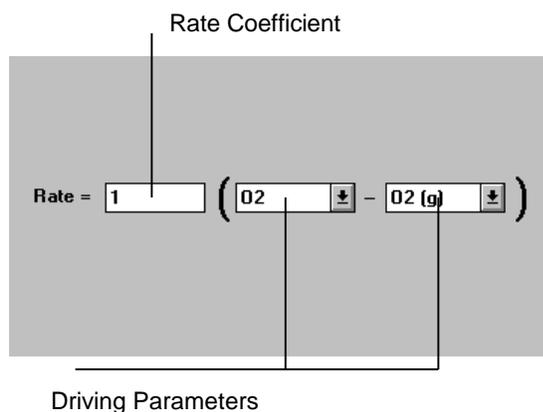
Figure 6.24 Mass Transfer Reaction

The mass transfer equation simply uses the difference between two parameter values to compute the rate of reaction.

6.13.15 Rule Curve Reaction

Figure 6.25 Rule Curve Reaction

The Rule Curve reaction can be used if all of the above reactions were not appropriate. In addition to accessing the values of parameters, this reaction can also use time as input. For example, an injection schedule could be entered. Independent variables (x) must be entered in acceding order. BUGS uses a simple lookup routine to find values in the list.

6.14 Opening the Reaction Systems Window

Reaction systems can be thought of as collections of reactions. This is necessary because not all subsurface processes may occur everywhere in the aquifer. For example, a well in an aquifer may be injecting methane at a constant concentration. This process only occurs at the well. Thus, the user can specify a reaction describing a constant source, and group it in a "well" reaction system. This reaction system in turn could be assigned to the node at the location of the well.

The Reaction Systems window has only one view, form views. To open the reaction systems window select the Reaction Systems from the Window menu. Figure 6.26 illustrates the corresponding window.
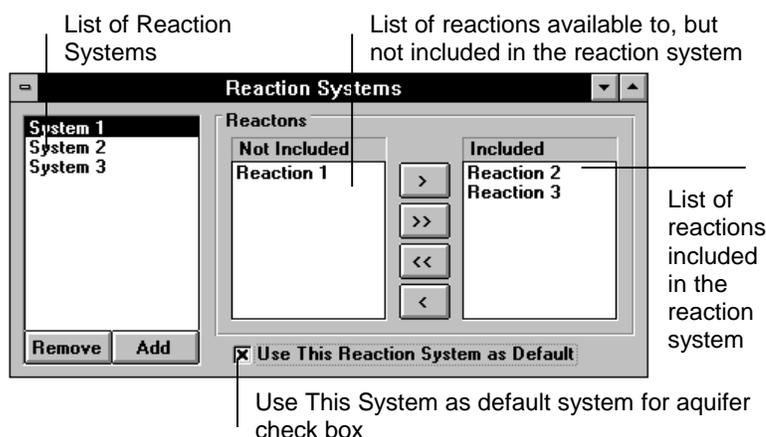
Figure 6.26 Reaction Systems Window

If the aquifer system contains no reaction systems, the user will be automatically prompted to enter a name for the first reaction system.

6.15 Adding and Deleting Reaction Systems

To add a reaction system, first display the reaction systems window (as discussed above). When the reaction systems window opens for the first time, there will be no reaction systems. The program automatically prompts the user to enter a name for a new reaction system. Figure 6.27 shows the add reaction systems dialog box.
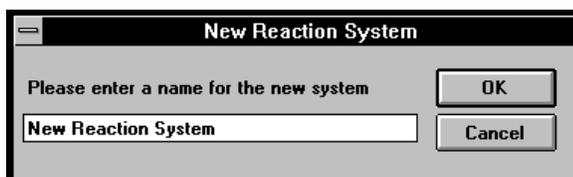
Figure 6.27 Add Reaction Systems Dialog Box

Simply type the new name of the reaction and press ENTER or click on the OK button. To add additional reaction systems, click on the Add button in the reaction systems window and follow the above procedure. Reaction system names must be unique. If the user specifies a name already used by a reaction system, no reaction system will be added.

To delete a reaction system, simply select the desired system in the reaction system list box, and click on the remove button. If only one reaction system exists, the remove button will not be enabled. Each aquifer system must have at least one reaction system. Deleting a reaction system is an irreversible process. It can not be undone.

6.16 Specifying a Reaction for a Reaction System

Figure 6.26 above depicts a typical aquifer system. The aquifer system has available to it a source pool of three reactions. It can be seen from the figure that reaction system 1 includes reactions 2 and 3, but not reaction 1.

To add a reaction to the reaction system, simply select the reaction to be added in the "available" list and click the ⌐ > ⌐ button. To remove a reaction from a reaction system, select the reaction from the "included" list and click on the ⌐ < ⌐ button. To include or exclude all reactions click on the ⌐ >> ⌐ or ⌐ << ⌐ buttons respectively. A shortcut to the ⌐ > ⌐ and ⌐ < ⌐ buttons is to double click on the reaction.

6.17 Specifying the Default Reaction System

To specify the default reaction system to occur at all nodes in the aquifer system, select the desired reaction system in the reaction system window. Then check the "use as default system" check box. This system will now be used by all nodes unless otherwise overridden from the nodes window as discussed earlier.

6.18 Changing Simulation Run Options

To change simulation run options, select Options from the Run menu. The following dialog box will appear.
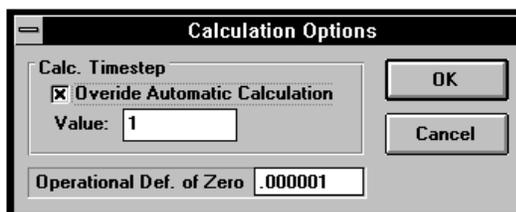
Figure 6.28 Simulation Run Options Dialog Box

Two simulation run options can be changed, the global calculation timestep and the operational definition of zero. The simulation routine uses the global calculation timestep to calculate advection and dispersion of mobile parameters. It is not recommended to override the automatic calculation of this variable. See the BUGS SCRATCHPAD Technical Reference for details on the calculation of the timestep.

The operational definition of zero can be thought as a tolerance factor in the iterative calculation of kinetic and equilibrium reactions. The higher the value, the faster simulations will run, but they will be less accurate.

7. Running a Simulation

After all the necessary data has been entered for an Aquifer System, the System can be simulated. To run the simulation, select Simulate from the Run menu When this option is selected, BUGS shows a dialog box describing the progress of the simulation. The user can not edit the aquifer system while the simulation is being run.

8. Viewing Output

After a simulation has been run or updated, the user has four output options. The user can view a profile of parameter values in a snapshot of time. Additionally, the user can view parameter values as a function of time at a given node in the aquifer. BUGS also produces a surface graph of parameters. Finally, numerical output can be viewed in a tabular format.

8.1 Parameter Profile Graph

Parameter profile graphs consist of a snapshot in time of parameters along a profile in the X or Y direction. To view a profile graph, select Profile Graph from the Windows menu. If the simulation is out of date with respect to the current input parameters, the user will be prompted to update it.
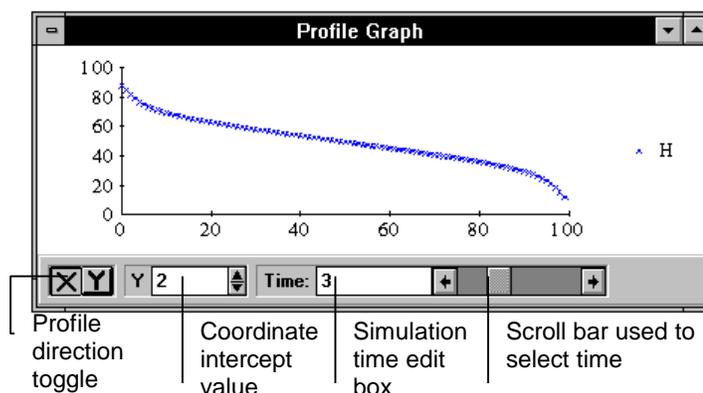
Figure 8.1 Parameter Profile Graph

Profile graphs can display more than one parameter at a time. In order to add or remove a parameter from the graph, select the desired parameter from the Parameters menu. If the menu does not display the desired parameter, select the More ... command. A dialog box with a list of all the parameters to chose from will appear.

A profile graph can only be displayed in the X or Y direction. To toggle the orientation of the graph, click on the ⊠ or ⓨ button for a profile in the X or Y direction respectively.

If the profile plot is oriented in the X direction, the coordinate intercept value refers to the point in the Y direction which the X profile passes through. The opposite is true for Y profile graphs.

The user can change the time of the profile plot in two ways. The easiest way is to use the scroll bar to quickly scan through the time periods for the desired time. The user can

also enter a time directly in the time edit box, the closest matching time period will be displayed.

8.2 Node Time Series Graph

Node time series graphs consist of a plot of parameters at a fixed point in the aquifer over the time period of simulation. To view a node graph, select Node Graph from the Windows menu. If the simulation is out of date with respect to the current input parameters, the user will be prompted to update it.
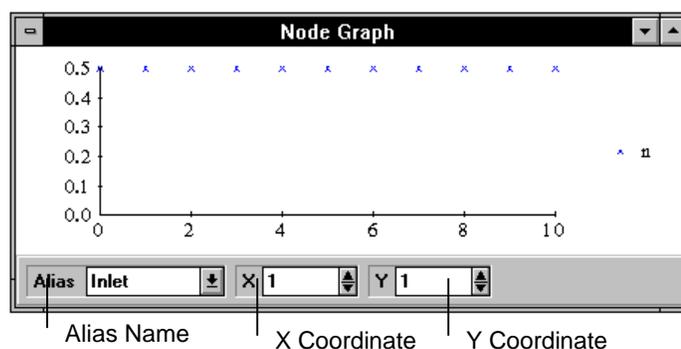

Figure 8.2 Node Profile Graph

Node graphs can display more than one parameter at a time. In order to add or remove a parameter from the graph, select the desired parameter from the Parameters menu. If the menu does not display the desired parameter, select the More ... command. A dialog box with a list of all the parameters to chose from will be displayed.

