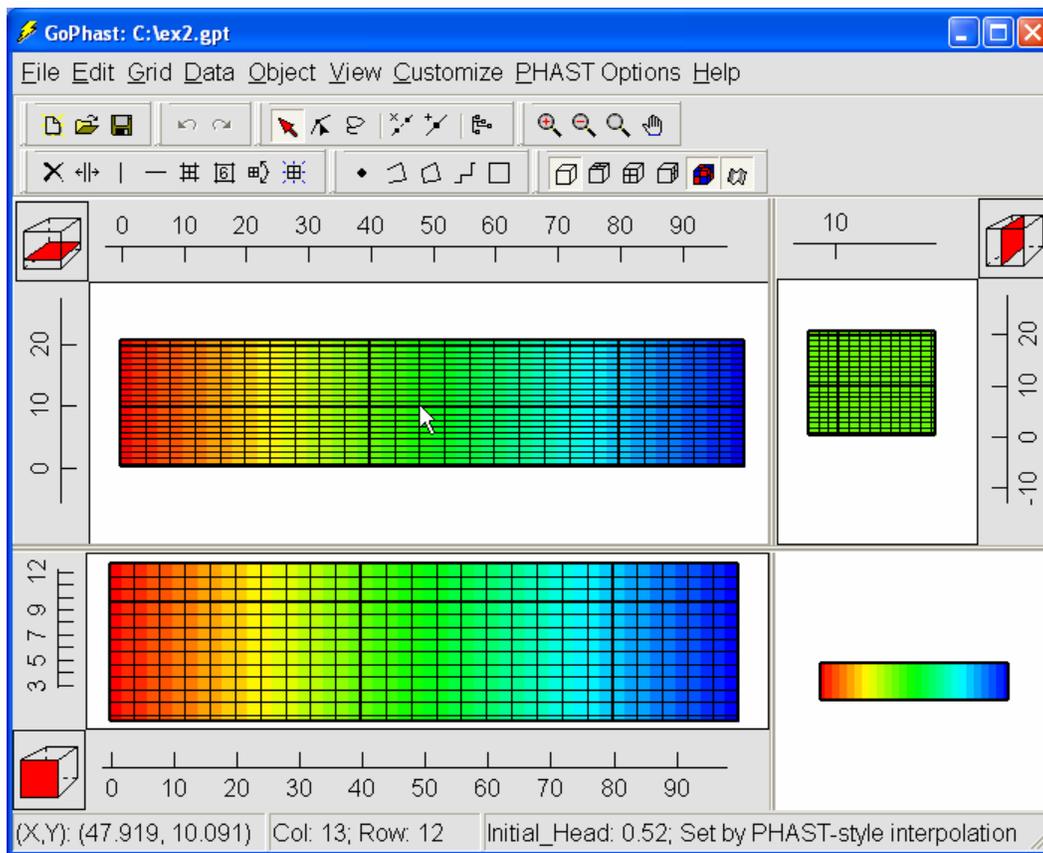




GoPhast: A Graphical User Interface for PHAST



Techniques and Methods 6-A20

U.S. Department of the Interior
U.S. Geological Survey

Cover: GoPhast screen view for Example 2 (p. 74). The grid has been colored to show the distribution of initial hydraulic head. The status bar (at bottom) shows the coordinates of the mouse cursor, the column and row numbers at the cursor position, the value of initial head in the user's choice of units at the cursor position, and a description of how the initial head value at that location was specified.

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By Richard B. Winston

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1. Abstract

GoPhast is a graphical user interface (GUI) for the USGS model PHAST. PHAST simulates multicomponent, reactive solute transport in three-dimensional, saturated, ground-water flow systems. PHAST can model both equilibrium and kinetic geochemical reactions. PHAST is derived from HST3D (flow and transport) and PHREEQC (geochemical calculations). The flow and transport calculations are restricted to constant fluid density and constant temperature. The complexity of the input required by PHAST makes manual construction of its input files tedious and error-prone. GoPhast streamlines the creation of the input file and helps reduce errors. GoPhast allows the user to define the spatial input for the PHAST flow and transport data file by drawing points, lines, or polygons on top, front, and side views of the model domain. These objects can have up to two associated formulas that define their extent perpendicular to the view plane, allowing the objects to be three-dimensional. Formulas are also used to specify the values of spatial data (data sets) both globally and for individual objects. Objects can be used to specify the values of data sets independent of the spatial and temporal discretization of the model. Thus, the grid and simulation periods for the model can be changed without respecifying spatial data pertaining to the hydrogeologic framework and boundary conditions. This report describes the operation of GoPhast and demonstrates its use with examples. GoPhast runs on Windows 2000, Windows XP, and Linux operating systems.

2. Introduction

GoPhast is a graphical user interface (GUI) for the PHAST ground-water simulation model (Parkhurst and others, 2004). GoPhast runs on Windows 2000, Windows XP, and Linux operating systems. PHAST simulates multicomponent, reactive solute transport in three-dimensional, saturated, ground-water flow systems. PHAST can model equilibrium and kinetic geochemical reactions. PHAST is derived from HST3D (flow and transport) (Kipp, 1987; 1997) and PHREEQC (geochemical calculations) (Parkhurst, 1995; Parkhurst and Appelo, 1999). The flow and transport calculations in PHAST are restricted to constant fluid density and constant temperature. GoPhast is a tool used to transform data about an aquifer system into a data input file for PHAST. GoPhast is used to create the flow and transport data file required by PHAST. GoPhast does not create the chemistry data file required by PHAST; PHREEQCI (Charlton and Parkhurst, 2002), PHREEQC for Windows (<http://www.geo.vu.nl/users/posv/phreeqc/index.html>), or a text editor can be used to create that file.

2.1 Reasons for Using Graphical User Interfaces

Tools such as GoPhast are a bridge between the conceptual model of an aquifer system and the numerical model used to represent that aquifer system. Graphical User Interfaces are useful because of the disparity between aquifers and the models used to understand them. Models are typically orderly; the aquifers are not. In PHAST, for example, the aquifer system consists of a series of nodes arranged in a grid; the aquifer, obviously, has no such grid. In PHAST, the grid is an isolated spatial domain, whereas, the aquifer system is embedded in a landscape with which it interacts. Boundary conditions are used to approximate the outside landscape but the boundary conditions allow only simplified interactions with the exterior. In PHAST, aquifer properties are defined in block-shaped zones that often encompass several nodes in the grid. In aquifers, zones, if they exist at all, will almost certainly not be block-shaped unless humans have engineered them to be so. Thus, the block-shaped zones of PHAST are an unnatural representation of the aquifer system.

Resolving disparities between the requirements of the model and the nature of the aquifer system is one of the ways in which a GUI can be most useful. A GUI can allow the user to specify the aquifer properties in ways that do not correspond directly to the requirements of the model. For example, instead of block-shaped zones, the aquifer properties and boundary conditions can be specified in ways that seem more natural such as zones with irregular boundaries. Hydrologists often conceive of an aquifer system as comprising a series of irregularly shaped zones with uniform properties within those zones. Because it is a purely mechanical process to transform the irregular zones as conceived by the user to the block-shaped zones required by the model, the GUI can make this transformation for the user.

The actual characteristics of the aquifer are imperfectly known. Often a property of interest is known at only a few sampling points and these data must be used to infer a likely value of the property elsewhere in the aquifer system. If the user wishes to interpolate among a series of data points to infer aquifer properties, those data points can be entered in the GUI and the GUI can perform the required interpolation. If the grid is changed, the GUI can automatically detect the change and reinterpolate the data to the new grid.

Another benefit of a GUI is its graphical representation of data. Models typically require that all or nearly all of the input be in the form of numbers. A river, for example, is represented in PHAST by a series of X and Y coordinates. A GUI can make those numbers more comprehensible by mapping them as a series of line segments on a computer screen. Graphical representation of the data, including the use of color, has enormous benefits. The graphical representation allows the user to specify and check the data much more rapidly and accurately than would otherwise be possible.

A detail that can be largely hidden from the user is the time discretization. Models typically require that time be broken up into a series of simulation periods. In each simulation period, the boundary conditions may need to be respecified. In the user's conception of the aquifer, only one or a few of the boundary conditions may change over time. Thus, there is no conceptual reason why the user must respecify the boundary conditions that have not changed. Instead, the GUI can hide this detail from the user.

The GUI of an aquifer system is most effective when it represents a system in two different ways: (1) as the user conceives it, and (2) as the model requires it. The latter representation can be largely hidden from the user. With current (2006) technology, the user must still be aware of the model requirements because the user is responsible for creating the grid. Similarly, the model may provide a number of different options and the user must decide which of these options to use. The GUI cannot hide those choices from the user. However, there are many aspects of the model the

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user does not need to know about. GoPhast is designed to simplify the process of translating conceptual models to numerical definitions and as much as possible to automate the tedious and error-prone parts of the process.