To change the node location, the user can use the X and Y coordinate edit boxes, or select the node name form the alias list.

8.3 Surface Plot

For the individual that prefers to see a larger picture than just a profile or time series at a particular point, BUGS can generate surface plots over the entire aquifer for a given parameter at a given point in time. To view a surface plot, select Surface Graph from the Window menu.

Simulation time edit box   Simulation time scrol bar
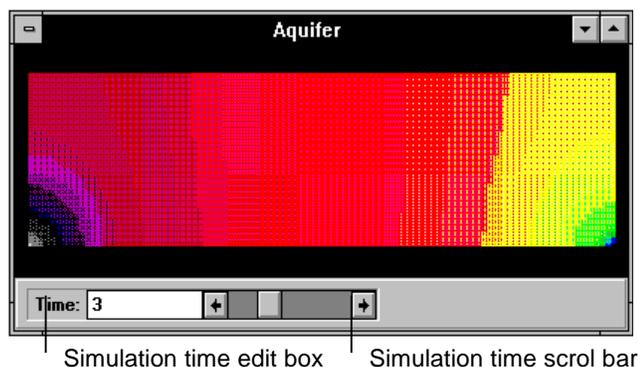
Figure 8.3 Surface Plot

The user can change the time of the profile plot in two ways. The scroll bar can quickly scan through the time periods for the desired time. The user can also enter a time directly in the time edit box, the closest matching time period will be displayed.

8.4 Tabular Output

The most useful output feature provided by BUGS is the tabular output table. The numbers in this table can be transferred to other programs via the clipboard. To view the output grid, from the Windows menu, select Output. Figure 8.4 illustrates a typical output screen.

	0	1	2	3	4
0	100.000	99.293	98.586	97.879	97.172
1	99.293	98.586	97.879	97.172	96.464
2	98.586	97.879	97.172	96.464	95.757
3	97.879	97.172	96.464	95.757	95.050
4	97.172	96.464	95.757	95.050	94.343
5	96.464	95.757	95.050	94.343	93.636
6	95.757	95.050	94.343	93.636	92.929
7	95.050	94.343	93.636	92.929	92.222
8	94.343	93.636	92.929	92.222	91.515
9	93.636	92.929	92.222	91.515	90.808
10	92.929	92.222	91.515	90.808	90.101
11	92.222	91.515	90.808	90.101	89.393
12	91.515	90.808	90.101	89.393	88.686

Figure 8.4 Numerical Output

The output grid can display information in any desired format or configuration. If the user desires time displayed in columns instead of Y coordinates, they simply need to position the mouse pointer over the Time caption, press down on the left mouse button, move the mouse pointer to the Y axis caption while keeping the button depressed, then release the mouse button. (This is also called Drag and Drop.) The corresponding window would then look like Figure 8.5.

	n	Kx	Ky	Qx	Qy	02
0	0.500	1.000	1.000	0.707	0.707	24.296
5534:	0.500	1.000	1.000	0.707	0.707	19.253
2274	0.500	1.000	1.000	0.707	0.707	12.785
9014	0.500	1.000	1.000	0.707	0.707	8.247
4548:	0.500	1.000	1.000	0.707	0.707	5.073
1288	0.500	1.000	1.000	0.707	0.707	3.241
B028(	0.500	1.000	1.000	0.707	0.707	2.067
3562:	0.500	1.000	1.000	0.707	0.707	1.263
D302:	0.500	1.000	1.000	0.707	0.707	0.802
7042(	0.500	1.000	1.000	0.707	0.707	0.508
2257(	0.500	1.000	1.000	0.707	0.707	0.308

Figure 8.5 Adjusted Numerical Output

In this way the output can be configured to the user's needs.

9. Communicating with Other Programs

This chapter describes how BUGS can exchange data with other programs. The primary way to exchange data is through the windows clipboard. However, the output files can be accessed directly when the use of the clipboard would be cumbersome or inappropriate. BUGS does not currently support Dynamic Data Exchange (DDE) or Object Linking and Embedding (OLE).

9.1 The Windows Clipboard

Currently, BUGS supports the windows clipboard cut, copy, and paste commands. The clipboard commands are found on the Edit menu. In addition to the edit menu, the user can use the shortcut keys Ctrl-X, Ctrl-C, and Ctrl-V for cut, copy, and paste respectively. These commands work with most text edit boxes, combo boxes, and editing grids. The utility of these commands can be easily seen with the use of editing grids. For example, say the user has a spreadsheet depicting the current concentrations of contaminant in an aquifer. The user needs to enter these initial concentrations into BUGS. Instead of entering the concentrations by hand, the user can use the copy and paste commands. Simply copy the values to the clipboard in the spreadsheet program, then switch to bugs, bring up the nodes window in grid view, select the contaminant and then use the paste command. The initial conditions are entered.

Not only can initial conditions be entered via the clipboard, output data can also be transferred. For example, if the user has a superior graphing package to that supplied by BUGS. The numerical values could be copied from the output grid and pasted into the graphing software.

9.2 Output File Format

In the case where use of the clipboard is too cumbersome or repetitive, the output file themselves can be accessed. The files are in binary format. The concentration file contains a stream of eight byte floating point numbers..

The numbers are grouped first by the parameters at a node first, then rows of nodes in the Y direction, followed by rows of nodes in the X direction, then time. For example, if the aquifer was the size of two nodes in both the X and Y directions with two parameters spanned over two time periods, the order of values would be:

Table 9.1 *.bgo Output File layout

Parameter	Y Coordinate	X Coordinate	Time Period
1	1	1	1
2	1	1	1
1	2	1	1
2	2	1	1
1	1	2	1
2	1	2	1
1	2	2	1
2	2	2	1
1	1	1	2
2	1	1	2
1	2	1	2
2	2	1	2
1	1	2	2
2	1	2	2
1	2	2	2
2	2	2	2

Future versions of BUGS may include export utilities that will port to multiple formats.

10. Menus

This chapter is presents a chronological listing of the commands available through the menu structure. They are listed in chronological order. For a discussion on a particular task to be accomplished, see Chapter 6, Editing an Aquifer System.

10.1 File Menu

The file menu contains commands associated with file operations such as loading, saving, and printing files.

New   Creates a new simulation file. If the current simulation has been changed since the last time it was saved, the user will be prompted to save it before creating the new simulation file.

Open   Opens a previously saved simulation file. If the current simulation has been changed since the last time it was saved, the user will be prompted to save it before opening the simulation file

Save   Saves the current simulation to disk under the present name.

Save As   Saves the current simulation to disk under a new file name.

10.2 Edit Menu

The edit menu contains the clipboard cut, copy and paste commands.

Cut   Instructs BUGS to copy the currently selected item to the clipboard and erase it. This command may not always be available.

Copy   Copies the currently selected item to the clipboard. This command may not always be available.

Paste   Places the current contents of the clipboard onto the selected item. Depending upon what is in the clipboard and what is selected, this command may not be available.

10.3 View Menu

This menu allows the user to change certain aspects of the working environment and types of screens shown.

Toolbar   Displays the toolbar below the menu bar. For more information on the toolbar, see the following chapter.

Status Bar   Makes the status bar visible at the bottom of the BUGS window. The status bar is a source of additional information to the user.

Form   Shows the form view of the active window. Depending on the currently active window, this command may not be available.

Grid   Displays the grid view of the active window. Depending on the currently active window, this command may not be available.

10.4 Run Menu

This menu allows the user to set simulation run time options and to run the simulation.

Simulate   Runs a simulation. It is only available if the simulation has been saved to disk.

Options   This command brings up a dialog box that allows the user to override the default global time calculation and to set the value of the operational definition of zero.

10.5 Parameters Menu

If this menu is visible, it allows the user to select a parameter from the list of available parameters. Depending on the active window, multiple parameters may be selected at a time. A check denotes a selected parameter. If there are more parameters than can be displayed on the menu, the More... command will be visible. Selecting this command will show a dialog box containing a list box of all the parameters to chose from.

10.6 Window Menu

Tells BUGS to display the various editing and output windows.

Aquifer Properties	This window allows the user to edit the size of an aquifer, grid spacing, starting and editing times, and the default reaction system.
Parameters	Displays a window which can add and remove parameters, edit parameter dispersion properties, and specify initial values.
Nodes	Displays window which specifies prescribed heads, placement of reaction systems, and edits parameter initial values.
Reactions	Displays a window which can add and delete reactions, specify reaction types, edit rate data, edit Stoichiometry data, and to link and unlink reactions and reactions systems.
Reaction Systems	Displays a window which can add and remove reaction systems and to link and unlink reactions and reaction systems.
Profile Graph	Displays a graph of parameters in a cross-section through the aquifer at a snapshot in time. This window is only available if the simulation is current or up to date.
Node Graph	Displays a graph of parameters at a give node over the time of simulation. This window is only available if the simulation is current or up to date.
Surface Graph	Displays a surface plot of a parameter throughout the aquifer at a given time. this window is only available if the simulation is current or up to date.
Output	Displays a configurable grid of output values. By using drag and drop, the grid can be configured for the display desired by the user. This window is only available if the simulation is current or up to date

11. Toolbar

The toolbar can be used as a shortcut to the menu system. The commands are carried out by simply clicking on the appropriate toolbar button. The standard BUGS toolbar is shown in Figure 11.1

Figure 11.1 BUGS Toolbar

The following is a description of the options.

New creates a new BUGS simulation file

Open opens an existing BUGS simulation file

Save saves the current BUGS simulation file

Form switches the active window to form view

Grid switches the active window to grid view

12. Command Keys

Some of the menu commands also have corresponding command keys, or shortcut keys. Table 12.1 lists the actions and associated command keys. "Ctrl" refers to the control key, "Alt" refers to the Alt key. The hyphen means to press the two keys simultaneously. For example, Ctrl-X means to hold down the Ctrl key and press the X key.

Table 12.1 Command Keys

Task	Key
Open	Ctrl-F12
Save	Shift-F12
Save As	F12
Cut	Ctrl-X
Copy	Ctrl-C
Paste	Ctrl-V
Run Simulation	F5
Exit	Alt-F4

13. Examples and Lessons

The purpose of this chapter is to give the user hands on experience in BUGS SCRATCHPAD. These step-by-step instructions will guide the user in quickly creating an aquifer simulation and viewing the results. It is recommended the user follow along with these lessons on the computer. However, this is not absolutely necessary as, all relevant pictures are included in the text.

Currently there are four lessons in this chapter, each is designed to build on the previous lesson. Lesson One shows how to create a one dimensional solute transport simulation using a conservative solute with a constant source at the inlet. Lesson Two adds kinetic sorption to the simulation. Lesson Three adds a first order decay reaction and Lesson Four expands the simulation to two dimensions. The lessons in this section provide a brief overview of some of the tools provided by BUGS SCRATCHPAD. Complete descriptions of all the tools were discussed in previous chapters.

13.1 Lesson 1, Conservative Solute Tracer Simulation

This tutorial will step through the tasks necessary to create a one dimensional, constant source conservative solute tracer simulation. The following table presents the input parameters in this tutorial.

Parameter	Value	Units
Aquifer Length	100	meter
Grid Spacing	1	meter
Starting Time	1	day
Ending Time	10	day
Output Timestep	1.0	day
Longitudinal Dispersitivity	1.0	meter
Transverse Dispersitivity	0.1	meter
Effective Diffusion	0.0	sq.meter/day
Constant Inlet Concentration	10.0	mg/l
Effective Porosity	0.5	cu.meter/cu.meter
Pore Water Velocity	2.0	meter/day

Roughly speaking, conducting this BUGS™ SCRATCHPAD simulation can be divided into 10 steps:

1. Starting the Program
2. Defining the Grid Mesh
3. Adding the Conservative Solute
4. Creating the Boundary Condition "Reaction"
5. Creating the Reaction Systems
6. Assigning Reaction Systems to Nodes
7. Setting the Hydraulic Flow Conditions
8. Saving the Simulation Project File.
9. Running the Simulation
10. Viewing Results

These steps are described below:

1.   Start BUGS SCRATCHPAD.

To start BUGS SCRATCHPAD, either double click on the program icon (Windows 3.1) or select BUGS SCRATCHPAD from the Start Menu -> Programs -> BUGS SCRATCHPAD program group (Windows '95).

After loading, BUGS SCRATCHPAD presents the main window. The program is ready to accept input for a new simulation.
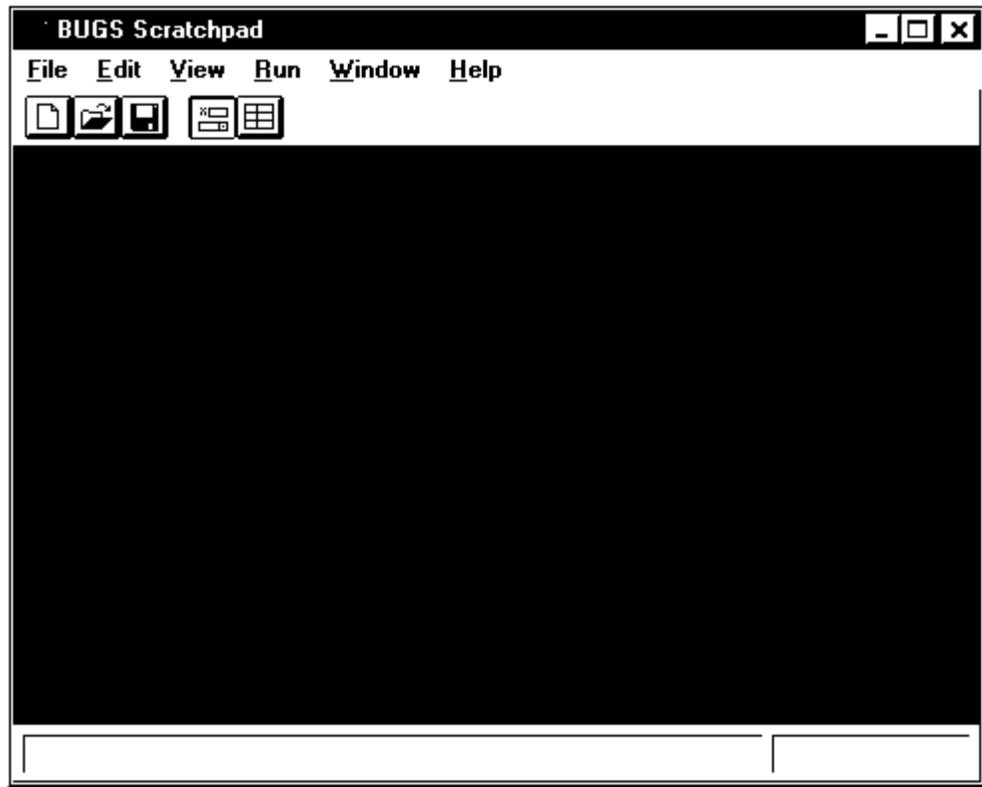
2.   Define the Aquifer Grid Mesh.

The first thing to is to define the size and shape of the aquifer mesh. This is done from the *Aquifer Parameters* window. To bring up this window select **Aquifer Properties** from the **Window** menu.
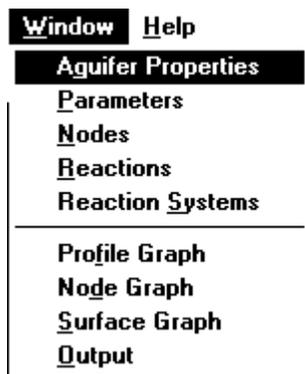
The *Aquifer Parameters* window will appear. The grid mesh spacing is 1.0 meters, which is the same as the default (the *dX* field). However, the number of nodes in the X direction needs to be changed to 100 (the *X* field). This will result in an aquifer length of 100 meters. (100 nodes spaced 1 meter apart).
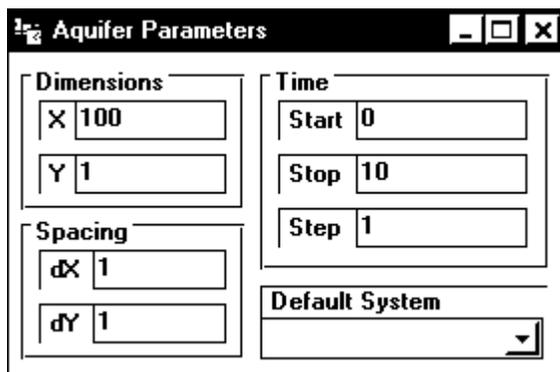
Also notice, the *Time* group, this is where the starting and ending times for the simulation are entered. Also, the *Step* field refers the timestep in which results are recorded. (The default is for recording the results every 1 time unit.) Since the default values are the same used for this tutorial, they do not need to be modified.

The *Default System* will be explained later below.

Close the *Aquifer Parameters* window.

3.   Add the Conservative Solute

The next step is to add the Conservative Solute. This will be done from the *Parameters* window. To display the *Parameters* window, select **Parameters** from the **Window** window.

Window **Help**

> **Aquifer Properties**
> **Parameters**
> **Nodes**
> **Reactions**
> **Reaction Systems**
>
> **Profile Graph**
> **Node Graph**
> **Surface Graph**
> **Output**
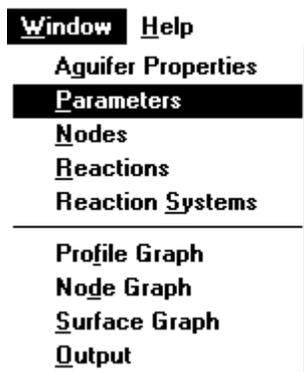
The *Parameters* window will appear.

Parameters   **_ □ ×**

H	**Default Initial Value** 0
Q	
n	┌ **Initial Value at Nodes** ┐
Kx	
Ky	**(none)** X 1
Qx	
Qy	Y 1
	Initial Value
	0
Remove | **Add**	**Reset All** **Default**
☐ **Mobile Parameter**	
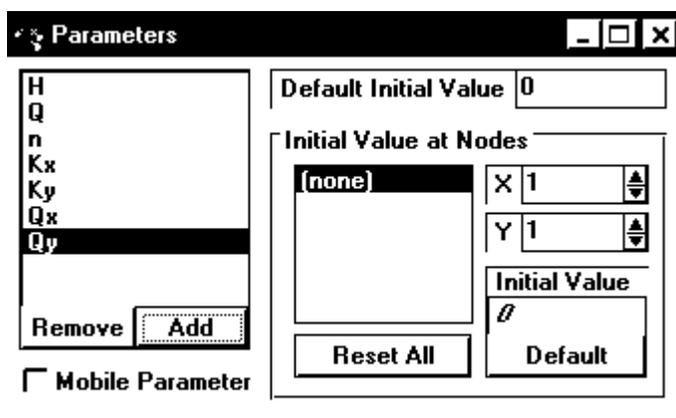
Parameters represent many things in a BUGS SCRATCHPAD simulation. They can represent system defined data such as porosity, hydraulic head, as well as user defined solutes and sorbed species. They are grouped together as "Parameters" for the convenience of providing a uniform method to enter simulation initial values.