2.2 Purpose and Scope

This report (1) describes the basic concepts needed to work with GoPhast, (2) documents the features of GoPhast, and (3) gives examples of how to use GoPhast.

Three of the examples are based on the examples provided with PHAST. The other example is new. Some of the text of this report consists of quotations from or paraphrases of the PHAST documentation (Parkhurst and others, 2004). Information for programmers is included in appendix 1.

It is anticipated that different users will use this document in different ways. Some will read this document from beginning to end before trying to use GoPhast. Others will use it as a reference volume and will read parts of it in an arbitrary order as the situation warrants while using GoPhast. Others will want to learn how to use GoPhast by following the instructions in the “Examples” section (p. 64). The separate sections of this report have been designed to be independent of one another to allow for all these uses; however, all users would benefit from reading the “Basic Concepts” section (p. 3). Extensive cross references within the text should help the user find desired information quickly.

2.3 Distribution

The software described in this report may be obtained from the U.S. Geological Survey (USGS) Ground-Water Software web page (http://water.usgs.gov/software/ground_water.html).

3. Basic Concepts

To work effectively with GoPhast, several basic concepts must be mastered. This section provides an introduction to those concepts and tells where in this document more information about them may be found.

3.1 The Grid

PHAST uses finite-difference techniques for spatial and temporal discretization. A **grid** is required for spatial discretization; PHAST uses a point-distributed grid. The nodes in this grid are at the corners of elements (fig. 1). Each node is surrounded by a cell that includes parts of one to eight elements (fig. 1). Boundary and initial conditions are specified by node; aquifer properties are specified by element.

Basic Concepts

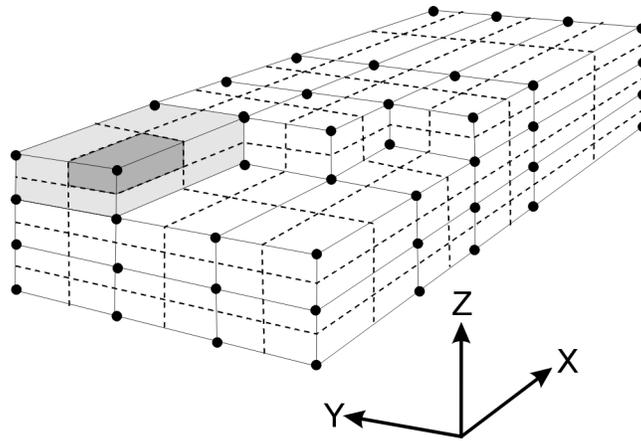


Figure 1. The grid in PHAST including nodes (black dots) and a light gray element and a dark gray cell. Solid lines represent element boundaries. Dashed lines represent cell boundaries.

In GoPhast, the grid can be at an angle to the global coordinate system. The coordinate system for the grid is aligned with the grid lines, but has the same origin as the global coordinate system. The coordinates of a point in the global coordinate system are referred to as X, Y, and Z; the coordinates of a point in the grid coordinate system are referred to as X', Y', and Z (X-prime, Y-prime, and Z). There is no Z' because the grid is never rotated away from the horizontal plane. Coordinate values at the cursor location in both the global and grid coordinate system are displayed on the status bar of the main window of GoPhast. More information about the grid can be found in the PHAST documentation (Parkhurst and others, 2004). GoPhast can be used to create the grid; rotate it; and add, move, or remove grid lines.

3.2 Data Sets

Data sets are used to represent spatially distributed data in PHAST. Each data set represents a two-dimensional (2D) or three-dimensional (3D) array of values. 3D data sets are defined for the entire extent of the model domain. 2D data sets are defined for a top, front, or side projection of the model domain. Because PHAST requires that some data be assigned to elements and other data be assigned to nodes, some data sets will have a value for each element and others will have a value for each node. The initial water table, which is a 2D data set, is only defined for the top layer of nodes in the model. The remaining data sets required by PHAST are 3D. If the number of rows, columns, or layers in the grid changes, the sizes of the data sets are also changed.

In addition to the data sets required by PHAST, the user can create additional data sets. The user-defined data sets can be used in “Formulas” to define the distribution of values in the data sets that are required by PHAST. See “Data Sets Dialog Box” on page 42 for more information on data sets.

3.3 Formulas

Formulas are used to help define the distribution of values in data sets. One simple example of a formula would be just the name of another data set. For example, a valid formula for

Basic Concepts

the **K_y** data set (which defines the hydraulic conductivity in the Y direction) would be “**K_x**.” (**K_x** is the data set that defines the hydraulic conductivity in the X direction.) Setting the formula for **K_y** to “**K_x**” would mean that the value of **K_y** in a given element would be equal to the value of **K_x** within that element.

Another simple example of a formula would be to set the formula for the **K_z** data set (**K_z** defines the hydraulic conductivity in the Z direction.) to “**K_x**/10.” This formula would mean that in a given element, the value of **K_z** would be equal to the value of **K_x** in that element divided by 10.

These examples only hint at the power of formulas. In addition to simple arithmetic operations, it is possible to use mathematical functions such as “sin” and “ln.” Geographic Information Systems (GIS) functions, logic functions, and functions related to the grid and objects are also available in formulas.

See “Formulas”, and “Formula Editor Dialog Box” on pages 17 and 44 respectively for more information about formulas.

3.4 Objects

Objects are points, polylines (a series of connected line segments), and polygons drawn in the main window of GoPhast or imported from external files. An object can have a formula for just a single surface or it can have no surfaces. An object without any additional surfaces is two-dimensional because it has only two coordinate directions defined. All objects, including point objects, with at least one surface defined are three-dimensional because they have three coordinate directions defined. Each object can have an upper and lower surface making it three-dimensional. For example, a polygon with an upper and lower surface is a solid. The surfaces associated with an object need not be flat. The surfaces are defined by formulas that allow them to have virtually any shape. There are some limitations: none of the line segments defining an object can cross another line segment of the same object; objects cannot have holes in them; and an object can have, at most, one upper and one lower surface.

Objects are used to modify the default values of data sets and to set boundary conditions. Objects can be used to set values of data sets in any of three ways: (1) values can be interpolated among objects; (2) values can be set for elements or cells whose centers or nodes are enclosed inside the object; and (3) values can be set for elements or cells intersected by the object. For the latter two methods, the order of the objects is important; because each object overwrites previous values, only the last value applied takes effect.

See “Creating, Selecting, and Editing Objects in GoPhast” and “Object Properties Dialog Box” on pages 28 and 49 respectively for more information about Objects.

3.5 Assigning Values to Data Sets

Values are assigned to data sets at nodes or elements using the following procedure.

1. First, a default value is assigned to every node or element by using either PHAST-style interpolation or mixtures (See “PHAST-Style Interpolation”, p. 16.), the selected interpolation method (See “Interpolation Methods”, p. 16.), or the default formula for the data set (See “Formulas”, p. 17 and “Data Sets Dialog Box”, p. 42.).
2. Next, each object that affects the data set is processed, and nodes or elements that are intersected or enclosed by each object are assigned values on the basis of PHAST-style interpolation or mixtures or by using the object’s formula for the data set.

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Interpolation can be useful to specify the boundaries between geologic units (see example in fig. 2). To do this, the user first creates a data set for each interface between adjacent geologic units. Then the user creates point objects to specify the elevations of the interfaces at known locations. Interpolation can then be used to specify the elevations throughout the grid. These data sets for the elevations can then be used in the formulas for the upper and lower surfaces of “3D Objects” that define properties of aquifers.

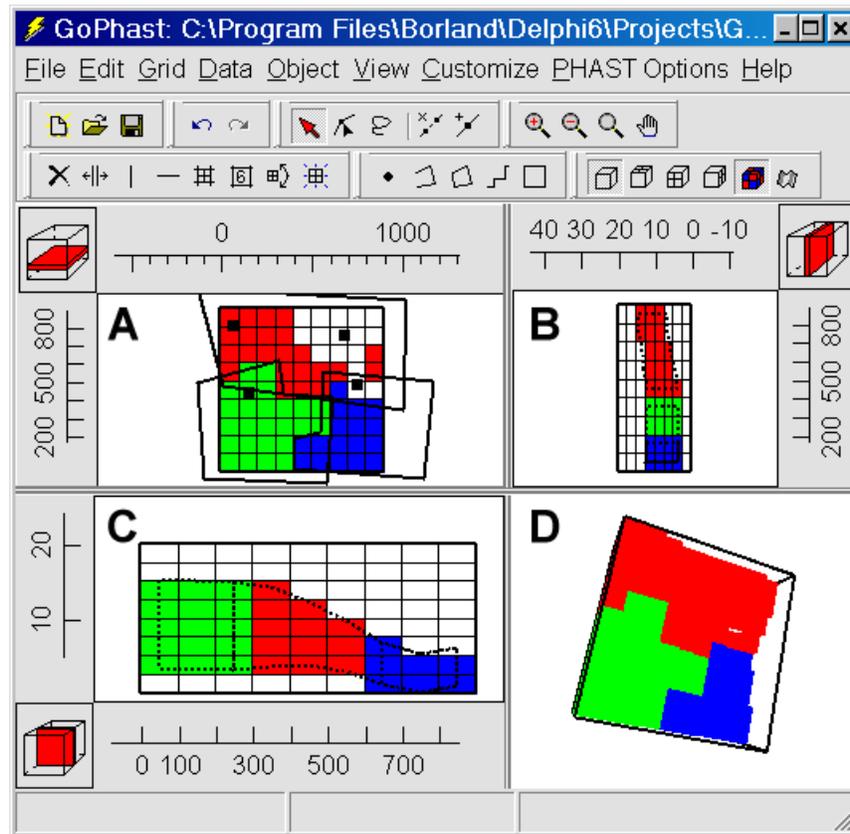


Figure 2. Example of 2D data sets used to define the top and bottom of a geologic unit. (A) Top view, (B) Side view, (C) Front view, (D) Three-Dimensional view. In the top view (A), point objects (black squares) were used to specify the top and bottom of a geologic unit by interpolation. Polygons were then used to define the value of the hydraulic conductivity of that unit. The colored cells represent the different values of hydraulic conductivity. Note the sloping surfaces of the geologic unit visible in the front (C) and side (B) views of the model.

Because values for data sets are specified using formulas and objects, the data for a given model are independent of the spatial discretization of the model. Values of a data set are needed when exporting the model input or when coloring the grid with the data set. Values for data sets are recalculated when the data are needed and the values for the data set are out-of-date. These values become out-of-date when any of the following occur:

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1. the grid changes,
2. any of the formulas used to set values of the data set change,
3. the interpolation method for the data set changes,
4. any of the objects used to set the value of the data set are edited, or
5. any of the data sets on which the data set in question depends become out-of-date.

3.6 Boundary Conditions

Boundary conditions are treated similarly to other “Data Sets” except that there is no global formula for boundary conditions; boundary conditions are specified only with objects (points, lines, and polygons). In addition, the user must specify starting times for each boundary condition. The values specified for each time apply until the model run is terminated or the values are overridden by values for a later time. The user does not need to define stress periods because GoPhast can determine the appropriate stress periods based on the times specified by the user. The user can also specify different starting times for different objects, making the specification of the boundary conditions independent of the time discretization.

4. Initial Dialog Boxes

When the user first starts GoPhast, the **Start-Up** dialog box is displayed. If the user chooses to create a new model in the **Start-Up** dialog box, the **Initial Grid** dialog box is displayed. After both these dialog boxes are closed, the main window of GoPhast is displayed (fig. 3).

4.1 Start-Up Dialog Box

The **Start-Up** dialog box is displayed when first starting GoPhast. It prompts the user either to start a new project or to open an existing GoPhast project. The five most recently opened files will be listed among the choices. If the user chooses to start a new project, the **Initial Grid** dialog box will be displayed.

4.2 Initial Grid Dialog Box

The **Initial Grid** dialog box is used to specify the grid for a new GoPhast project either when first starting GoPhast or by selecting **File|New**. In it, the user specifies the dimensions of the grid (the number of columns, row, and layers of nodes) and the spacing between nodes in the column, row, and layer directions. The user must also specify the X, Y, and Z coordinates of the grid origin. The grid origin is the location of the node in the first column, row, and layer. Columns are numbered from left to right. Rows are numbered from front to back. Layers are numbered from bottom to top. Thus the grid origin is the node at the left, front, bottom corner of the grid. The grid angle must also be specified. The angle is measured in degrees counterclockwise from the X-axis. The vertical exaggeration must also be specified.

Clicking the **Finish** button will create a grid with the dimensions and location specified. If the **Do not create initial grid** button is clicked instead, a new project will be created without a grid.

5. Main Window

The main window of GoPhast has several parts as listed below and shown in figure 3.

- the Main Menu and Buttons
- the Top, Front, and Side Views of the model,
- the 3D View of the model, and
- the Status Bar.

The menu and buttons are described in “Main Menu and Buttons” on p. 31. The other parts are described below.

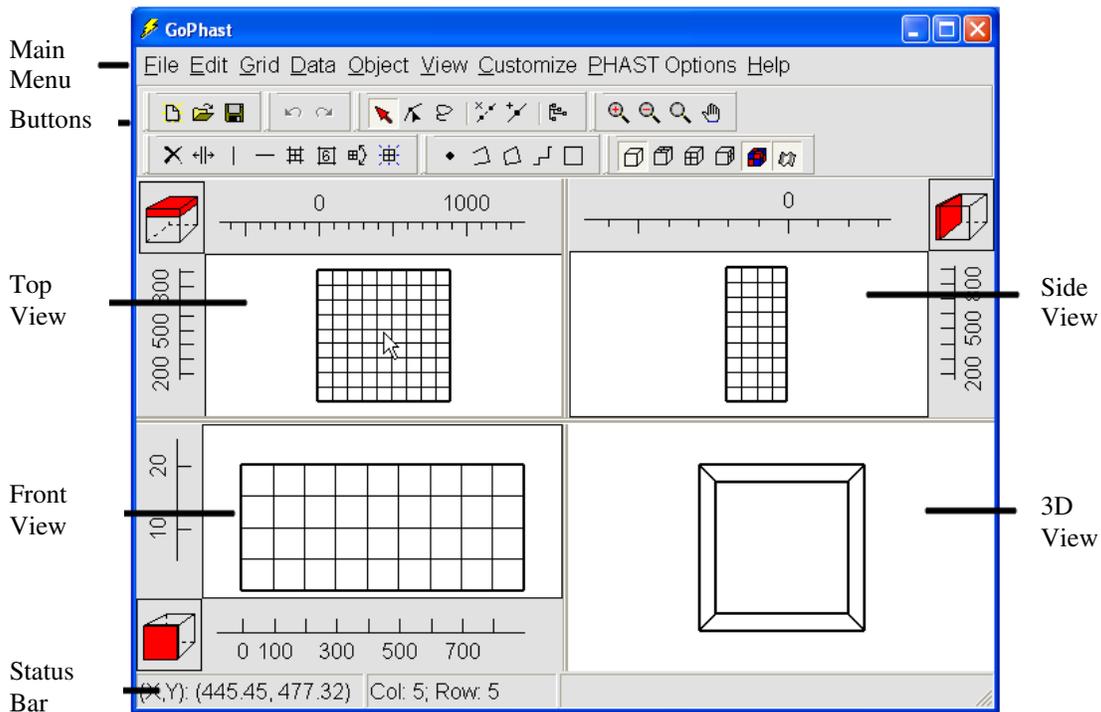


Figure 3. The main window of GoPhast.

5.1 Top, Front, and Side Views

The main GoPhast window includes four panes. Three of these panes contain the top, front, and side views of the model. The other pane is a 3D view of the model. Each pane can be resized by clicking on the space between the panes, moving the mouse while holding the mouse button down, and releasing the mouse button at the new position.

The top, front, and side views of the model are each composed of several parts (fig. 4):

- the Selection Cube,
- the two Rulers, and
- the Working Area.

Main Window

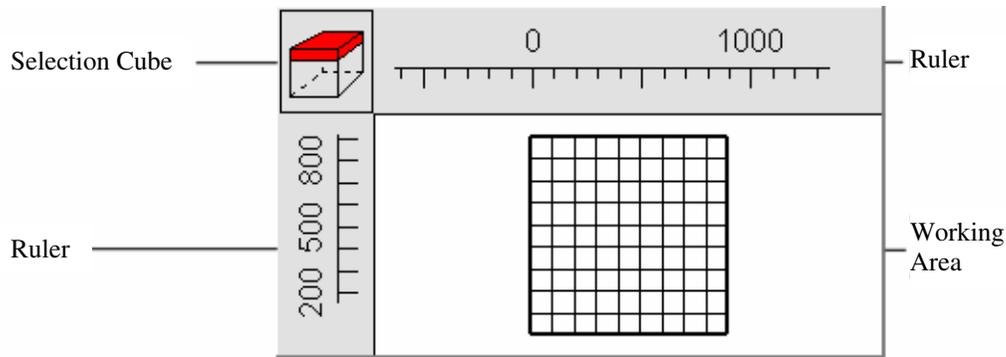


Figure 4. The parts of the top, front, or side views of the model.

5.1.1 The Selection Cube

The **Selection Cube** (fig. 5) shows the selected column row or layer. It can also be used to change the selected column row or layer.