The first thing to do is add the conservative solute. This will be a user defined parameter. To add the parameter, click on the *Add* button.

Add

The *New Parameter* dialog box will appear. Enter "O2" as the name for the new parameter (conservative solute) and click the *OK* button.

New Parameter   **×**

> **Please Enter a name for the new parameter.**   **OK**
>
> O2   **Cancel**
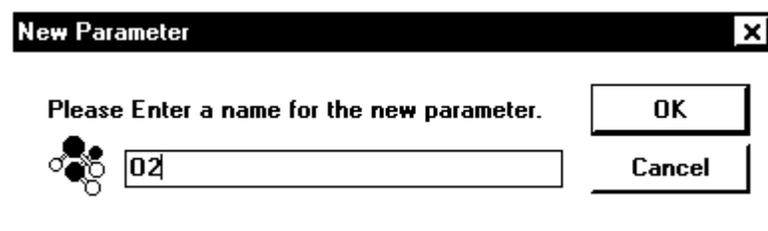
The *Parameters* window will change to the following.
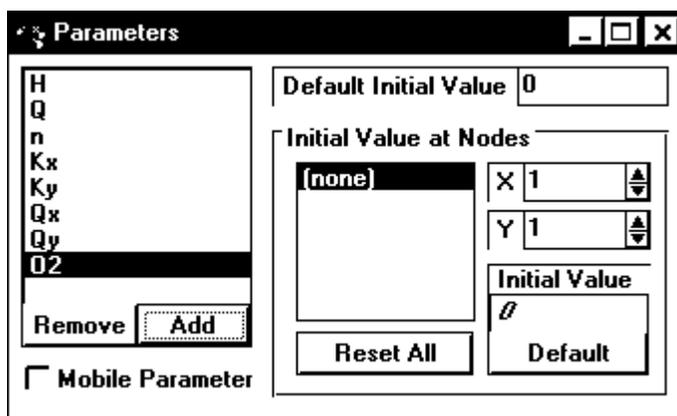
The default parameter type for a user parameter is an *Imobile* parameter (sorbed species). This needs to be changed to a *Mobile* parameter (mobile solute species). To change the new parameter from a *Imobile* to a *Mobile* parameter, first make sure that "O2" is selected in the list box, then check the *Mobile Parameter* checkbox.

The *Parameters* window expands to show some additional data entry fields for a mobile parameter (solute species).
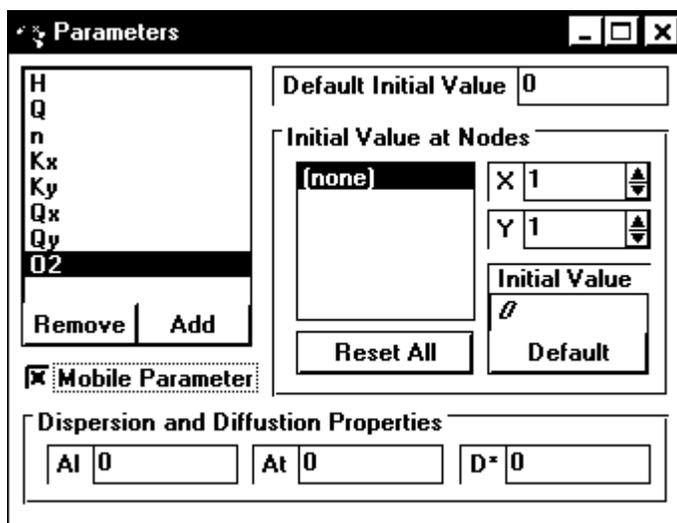
Al, At, and *D** are the longitudinal dispersitivity, transverse dispersitivity, and effective diffusion coefficients respectively. Change the default values of the longitudinal and transverse dispersitivity to 1.0 and 0.1 respectively. The effect of diffusion is ignored in this simulation.
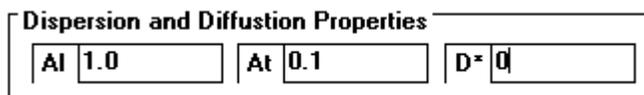
Close the *Parameters* window.

4. Create the Boundary Condition "Reaction"

Next, it is necessary to create the constant source boundary condition. In BUGS SCRATCHPAD, boundary conditions are entered a bit differently than in traditional groundwater modeling programs. BUGS SCRATCHPAD represents boundary conditions using *Reactions*. The primary way BUGS SCRATCHPAD manipulates the values of parameters in a simulation is through *Reactions*, therefore it makes sense to describe a constant source boundary condition through a *Reaction*. This opens the door to many possibilities with specialized boundary conditions. For example, BUGS SCRATCHPAD provides a *Reaction* that is dependent upon the simulation time, thus a timed pulsing nutrient injection well boundary condition can be represented by a reaction almost as easily as a constant source can be, as in this simulation.

To create the reaction to represent the constant source boundary, select **Reactions** from the **Window** menu.
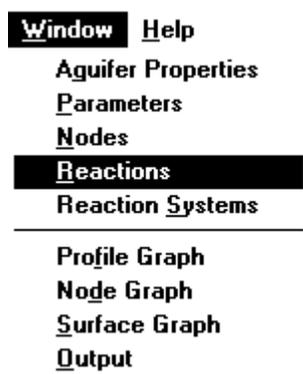
Since this as a new simulation, no reactions have been defined yet. BUGS SCRATCHPAD immediately prompts for a new reaction name.
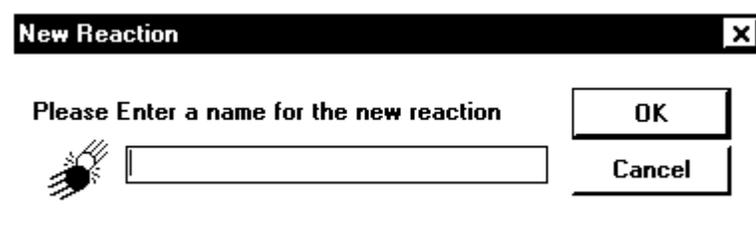
Enter "Constant Source" for the name of the reaction and press the *OK* button.

New Reaction ☒

Please Enter a name for the new reaction   [OK]

[Constant Source]   [Cancel]
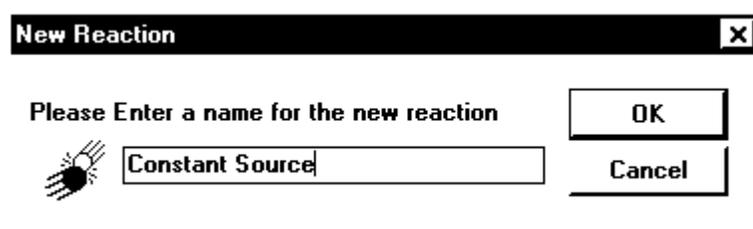
BUGS SCRATCHPAD displays the *Reactions* window with the "Constant Source" *reaction* highlighted in the list box.

Reactions   _ ▢ ☒

| Type | Rate | Stoichiometry | Systems |

Name
Constant Source

Equilibrium
⦿ Standard
○ Equality
○ Target

Ordered
○ Single
○ Mixed

Eq. Isotherm
○ Linear
○ Langmuir
○ Freundlich

Other
○ Mass Tr.
○ Rule Cv.

Monod
○ Single
○ Double
○ Competitive

Kin. Isotherm
○ Linear
○ Langmuir
○ Freundlich

[Remove] [Add]
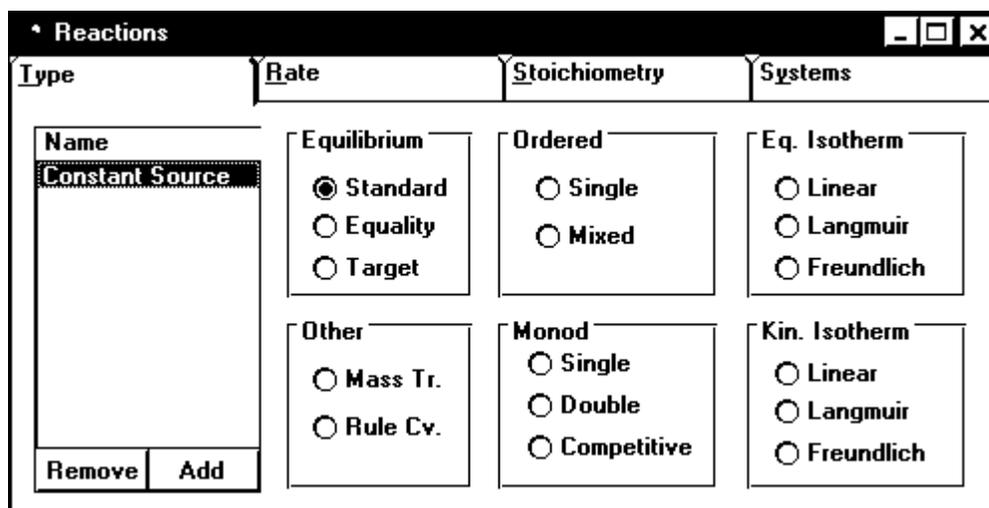
Since the *Type* tab in the *Reactions* window is already activated, the window displays the available types of reactions. The default is *Standard Equilibrium*. The type of reaction used to represent a constant source is the *Equality Equilibrium* reaction. This type of reaction is the simplest of all reactions that BUGS SCRATCHPAD provides. It simply adjusts the value of a parameter to the set value at every timestep (just what a constant source does).