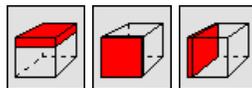


Figure 5. The top, front, and side Selection Cubes.

- To change the selected column, row, or layer with the Selection Cube, click on the Selection Cube. The selected column, row, or layer will move by one node or element toward the position that was clicked.
- If the Shift key on the keyboard is held down when the mouse button is clicked, the selected column, row, or layer will move by 10 nodes or elements toward the position that was clicked.
- If the Ctrl key on the keyboard is held down when the mouse button is clicked, the selected column, row, or layer will move to the position that was clicked.
- If the left mouse button is kept held down while the cursor is on the Selection Cube, the selected column row or layer will start to move toward the cursor position after a wait of one second. It will then move rapidly toward the cursor.

See also: “Select Column, Row, and Layer Dialog Box” on p. 41.

5.1.2 The Ruler

The **Ruler** (fig. 6) is used to show the position of the model. The format of the numbers on the Ruler can be changed by double clicking on a Ruler or selecting **Customize|Ruler Format...** See “Ruler Format Dialog Box” on p. 58.

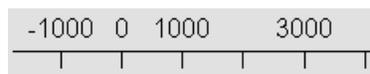


Figure 6. Ruler in GoPhast.

Main Window

5.1.3 The Working Area

The **Working Area** is used to display and edit the model. All objects are created and edited in the **Working Area**. It is also possible to edit the grid in the Working Area. The **Zoom** , **Zoom In** , **Zoom Out** , and **Pan**  buttons allow the user to navigate in the **Working Area**. See the “Grid” (p. 38), “Object” (p. 48), and “View” (p. 55) menu items under “Main Menu and Buttons” for more details.

5.2 Three-Dimensional View

The 3D view of the model (fig. 7) allows the user to view (but not edit) the model. A number of items in the **View** menu (p. 55) change the appearance of the 3D view. The following mouse actions can be used to navigate in the 3D view.

- To rotate the 3D view, click in the 3D view and drag with the mouse.
- To pan the 3D view, hold down the shift key while dragging with the mouse.
- To change the magnification of the 3D view, hold down the right mouse key and click in the 3D view. Then, while holding the right mouse key down, move the mouse up or down.

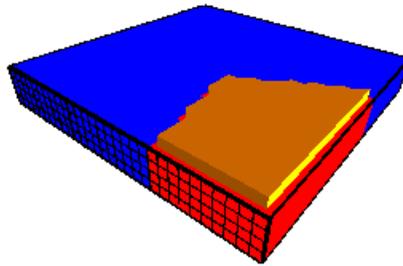


Figure 7. A 3D view of a model in GoPhast.

5.3 Hints and the Status Bar

When the mouse is held briefly over a menu item or button in the main GoPhast window, a hint will appear on the status bar briefly describing the function of the menu item or button. In addition, with buttons, a shorter version of the “hint” will appear in a small window above the button. The hint will remain visible for a short time and then disappear.

Hints that are related to the **Working Area** are also displayed on the status bar. When the cursor is moved over the Working Area, the coordinates of the cursor are displayed on the left panel of the status bar. When the cursor is over the grid, the column, row, and/or layer number is displayed on the middle panel of the status bar. When the grid is colored, the value of the data set used to color the grid in the current node or element is displayed on the right hand panel of the status bar along with a description of how the value was assigned.

To resize the individual panels on the status bar, click on the dividers between the panels and drag with the mouse.

See also “Hint Display Time Dialog Box” on p. 58

6. Generating Grids

There are four ways to generate a grid.

1. When a new model is first created, a uniform grid can be specified.
2. The commands **Grid|Specify Grid Angle...** and **Grid|Specify Grid Lines...** can be used to specify the grid numerically.
3. A grid can be drawn and rotated with the mouse.
4. The user can use objects to define where the grid should be and then use the **Grid|Generate Grid...** command to create it.

These four options are explained in greater detail in the following sections.

6.1 Specifying a Uniform Initial Grid

When the user chooses to create a new model, the “Initial Grid Dialog Box” gives the user the opportunity to specify a uniform grid (see p. 7).

6.2 Specifying a Grid with Numbers

If precise control over the position of the grid is desired, the menu items **Grid|Specify Grid Angle...** and **Grid|Specify Grid Lines...** can be used to locate the grid at an exact position. Normally, it is best to specify the grid angle first. When the grid angle is changed, the grid is rotated relative to its own center. The positions of the grid lines are measured relative to the origin of the coordinate system so when the grid is rotated, those positions change, as illustrated in the front and side views of the model in figure 8. The objects are not rotated when the grid is rotated (fig. 8). See “Grid Angle Dialog Box” on p. 39 and “Grid Spacing Dialog Box” on p. 40 for more information.

Generating Grids

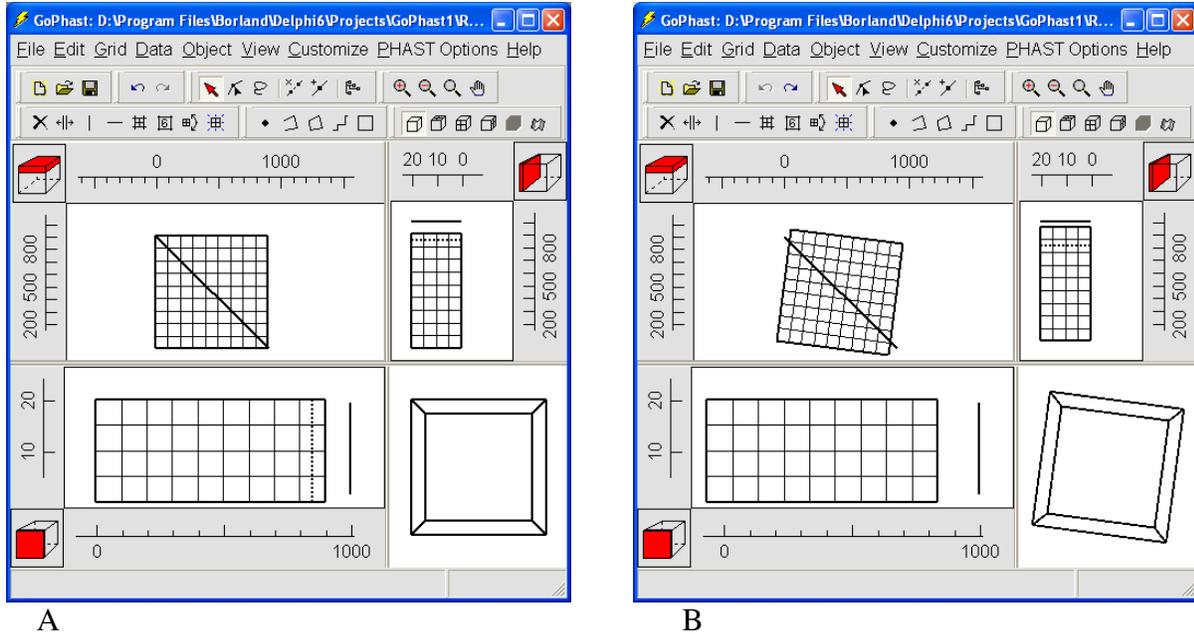


Figure 8. Unrotated (A) and rotated (B) grid with unmoved objects.

6.3 Drawing the Grid

If the user selects **Grid|Add Vertical Grid Line**  or **Grid|Add Horizontal Grid Line**  and then clicks on the top, front, or side view of the model, a horizontal or vertical grid line will be drawn at the mouse position. By doing this repeatedly, a complete grid can be drawn. The grid can be rotated around its center by selecting **Grid|Drag to Rotate**  and then dragging with the mouse on the top view of the model. Other menu items that are useful in drawing the grid include **Grid|Delete Grid Line** , **Grid|Move Grid Line** , **Grid|Subdivide Grid Elements** , **Grid|Set Width** , and **Grid|Smooth Grid...**

See “Editing the Grid” on p. 38 for more information on these menu items.

6.4 Using Objects to Specify the Grid

Objects can be used to set the size of elements in a grid. Multiple objects can be used in determining the grid location and node spacings. An object drawn on the top view of the model specifies the column and row width. Polygons drawn on the top view of the model specify the grid location in addition to specifying the grid element size. The grid will be drawn to completely enclose the polygon or polygons. An object drawn on the front or side view of the model specifies the layer height and the vertical extent of the grid. For an object to be used to specify the grid, the **Use to set grid element size** checkbox in the “Object Properties Dialog Box” (p. 49) must be checked. When it is checked, the user can enter the desired size in the **Grid element size** edit box.