To select the *Equality Equilibrium*, click on the *Equality* in the *Equilibrium* group.

Equilibrium
○ Standard
⦿ Equality
○ Target
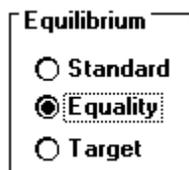
Now to show the window to describe the details of this constant source reaction, click the *Rate* tab.

Rate

This reaction allows the user to specify that a parameter will be adjusted to equal a value defined by a linear combination of all the available parameters at that node. However, this simulation is only interested in a constant value, so this extra ability will be ignored for now. The only two data values that need to be entered are the dependent parameter (O2) and the value to set the dependent parameter to (10).

In the *Depndt.* combo box, select "O2".

Depndt.	O2	▼

Constant
- H
- Q
- n
- Kx
- Ky
- Qx
- Qy
- **O2**

In the *Coeffient.* field, enter "10".

Constant	10

Notice that BUGS SCRATCHPAD echoes the equality reaction equation as it is being built in the window below the *Coefficnt.* field. (O2 = 10).

• Reactions 　　　　　　　　　　　　　　 ＿□✕

Type	Rate	Stoichiometry	Systems

Name				Parameter	Coeff.	▲
Constant Source	Depndt.	O2 ▼		H	0	
	Constant	10		Q	0	
				n	0	
				Kx	0	
				Ky	0	
		O2 = 10		Qx	0	
				Qy	0	
				O2	0	
Remove	Add					▼

This is all that needs to be done with this window, the *Systems* tab will not be used at this time. *Reaction Systems* are explained below.

Close the *Reactions* window.

5.　　Create the Reaction Systems

Reaction Systems are the means by which the user tells BUGS SCRATCHPAD which reactions occur at which nodes in an aquifer simulation. They allow the user to group different sets of reactions and name the set of reactions. Then the user tells BUGS SCRATCHPAD that this collection of reactions occurs at a particular region in the aquifer. A *Reaction* can belong to any number of *Reaction Systems* but only one *Reaction System* can occur at any one node.

This particular simulation requires two *Reaction Systems*. One for the boundary condition, and one for the remainder of the aquifer.

To bring up the *Reaction Systems* window, select **Reaction Systems** from the **Window** menu.
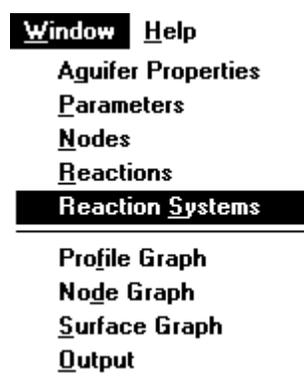
Since this as a new simulation, no *Reaction Systems* have been defined yet. BUGS SCRATCHPAD immediately prompts for a new *Reaction System* name.
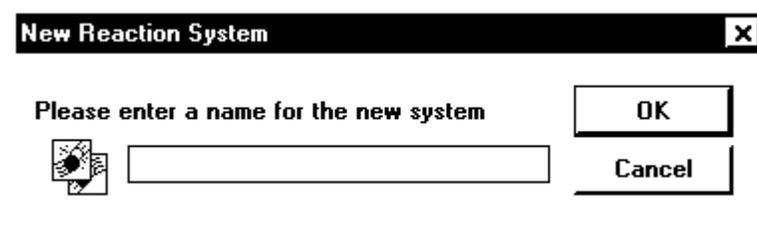
Enter "Boundary Condition" for the new *Reaction System* name and press the *OK* button.
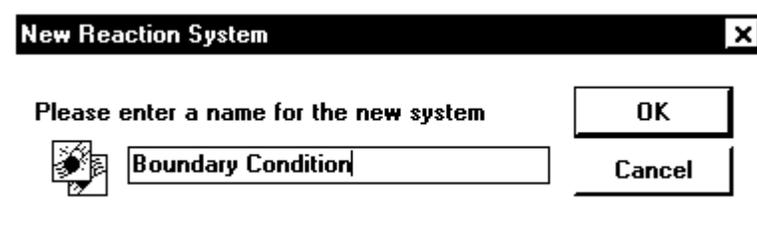
BUGS SCRATCHPAD displays the *Reaction Systems* window with the "Boundary Condition" *Reaction System* highlighted in the list box.
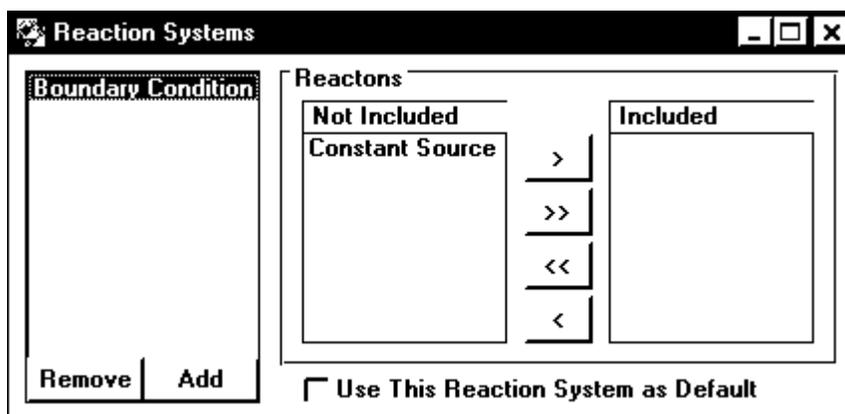
Notice that the "Constant Source" *Reaction* is also displayed in the *Not Included* list. This means that "Constant Source" is not included in the "Boundary Condition" *Reaction System*. This needs to be changed. To include the "Constant Source" *Reaction* in the "Boundary Condition" *Reaction System*, first click on "Constant Source" in the *Not Included* list ("Boundary Condition is already

selected) and click on the ▷ button. The *reaction* now appears in the *Included* list.
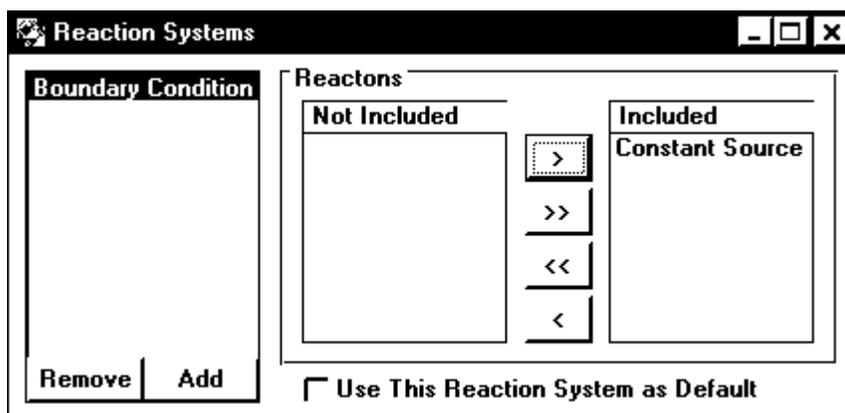
The "Boundary Condition" *Reaction System* will be placed at the inlet node, as described later. Now it is necessary to define the *Reaction System* that will represent the remainder of the aquifer. Since this is a conservative tracer simulation, the second reaction system will contain now reactions, but it still must be defined anyway.

Click on the *Add* button to bring up the *New Reaction System* Dialog. Enter "Interior" for the name of the new *Reaction System* and press the *OK* button.
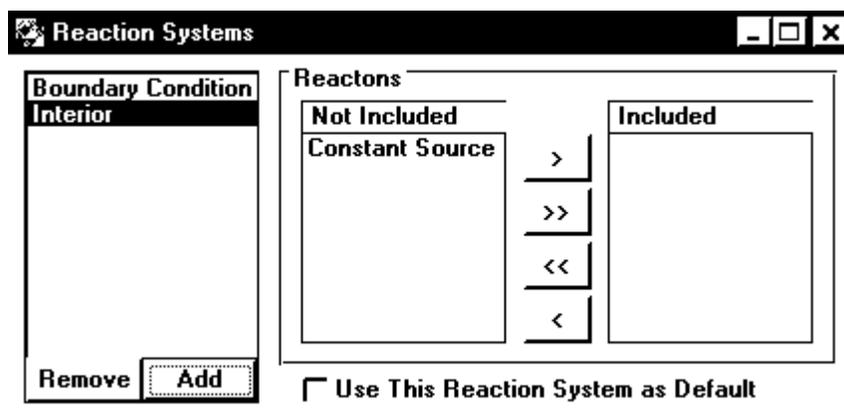
The "Interior" *Reaction System* will reside at every node in the aquifer except for the inlet. Therefore it will become the *Default System* (so that each node does not have to be specifically assigned this reaction system). Check the *Use This Reaction System as Default* checkbox at the bottom of the *Reaction Systems* window.

Close the *Reaction Systems* window.

6. Assign Reaction Systems to Nodes

The next step is to tell BUGS SCRATCHPAD where the reaction systems are located in the aquifer. This is done through the *Nodes* window.

To bring up the *Nodes* window, select **Nodes** from the **Window** menu.
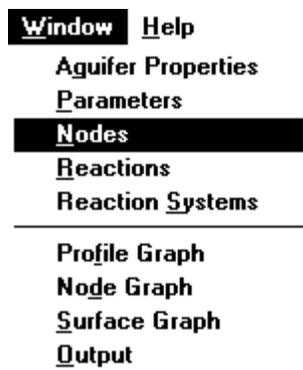
BUGS SCRATCHPAD will display the *Nodes* window.

The *Nodes* window provides the interface for the user to tell BUGS SCRATCHPAD which *Reaction Systems* occur at which nodes in the aquifer. Since constant source the boundary condition occurs only at the aquifer "inlet" (node 1), this well be an easy task. The current node is already set at coordinate (1,1) which will be the inlet node for the aquifer. To change the default *Reaction System* for this node, select "Boundary Condition" from the *System* field.

Since "Interior" is the default *Reaction System*, the rest of the nodes will use "Interior" as their *Reaction System*.

Leave the *Nodes* window open for the next step.

7. Set the Hydraulic Flow Conditions.

The last data entry step is entering data on the flow conditions. The desired pore water velocity is 2.0 m/d. Since the effective porosity is 0.5, this would correspond to a darcy velocity of 1.0 m/d. Since hydraulic conductivity was not given, (nor is it important for this tutorial) we'll assume it to be 1.0 m/d, resulting in a desired head gradient of 1.0 m/m. Now assuming a free outlet condition at the end of the aquifer, and a relative head of 0.0 m; the head at the entry of the aquifer would be 99 m. (Since node coordinates are block centered, the actual distance is 99 m between end nodes for this simulation.)

Therefore, to set the desired flow conditions, the initial hydraulic heads at both ends of the aquifer should be entered, and BUGS SCRATCHPAD should be notified that both end nodes in the aquifer are *Prescribed Head* nodes.

Since the current node is (1,1), it is easy to start there. To notify BUGS SCRATCHPAD that this is a *Prescribed Head* node, check the *Prescribed Head* checkbox.

☒ Prescribed Head

Next, With *Parameter* selected to hydraulic head ("H"), enter "99" in the *Value* field in the *Initial Parameter Values* group.

Initial Parameter Values
Value 99

Parameter
H
Kx
Ky
n
O2

Use Default Value

Next, BUGS SCRATCHPAD needs to be told that the outlet node is also a prescribed head. Change the coordinates to node (100,1). (A trick is to click on the up arrow in the spin control for *X*, it will automatically wrap around to the end of the aquifer).

Coordinates
X 100   99
Y 1   0

As before, check the *Prescribed Head* checkbox.

☒ Prescribed Head

Now the necessary information for the flow conditions has been entered (The default hydraulic head value at the end node is 0, so there is no need to change it). BUGS SCRATCHPAD will automatically calculate the hydraulic heads and flow field for the remainder of the nodes in the aquifer grid during calculation initialization.

Close the *Nodes* window.

8.   Save the Project File

Before running an aquifer simulation in BUGS SCRATCHPAD, the project file must be saved. To save the file, select **Save** from the **File** menu.

```
File  Edit  View  Run  Window  H
   New
   Open           Ctrl+F12
   Save           Shift+F12
   Save As        F12
   Save Special ...

   Print          Shift+Ctrl+F12
```
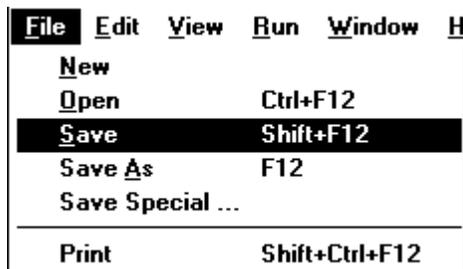
The user will be prompted with the standard windows save dialog. Enter whatever is appropriate for your system and press *OK*.

```
Save As                                    ? X

File name:          Folders:              OK
csource.bgs         c:\bugs
                                          Cancel
                    c:\
                    bugs                  Network...

Save file as type:  Drives:
Bugs File (*.bgs)   c: deuteronomy
```
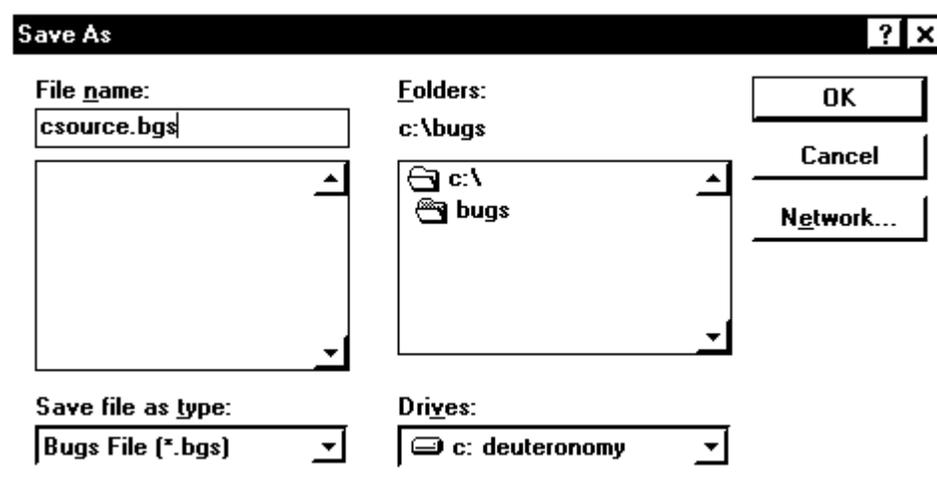
9.   Run the Simulation

The next step is to run the simulation, and save the file afterwards. To run the simulation select **Simulate** from the **Run** menu.

```
Run  Window  He
   Simulate  F5

   Options
```

BUGS SCRATCHPAD launches a separate calculation program and waits for its termination.
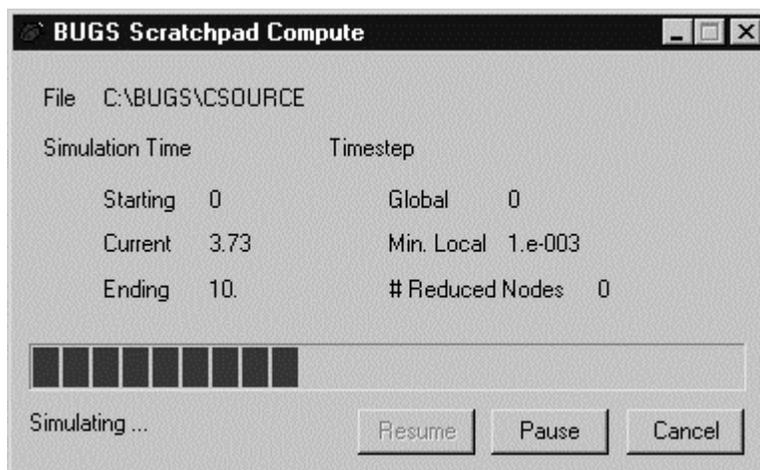
Save the file by selecting **Save** from the **File** menu.
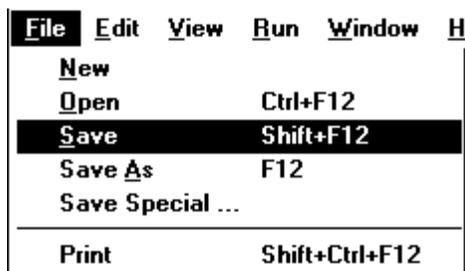
Now the results of this simulation can be viewed.

10. Viewing Results

BUGS SCRATCHPAD provides two primary ways to view results, table output and graphs. The output graphs come in two varieties as well, profile and node. The profile graphs show concentration profiles through the aquifer at a given point in time. The node graphs plot the concentration value over time at a single location within the aquifer.

To view a profile graph, select **Profile Graph** from the **Window** menu.
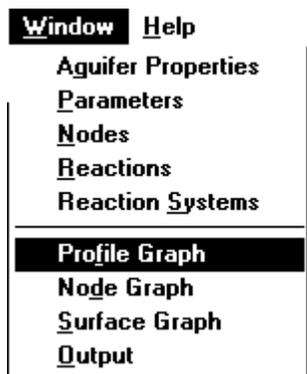
BUGS SCRATCHPAD displays the *Profile Graph* in the default configuration.
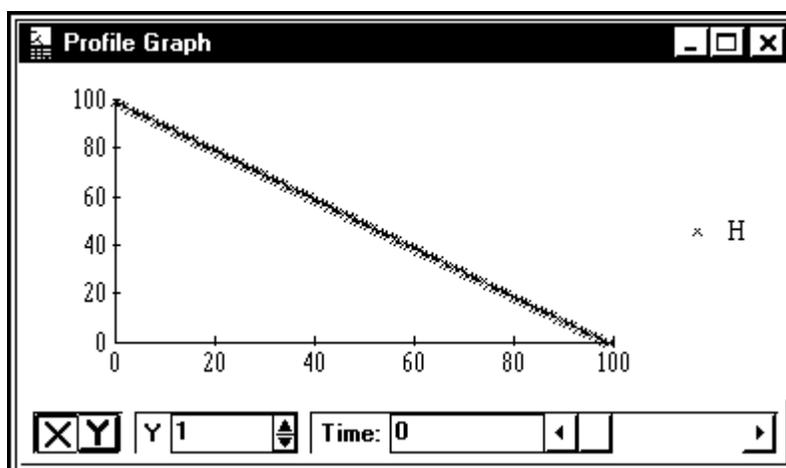
The profile of hydraulic head is not all that interesting, lets look at the conservative solute profile at the ending timestep.