In PHAST it can be useful to have an area with a refined grid where results need to be more accurate. To support this, GoPhast allows the user to specify overlapping objects that specify different element sizes. The final sizes of the elements will be determined by the smallest element

Generating Grids

size specified for a region. In some models (but not PHAST) it is important that the contrast in element size in adjacent elements not be too large. When the user creates a grid using objects, the **Grid smoothing criterion** in the “Generate Grid Dialog Box” (p. 40) allows the user to specify the maximum ratio of lengths between nodes for adjacent rows, columns, or layers that will be accepted. The default value is 1.2, which is well below the usual limit of 1.5.

Figures 9 to 14 illustrate examples of creating grids by using objects.

1. The user draws two objects to define the grid location and the size of the elements: a polygon on the top view of the model and a line on the front view of the model (fig. 9). (To create objects, see “Creating, Selecting, and Editing Objects in GoPhast” on p. 28 and the **Object** menu item on p. 48.) In this example, the size of the elements are set in the **Object Properties** dialog box (p. 49) to 500 meters in the horizontal direction (top view, fig. 9) and 10 m in the vertical direction (front view, fig. 9).

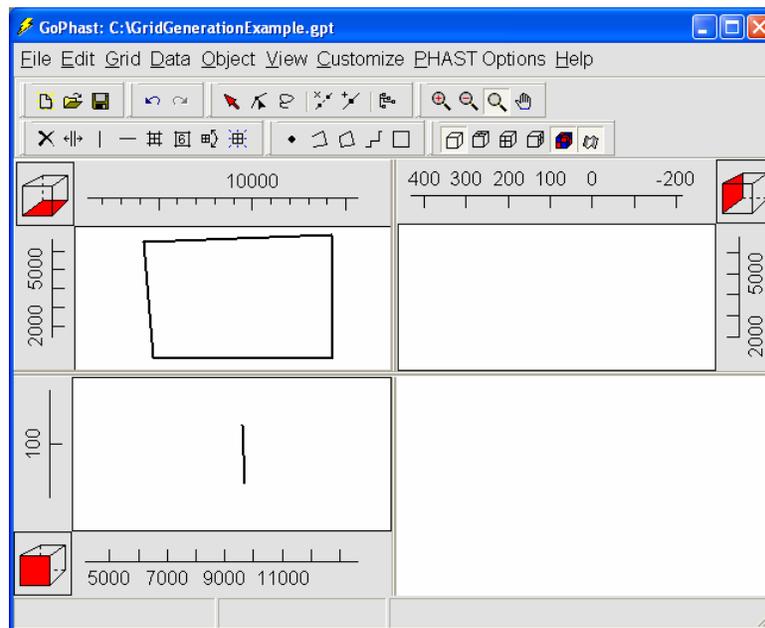


Figure 9. The objects used to define the position of the grid.

2. The user selects **Grid|Generate Grid...** and the **Generate Grid** dialog box appears (fig. 10). When the user clicks on the **OK** button, the grid is created (fig. 11).

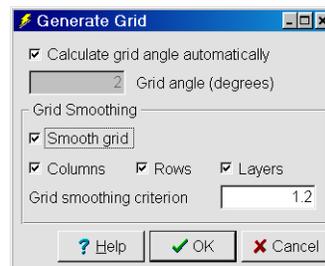


Figure 10. The **Generate Grid** dialog box.

Generating Grids

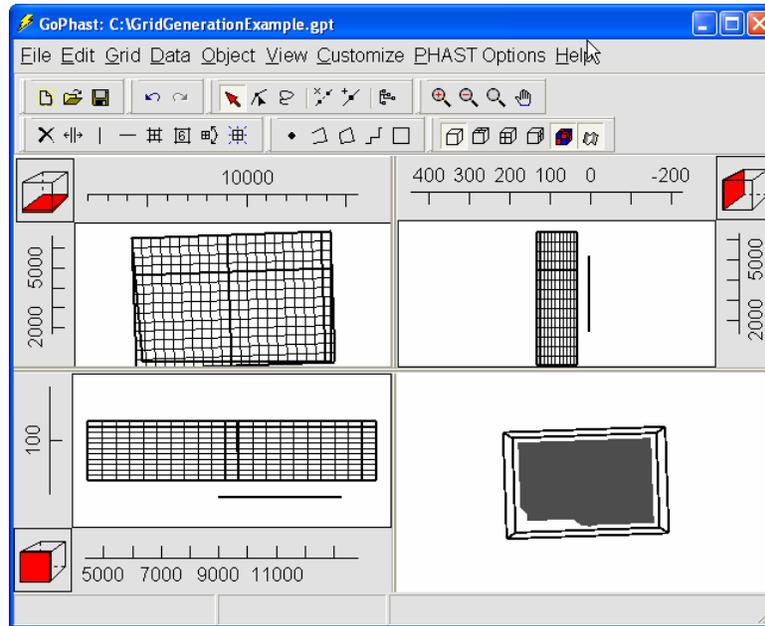


Figure 11. Grid and objects.

3. It may be desirable to have a finer grid in some regions than others. To do this, additional objects can be used to specify a zone where a fine grid will be used (fig. 12). In this example, the object specifies an element size of 200 m in the **Grid element size** edit box of the **Object Properties** dialog box.
4. After choosing **Grid|Generate Grid...** again, a new grid is created with a smaller element size in the area enclosed by the object (fig. 12).

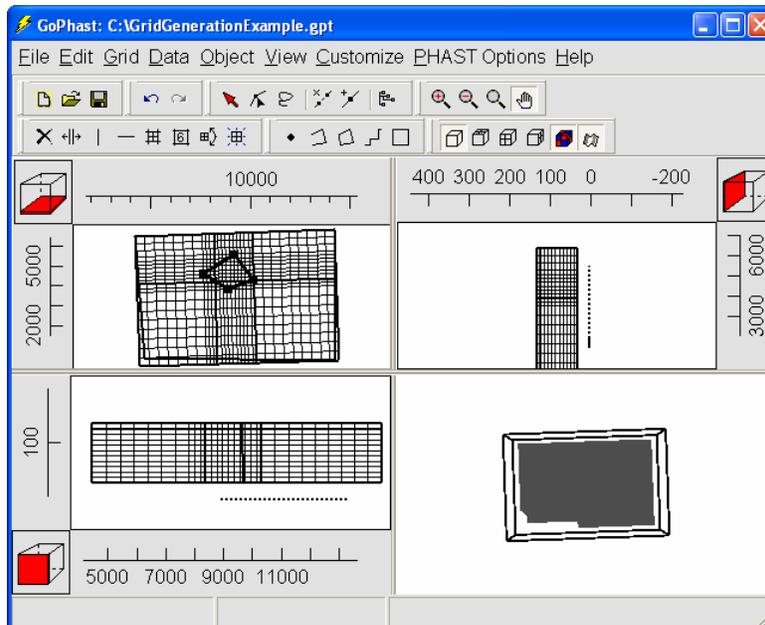


Figure 12. Grid with region with smaller elements specified by polygon object.

Generating Grids

5. In some cases, it may be desirable to have a gradual transition in element size. A size transition can be achieved by checking the **Smooth grid** checkbox in the **Generate Grid** dialog box (fig. 13). When it is checked, the widths of the columns, row, or layers will be adjusted so that the maximum ratio of the widths of adjacent cells is less than or equal to the grid smoothing criterion. An example of such a grid is shown in figure 14. See “Editing the Grid” on p. 38 for more information on grid smoothing.

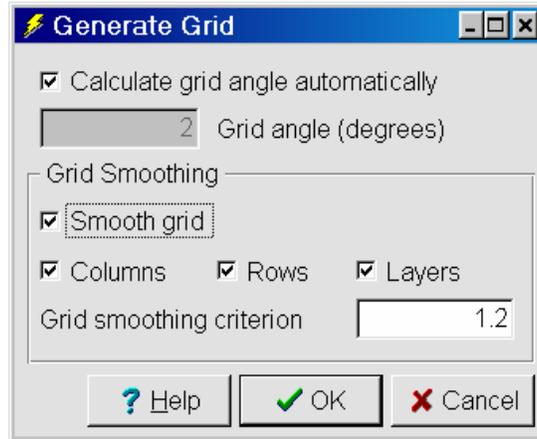


Figure 13. Generate Grid dialog box with grid smoothing activated.

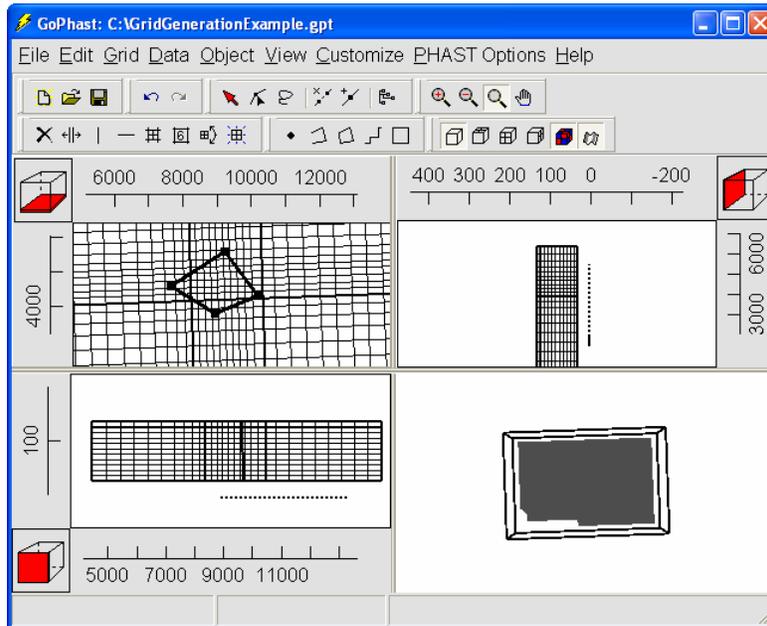


Figure 14. Grid generated with grid smoothing.

7. Interpolation Methods

The interpolation method is used to determine how values should be interpolated among a group of objects. Interpolation can only be used for 2D data sets. Only one of the PHAST data sets, **Initial_Water_Table**, is a 2D data set; however, the user can define his or her own 2D data sets and use interpolation in them. One appropriate use of such 2D data sets would be to define the tops and bottoms of geologic units. Three interpolation algorithms are available in GoPhast: **Nearest**, **Nearest Point**, and **Inv. Dist. Sq.** (Inverse Distance Squared).

The **Nearest** interpolation method (fig. 15A) works by determining the object that is closest to the location where the data set in question is being evaluated. Then the formula of that object is evaluated at that location.

The **Nearest Point** interpolation method (fig. 15B) is similar to the **Nearest** interpolation method except that only the vertices of objects are considered, rather than the lines connecting the vertices. If only point objects are being used, the results are identical. The **Nearest Point** interpolation method uses an algorithm that is faster than the **Nearest** interpolation method when the number of points is greater than several hundred.

With the **Inv. Dist. Sq.** interpolation method (fig. 15C), the formula for each object is evaluated at the location under consideration. The final value is a weighted average of these values. The weights are the inverse of the distance from the location to the closest point on each respective object. The **Inv. Dist. Sq.** interpolation method may only be used with data sets containing real numbers.

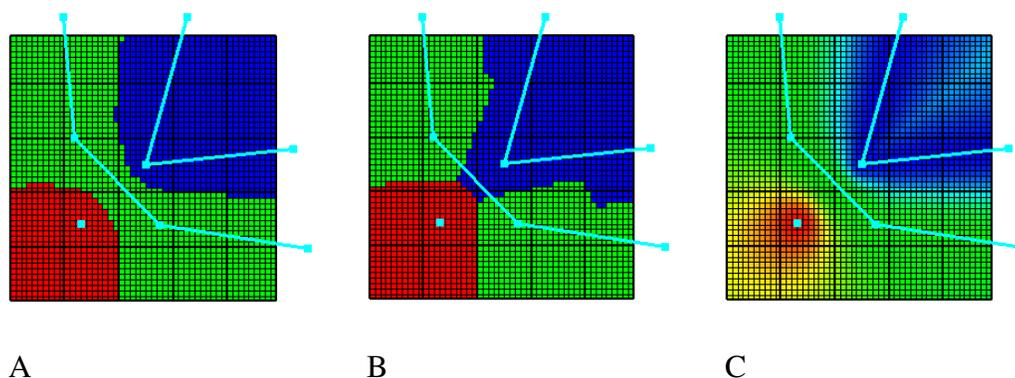


Figure 15. Interpolation methods. A. **Nearest** interpolation method. B. **Nearest Point** interpolation method. C. **Inv. Dist. Sq.** interpolation method.

8. PHAST-Style Interpolation

PHAST has a built in interpolation method using the grid coordinate system that can be applied to some CHEMISTRY_IC, FLUX_BC, HEAD_IC, LEAKY_BC, MEDIA, and SPECIFIED_HEAD_BC properties (Parkhurst and others, 2004). In PHAST-style interpolation, the user specifies a coordinate direction (X, Y, or Z), two distances, and two values. (The coordinate direction is relative to grid so if the grid is at an angle these are actually the X', Y' and Z directions.) If the X', Y', or Z coordinate of the current node is less than or equal to the first distance, the first value (Value 1) is used. If the X', Y', or Z coordinate of the current node is greater

PHAST-Style Interpolation

than or equal to the second distance, the second value (Value 2) is used. For intermediate distances, linear interpolation between the two values is used.

A related capability in PHAST is the ability to specify mixtures between two chemical compositions. In PHAST-style mixtures, the user specifies two values that represent chemical compositions and a series of proportions (between 0 and 1). The proportion represents the fraction of Value 1 in the mixture.

The following controls are used to specify the values needed for PHAST-style interpolation.

- **Interp. dir. or mixture:** **Interp. dir. or mixture** indicates the direction in which the interpolation will take place. For some data sets, the user can specify **Mix**. If **Mix** is specified, the mixture formula is used to specify the fraction of **Value 1** in the mixture.
- **Distance 1 and Distance 2:** **Distance 1** is the lower end of the distances used for interpolation. **Distance 2** is the upper end of the distances used for interpolation. If the position of a cell or element is between **Distance 1** and **Distance 2**, the value applied to a cell will be interpolated between **Value 1** and **Value 2**. Otherwise, either **Value 1** or **Value 2** will be applied depending on which end of the range of distances is closest to the position of the cell or element.
- **Value 1 and Value 2:** **Value 1** and **Value 2** are the two values that will be used for interpolation.
- **Mixture formula:** **Mixture formula** is the fraction of **Value 1** to use in the mixture of **Value 1** and **Value 2**. The **Mixture formula** should range between 0 and 1. If the **Mixture formula** is outside the range of 0 to 1, a value of either 0 or 1 will be used depending on which is closest to the value of the mixture formula.

PHAST-style interpolation in GoPhast can only be applied to data sets in PHAST that allow PHAST-style interpolation. This includes all the data sets directly used in the PHAST transport data file except **Active**, **Print_Chemistry**, and **Print_XYZ_Chemistry**. PHAST-style interpolation cannot be used with data sets created by the user. However, the user could specify a formula that would have the same effect as PHAST-style interpolation. Either of the following will emulate PHAST-style interpolation when applied to a real-number data set:

- $\text{If}((X_Prime < 1000.), 25., \text{If}((X_Prime > 10000.), 50., (((X_Prime - 1000.) / 9000.) * 25.) + 25.))$
- $\text{MultiInterpolate}(X_Prime, 25, 1000, 50, 10000)$

In these formulas, the interpolation direction is X', the two distances are 1,000 and 10,000, and the two values are 25 and 50.

Data sets that store integers and whose values are set by PHAST-style interpolation or mixtures should not be used in formulas for other data sets because the value used in the formula will be rounded to the nearest integer rather than representing a mixture between the two end member compositions. The formulas used in GoPhast are strictly mathematical and are unable to interpret those numbers as chemical compositions.

9. Formulas

Formulas are used to assign values to nodes or elements and help to define the geometry of 3D objects. The simplest formula is simply a numerical value such as "100." or "1." In a new model, if the user selects **Data|Edit Data Sets...**, the **Data Sets** dialog box (p. 41) will appear and it

Formulas

can be seen that the default formulas for **Kx** and **Kz** respectively are "100." and "1." This means that, in the absence of any other method (see “Assigning Values to Data Sets” on p. 5) for assigning a value to an element, **Kx** and **Kz** for all elements will be 100 and 1, respectively. By using a slightly more complicated formula, it is possible to see the power of formulas. Here is an example:

- Click on the cell in the table for the default formula for **Kz**. A button will appear in that cell. Ignore the button.
- Click in the cell again. The button will disappear and it will be possible to type a formula.
- Type "Kx/100" (without the quotation marks).

In the absence of any other method for assigning a value of **Kz** to an element, **Kz** for all elements will be equal to the value of **Kx** for that element divided by 100. Now by specifying the spatial distribution of **Kx**, the spatial distribution of **Kz** is also specified.

If the user selects the cell for the default formula for **Kz** again and clicks the button labeled **F()** that appears in the cell, the **Formula Editor** will appear. The **Formula Editor** can help set up complex formulas correctly. See the “Formula Editor Dialog Box” on p. 44 for more information.

When a Formula is applied to a data set or boundary condition in the **Data Sets** tab of the **Object Properties** dialog box, the formula will only be used for those nodes or elements that the object affects. (See “Objects” on p. 5.)