From the **Parameters** select "O2" and then un-select "H".
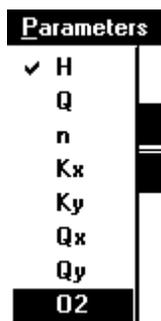
Now, slide the scroll bar all the way to the right to select the last timestep.
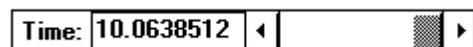
The *Profile Graph* is now configured to show the concentration profile at the last timestep.
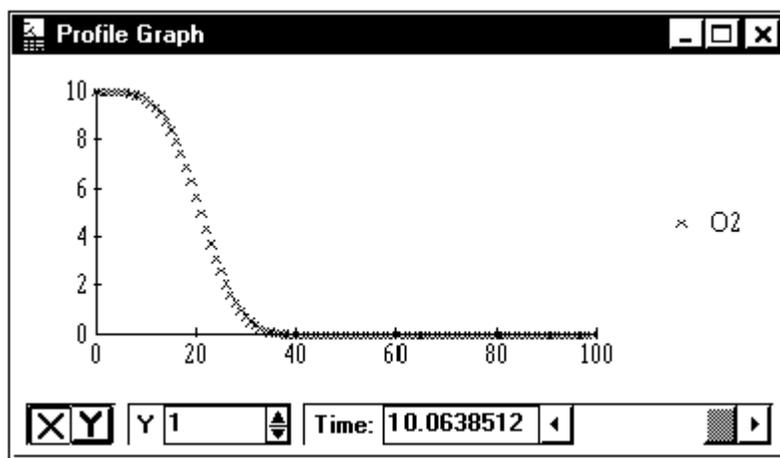
To review tabular results, select **Output** from the **Window** menu. Viewing various results in this window is left for the reader to discover. However, it is worth mentioning that the output grid can be configured by draging lables around via. Windows Drag and Drop. Poke around a bit to see how it works.

13.2 Lesson 2, Kinetic Sorption and Desorption

This lesson will demonstrate how to add a partitioning reaction to a simulation. This lesson uses the simulation created in Lesson One. If the simulation in lesson one is still open, close all windows and save it. If it is not open, then open it with the Open command from the file menu.
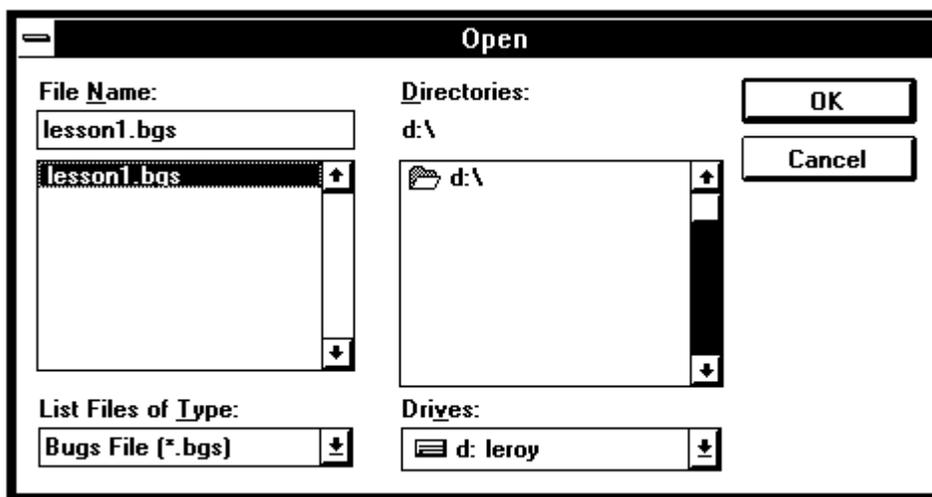
First, save the simulation under another name. From the File menu, select Save As. In the save as dialog box enter any appropriate name, for example "Lesson2".
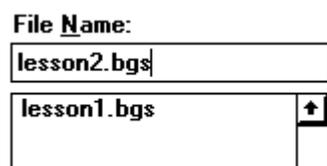
It is necessary to add a parameter to the simulation to represent the sorbed phase of O2. From the Windows menu, select Parameters.
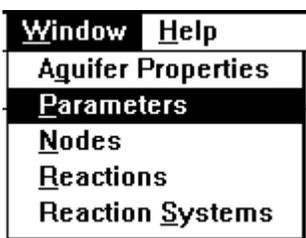
Click the Add button and enter "O2 (s)" as the name of the new parameter (sorbed species.)

This is an immobile (sorbed) parameter, therefore all the default values are adequate. Close the Parameters window. From the Windows menu, select Reactions.

Next we'll add a reaction representing the partitioning of the solute and sorbed phase (partitioning "O2" and "O2 (s)"). Click on the Add Button and enter "O2 Partitioning" as the name of the reaction.

This reaction will be a kinetic linear isotherm partitioning reaction. Bring up the Type screen by clicking on the Type tab if necessary.

Select Linear under the Kinetic Sorption reaction type.

Next we'll add the rate data for the partitioning reaction. Select the Rate tab.

The rate data will appear. The linear driving force will be a one to one ratio between "O2" and "O2 (s)". Enter values so that they match the following example.

$$\text{Rate} = \boxed{.5}\ \left(q^* - \boxed{O2 \text{ (s)}\ \boxed{\pm}}\right)$$

$$q^* = \boxed{1}\ \times\ \boxed{O2\ \boxed{\pm}}$$

Now that the rate data is entered, enter the Stoichiometry data. Click on the Stoichiometry tab.

Stoichiometry

The solute, O2, will be moving to the Sorbed phase, O2 (s), when the rate is positive. For O2 enter -1.0. For O2 (s) enter 1.0.

qy	0
O2	-1.0
O2 (s)	1.0

BUGS will then display the Stoichiometry reaction.

1 O2 --> 1 O2 (s)
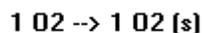
Next, add this reaction to the entire aquifer system. Click on the Systems tab.

Systems

To include this reaction in all of the reaction systems, click on the include all button, this includes the reaction in both the "Boundary Condition" reaction system and "Interior" reactions system.

>>

Now this reaction will be included both in the boundary condition reaction system and the interior reaction system.

Contained In
Boundary Condition
Interior

Close the reactions window. Save the simulation data before running the simulation. A shortcut way of saving a simulation is to click the Save button on the tool bar.

Run the simulation, chose Simulate from the Run Menu

```
Run  Window
 Simulate F5
 Options
```

The screen will appear similar to the following.

```
Reading in Data . . .
Allocating Arrays . . .
      2400 for Diffusion Properties
      24 for Dispersion Properties
      14400 for Parameters
      200 for Nodes
      1616 for Coorinates
Initializing Hydraulic Heads . . . Done
Computing Flows. . Done
Starting Simulation
Global Timestep is 0.12375
    Global Timestep 0
    Global Timestep 1.11375
    Global Timestep 2.10375
    Global Timestep 3.09375
    Global Timestep 4.08375
    Global Timestep 5.07375
    Global Timestep 6.06375
    Global Timestep 7.05375
    Global Timestep 8.04375
    Global Timestep 9.03375
    Global Timestep 10.0237

Pogram Terminated Normally
```

To view the profile output select Profile Graph from the Windows menu. From the Parameters menu ensure O2 and O2 (s) are checked. Move the time period to 7. The graph should appear to be similar to the following.
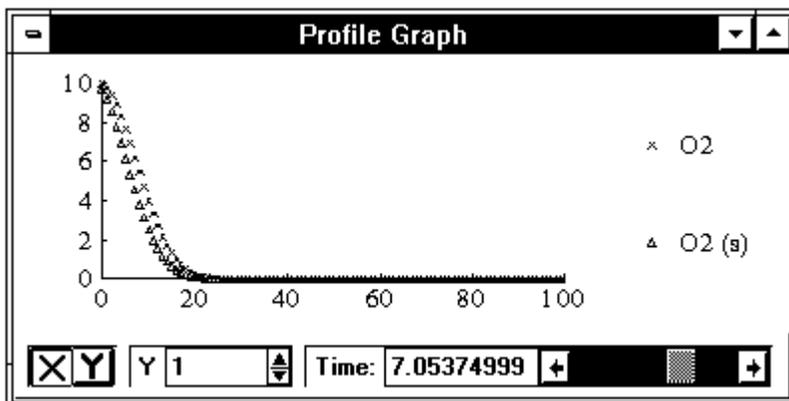
Notice, the O2 (s) front lags behind the O2 Solute front, as it should with kinetic sorption.

This concludes lesson two.

13.3 Lesson 3, First Order Decay

This lesson demonstrates how to set the default initial value of a parameter and add first order decay to a simulation. This lesson uses the simulation created in lesson one. If the simulation in lesson one is still open, close all windows and save it. If it is not open, then open it with the Open command from the file menu.
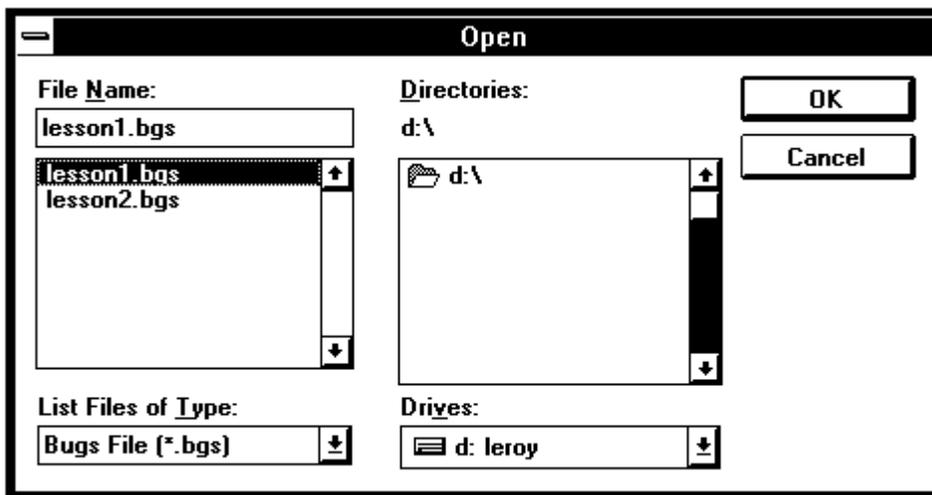
Save the simulation under another name. From the File menu, select Save As. In the save as dialog box enter any appropriate name, for example "Lesson3".
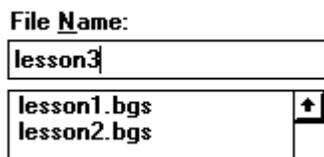
For this simulation, the aquifer will have an initial uniform concentration of O2 of 10 throughout the aquifer. From the Windows menu, Select Parameters.
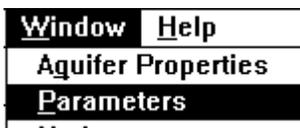
Select "O2" in the list box and then enter a default concentration of 10.