Formulas are, in essence, mathematical expressions that can be evaluated to produce real-numbers, integers, Booleans, or text. A formula can include constants and any of the operators or functions described in the following two sections. Text constant must be enclosed in double quotes. Boolean constants must be either **True** or **False**. Numeric constants that do not have a decimal point and that are not expressed in engineering notation (such as 1E0) are considered integers. Other numeric constants are real numbers. Integers are 32-bit values. Real numbers are double-precision values. Spaces, tabs, and line breaks in formulas are considered white space and are otherwise ignored. Loop constructs such as “while”, “for”, and “do” are not supported.

9.1 Operators

The operators in table 1 can be used in formulas.

Table 1. Operators in GoPhast formulas

Operator	Meaning	Data Types	Result type
=	equals	real numbers, integers, Booleans, text	Boolean
<>	not equals	real numbers, integers, Booleans, text	Boolean
>	greater than	real numbers, integers, Booleans, text	Boolean
<	less than	real numbers, integers, Booleans, text	Boolean
>=	greater than or equals	real numbers, integers, Booleans, text	Boolean
<=	less than or equals	real numbers, integers, Booleans, text	Boolean
and	and	Booleans	Boolean
or	or	Booleans	Boolean
xor	exclusive or	Booleans	Boolean
not	not	Booleans	Boolean
mod	modulus (remainder)	integers	integer
div	integer division	integers	integer
*	multiplication	real numbers, integers	real number, integer
/	division	real numbers, integers	real number, integer
+	addition or concatenation	real numbers, integers, text	real number, integer, text
-	subtraction	real numbers, integers	real number, integer

Formulas

The operator precedence rules are shown in table 2. Operators that are part of the same group have equal precedence. Operators of equal precedence are evaluated in order from left to right.

Table 2. Operator precedence rules in GoPhast formulas

Operators	Precedence
()	first (highest)
not	second
and, mod, div, *, /	third
or, xor, +, -	fourth
=, <>, >, <, >=, <=	fifth (lowest)

9.2 Functions

Functions that can be used in formulas are grouped into the following categories.

- GIS
- Grid
- Logical
- Math
- Object
- Text
- Trig

In each function, optional arguments are listed inside curly braces {}. If a function has more than one argument, the arguments must be separated by a single comma and/or one or more spaces or tab characters.

9.2.1 GIS

The GIS functions return values related to location.

X returns the X coordinate of a node or the element center in global coordinates (fig. 16). (See “The Grid” on p. 3.)

X_Prime returns the X coordinate of a node or the element center in grid coordinates (fig. 16). (See “The Grid” on p. 3.)

Y returns the Y coordinate of a node or the element center in global coordinates (fig. 16). (See “The Grid” on p. 3.)

Y_Prime returns the Y coordinate of a node or the element center in grid coordinates (fig. 16). (See “The Grid” on p. 3.)

Z returns the Z coordinate of a node or the element center in global coordinates. (Because this is also the Z coordinate in grid coordinates, there is no Z_Prime function) (fig. 16). (See “The Grid” on p. 3.)

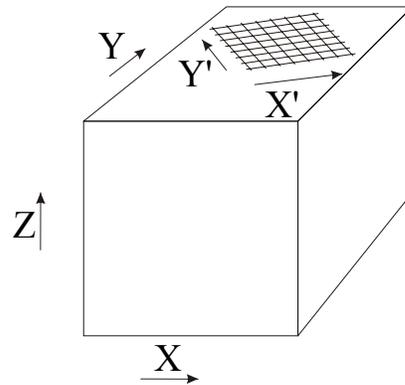


Figure 16. Global and grid coordinate systems in GoPhast.

9.2.2 Grid

The Grid functions return values related to the grid.

BlockAreaFront({Column, Layer}) returns the cross-sectional area of an element or cell as seen from the front of the grid (fig. 17). The function has two optional arguments: Column and Layer. If these arguments are provided, they specify the element or cell for which the area should be calculated. If they are not provided, the function uses the column and layer of the element or cell for which the formula is being calculated. If either of the arguments has an invalid value, the function returns zero.

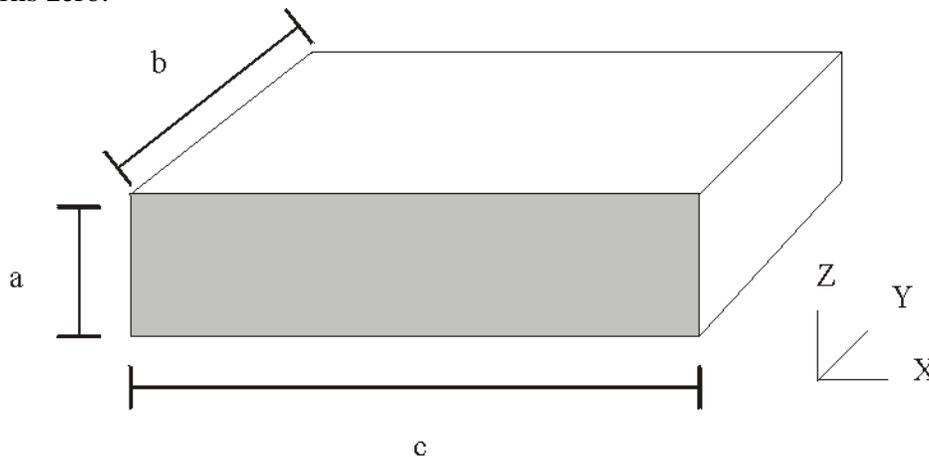


Figure 17. BlockAreaFront returns the product of a times c.

Formulas: Grid

BlockAreaSide({Row, Layer}) is like **BlockAreaFront** except that the value returned is the cross-sectional area of an element or cell as seen from the side of the grid (fig. 18).

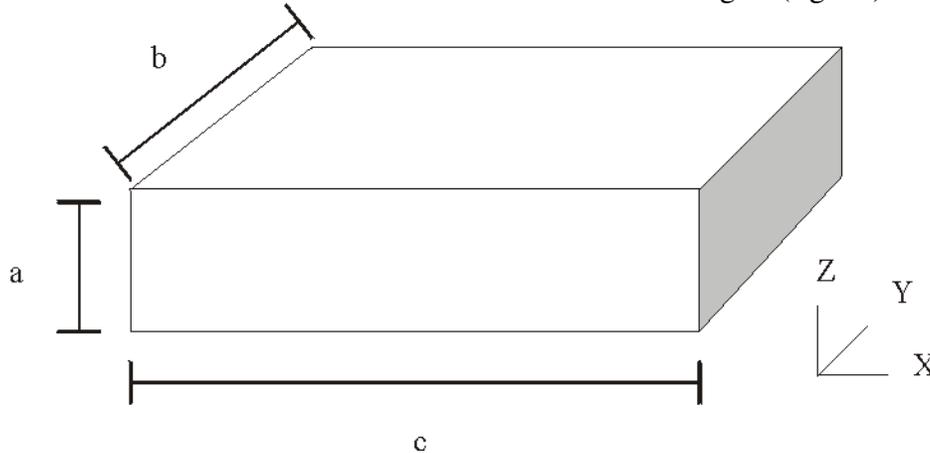


Figure 18. **BlockAreaSide** returns the product of a times b.

BlockAreaTop({Column, Row}) is like **BlockAreaFront** except that the value returned is the cross-sectional area of an element or cell as seen from the top of the grid (fig. 19).

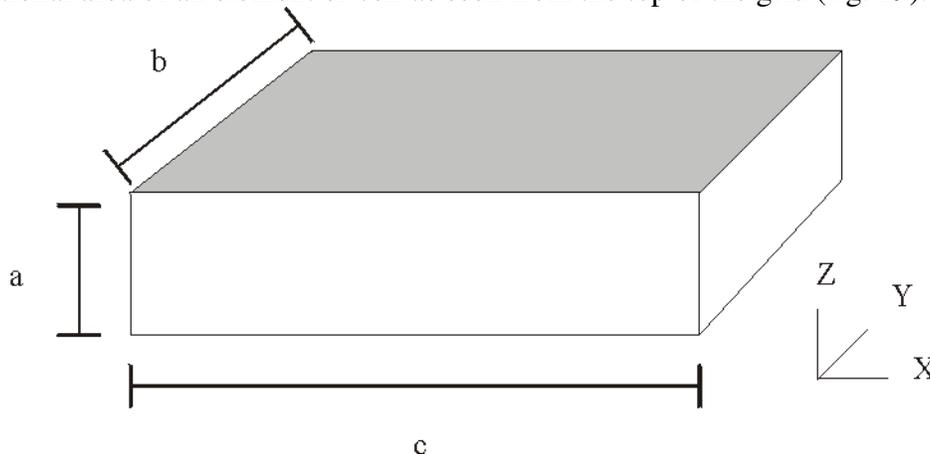


Figure 19. **BlockAreaTop** returns the product of b times c.