A first order decay reaction will be added to the simulation. From the Windows menu, select Reactions.

Window   Help
- **A**quifer Properties
- **P**arameters
- **N**odes
- **R**eactions
- **Reaction S**ystems
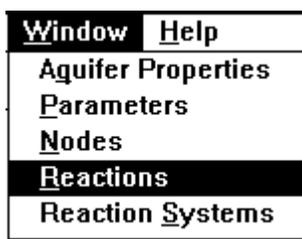
Click the Add button and enter "Decay" as the name for the new reaction.

New Reaction

Please Enter a name for the new reaction   **OK**

Decay| **Cancel**
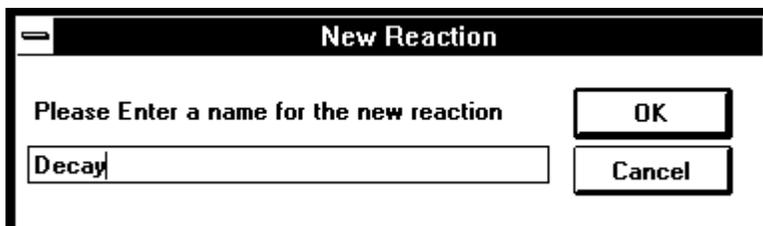
Click on the Type Tab to bring up the type information screen if necessary:

Type
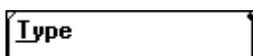
Select the first order reaction option.

Ordered
- ⦿ Single
- ◯ Mixed
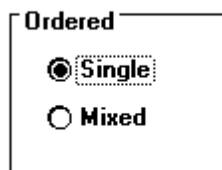
Now, enter rate data. Click on the Rate tab.

Rate

The first order reaction will have a rate constant of 0.5, enter the values on the screen as they appear below.

Rate = .5   × O2 ▼   1

Now, define the Stoichiometry for the reaction. Click on the Stoichiometry tab.

Stoichiometry

"O2" will be decaying to nothing. Enter -1 for the coefficient for O2.

uy	u
O2	-1

BUGS will echo the Stoichiometry reaction.

1 O2 --> Nothing

Add this reaction to a reaction system. Click on the Systems tab.

Systems
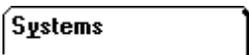
Select "Interior" in the unused list box

Not Contained In
Boundary Condition
Interior
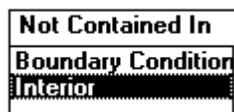
and click the include button.

>

The simulation is now ready to run. Close the reactions window and save the file.

File Edit View Ru
New
Open   Ctrl+F12
Save   Shift+F12
Save As F12   or

Select Simulate from the Run menu:

Run Parameter
Simulate F5
Options
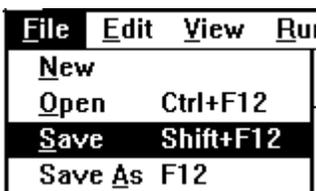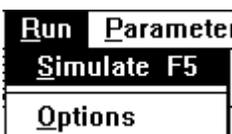
When the simulation is done, save the file once again. Now, from the Windows menu select Profile Graph. Below is an example of the O2 profile at timestep seven.

Profile Graph
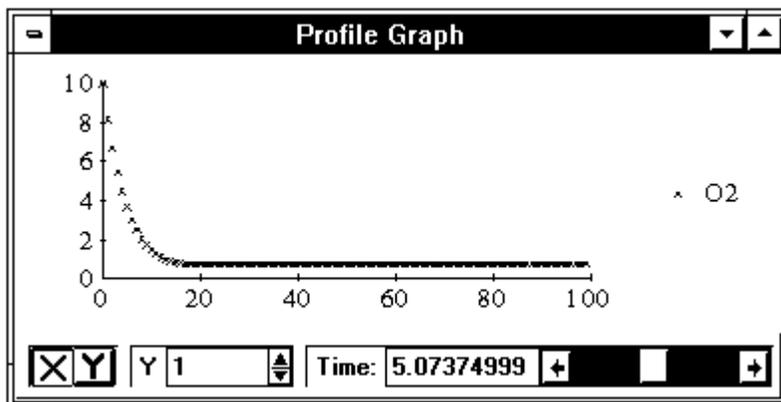
This concludes lesson 3.

13.4 Lesson 4, Two Dimensional Tracer Simulation

This lesson explains how to expand a one dimensional simulation into a two dimensional simulation. This lesson uses the simulation created in lesson one. If the simulation in lesson one is still open, close all windows and save it. If it is not open, open it with the Open command from the file menu.
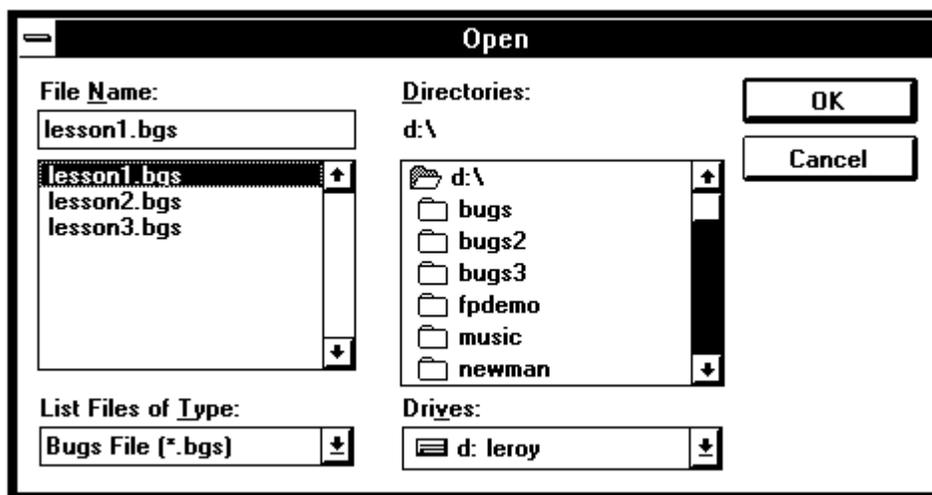
First, expand the aquifer size. From the Windows menu, select Aquifer Properties.

In the number of Y coordinates box, enter 30.
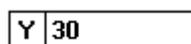
All other values are satisfactory. Close the window. A uniform velocity in the X direction will be used for this simulation. From the Windows menu, select Nodes.
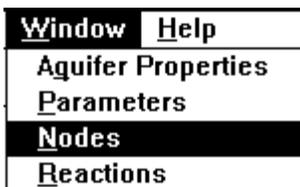
Change all of the coordinates along the Y axis where X is 1. For each node along the Y axis where X is 1, ensure the prescribed check box is checked, and the value of head is 100. (This is the time consuming way of doing it, for quicker ways of entering prescribed conditions, see Specifying Initial Values of Parameters.)

Coordinates
X | 1 | | 0
Y | 2 | | 1

and

☒ Prescribed Head

and

Initial Parameter Values
Value | 100

Parameter
H
Kx
Ky

Each node along the Y axis where X = 100 must be set to a prescribed head as well. The value for prescribed head of zero need not be changed.

Coordinates
X | 100 | | 99
Y | 2 | | 1

and

☒ Prescribed Head

Next, the constant source will be moved to the middle of the edge of the aquifer. The reaction system at node (1,1) should be set to "Interior"

System | *Interior*

and the reaction system at node (1,15) should be set to "Boundary Condition".

Coordinates
X | 1 | | 0
Y | 15 | | 14

and

System | Boundary Cond

All the necessary changes have been made, save the file as "lesson4.bgs" and run the simulation. When the simulation is done, select Surface Graph from the Windows menu. Then ensure O2 is checked in the Parameters menu. The surface plot of O2 at time period 7 is
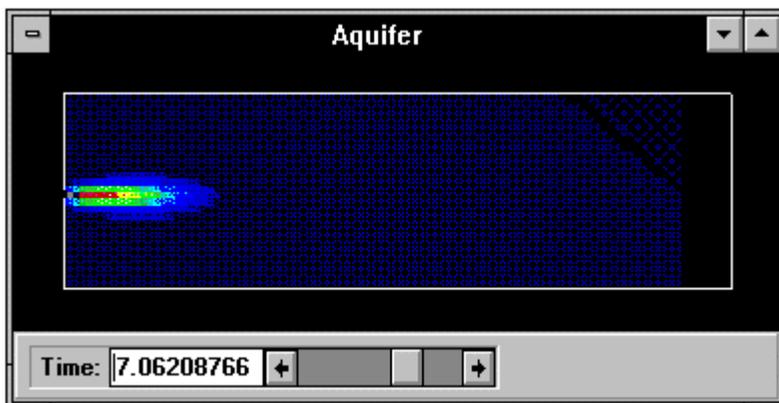
This concludes lesson 4.

14. References

Fabritz, Jason E., (1994). *A Two-Dimensional Numerical Model for Simulating the Movement and Biodegradation of Contaminants in a Saturated Aquifer*, Master's Thesis, Department of Civil Engineering, The University of Washington.

Fetter, C. W., (1993), *Contaminant Hydrogeology,* Macmillan Publishing Company, New York, New York.

15. Index