BlockVolume({Column, Row, Layer}) returns the volume of an element or cell. The function has three optional arguments: Column, Row, and Layer. If these three arguments are provided, they specify the element or cell for which the volume should be calculated. If they are not provided, the function uses the column, row, and layer of the node or element for which the formula is being calculated. If any of the three arguments has an invalid value, the function returns zero.

Column returns the column number of the node or element for which the formula is being calculated.

ColumnBoundaryPosition({Column}) returns the X coordinate in the grid coordinate system of the column boundary specified by its one optional argument Column. If the optional

Formulas: Grid

argument is not included, the function uses the column number of the node or element for which the formula is being calculated.

ColumnCount returns the number of column boundaries in the grid, which equals the number of nodes in the X direction.

ColumnWidth({Column}) returns the width of the cell or element column specified by its one optional argument Column. If the optional argument is not included, the function uses the column of the node or element for which the formula is being calculated.

Layer returns the layer number of the node or element for which the formula is being calculated.

LayerBoundaryPosition({Layer}) returns the Z coordinate in the grid coordinate system of the position of the layer boundary specified by its one optional argument Layer. If the optional argument is not included, the function uses the layer number of the node or element for which the formula is being calculated.

LayerCount returns the number of layer boundaries in the grid, which equals the number of nodes in the Z direction.

LayerHeight({Layer}) returns the height of the cell or element layer specified by its one optional argument Layer. If the optional argument is not included, the function uses the layer of the node or element for which the formula is being calculated.

Row returns the row number of the node or element for which the formula is being calculated.

RowBoundaryPosition({Row}) returns the Y coordinate in the grid coordinate system of the position of the row boundary specified by its one optional argument Row. If the optional argument is not included, the function uses the row number of the node or element for which the formula is being calculated.

RowCount returns the number of row boundaries in the grid, which equals the number of nodes in the Y direction.

RowWidth({Row}) returns the width of the cell or element row specified by its one optional argument Row. If the optional argument is not included, the function uses the row of the node or element for which the formula is being calculated.

9.2.3 Logical

The logical functions are used to choose between two or more possible choices based on a criterion.

Case(Index, Result1, Result2, ...). Case uses Index to determine which of the Result1, Result2... arguments will be returned as a result. If Index equals 1, Result1 is returned; if Index equals 2, Result2 is returned; if Index equals 3, Result3 is returned; and so forth. Only "Index", constant expressions, and the result that is returned will be evaluated. The types of Result1, Result2... must all be the same but they can be of any type. The type that is returned will be the same as the type of Result1, Result2, ...

CaseB(Index, Boolean_Result1, Boolean_Result2, ...) is like Case except that the value returned is always a Boolean.

CaseI(Index, Integer_Result1, Integer_Result2, ...) is like Case except that the value returned is always an integer.

CaseR(Index, Real_Result1, Real_Result2, ...) is like Case except that the value returned is always a real number.

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CaseT(Index, Text_Result1, Text_Result2, ...) is like Case except that the value returned is always text.

If(Boolean_Value, If_True_Result, If_False_Result) If uses Boolean_Value to determine whether If_True_Result or If_False_Result is returned as a result. If Boolean_Value is true, If_True_Result returned; if Boolean_Value is false, If_False_Result is returned. Only “Boolean_Value”, constant expressions, and the result that is returned will be evaluated. The types If_True_Result and If_False_Result must be the same but they can be of any type. The type that is returned will be the same as the type of If_True_Result and If_False_Result.

IfB(Boolean_Value, If_True_Boolean_Result, If_False_Boolean_Result) is like If except that the value returned is always a Boolean.

IfI(Boolean_Value, If_True_Integer_Result, If_False_Integer_Result) is like If except that the value returned is always an integer.

IfR(Boolean_Value, If_True_Real_Result, If_False_Real_Result) is like If except that the value returned is always a real number.

IfT(Boolean_Value, If_True_Text_Result, If_False_Text_Result) is like If except that the value returned is always text.

9.2.4 Math

The math functions supply general mathematical capabilities beyond the simple operations of addition, subtraction, multiplication, and division.

Abs(Value) returns the absolute value of Value. Value can be either an integer or a real number. The value returned by Abs will be the same type as Value.

AbsI(Value) returns the absolute value of Value. Value must be an integer. The value returned by AbsI will be an integer.

AbsR(Value) returns the absolute value of Value. Value can be either an integer or a real number. The value returned by AbsR will be a real number.

Distance(X1, Y1, X2, Y2) calculates the distance between points (X1, Y1) and (X2, Y2).

FactorialI(Value_Less_than_13) returns the factorial of Value_Less_than_13 as an integer.

FactorialR(Value_Less_than_171) returns the factorial of Value_Less_than_171 as a real number.

Frac(Value) returns the fractional part of Value. Value is a real number.

Interpolate(Position, Value1, Distance1, Value2, Distance2). Interpolate returns $(\text{Position} - \text{Distance1}) / (\text{Distance2} - \text{Distance1}) * (\text{Value2} - \text{Value1}) + \text{Value1}$. As its name implies, this is an interpolation between Value1 and Value2 based on where Position is between Distance1 and Distance2. If Position is not between Distance1 and Distance2, Interpolate extrapolates a value. See also MultiInterpolate.

IntPower(Base, Exponent) returns Base raised to the Exponent power. Base is a real number or integer. Exponent is an integer. IntPower returns a real number. See also **Power**.

ln(Value) returns the natural log of Value.

log10(Value) returns the log to the base 10 of Value.

logN(Base, Value) returns the log to the base N of Value.

Max(Value1, Value2, ...) returns whichever of its arguments is the largest. Its arguments must be either integers or real numbers. The result will be a real number if any of the arguments is a real number. If all the arguments are integers, the result will be an integer.

Formulas: Math

MaxI(Integer_Value1, Integer_Value2, ...) returns whichever of its arguments is the largest. Its arguments must be integers. The result will be an integer.

MaxR(Real_Value1, Real_Value2, ...) returns whichever of its arguments is the largest. Its arguments must be either integers or real numbers. The result will be a real number.

Min(Value1, Value2, ...) returns whichever of its arguments is the smallest. Its arguments must be either integers or real numbers. The result will be a real number if any of the arguments is a real number. If all the arguments are integers, the result will be an integer.

MinI(Integer_Value1, Integer_Value2, ...) returns whichever of its arguments is the smallest. Its arguments must be integers. The result will be an integer.

MinR(Real_Value1, Real_Value2, ...) returns whichever of its arguments is the smallest. Its arguments must be either integers or real numbers. The result will be a real number.

MultiInterpolate(Position, Value1, Distance1, [Value2, Distance2,] ...). If Position is less than or equal to Distance1, MultiInterpolate returns Value1. If Position is greater than or equal to DistanceN, MultiInterpolate returns ValueN. If Position is between any two adjacent distances, linear interpolation between the associated values will be used to determine the value that will be returned. Each distance after Distance1 must be greater than its predecessor. See also Interpolate.

Odd(Value) returns True if Value is an odd number. Otherwise it returns False. Value must be an integer.

Pi returns the ratio of the circumference of a circle to its diameter.

Power(Base, Exponent) returns Base raised to the Exponent power. Base and Exponent are real numbers or integers. Power returns a real number. See also **IntPower**.

Round(Value) converts Value to the nearest integer. In the case of a number that is exactly halfway between two integers, it converts it to whichever one is even. See also Trunc.

Sqr(Value) returns Value squared. Value can be either an integer or a real number. The result of Sqr will be an integer if Value is an integer. Otherwise it will be a real number.

SqrI(Integer_Value) returns Integer_Value squared. Integer_Value must be an integer. The result of SqrI will be an integer.

SqrR(Real_Value) returns Real_Value squared. Real_Value can be either an integer or a real number. The result of SqrR will be a real number.

Sqrt(Value) returns the square root of Value.

Trunc(Value) truncates Value to an integer by rounding it towards zero. See also Round.

9.2.5 Object

The object functions return values that are related to the properties of objects. (See “Objects” on p. 5 and “Creating, Selecting, and Editing Objects in GoPhast” on p. 28 for more information.)

FractionOfObjectLength is intended for use with objects that are lines rather than points or polygons. If the object being evaluated does not intersect the cell or element being evaluated, FractionOfObjectLength returns zero. If the object being evaluated intersects the cell or element being evaluated, FractionOfObjectLength returns zero if the first vertex of the object is in the element or cell, and returns one if the last vertex of the object is in the element or cell. It returns a fraction between zero and one for all other elements or cells. The value that is returned represents the fraction of an object’s length between the start of the object and the midpoint of an object’s intersection with a cell or element (fig. 20). If an object intersects a cell or element more than once,

Formulas: Object

the value that will be applied is the result of the last intersection between the object and the cell or element.

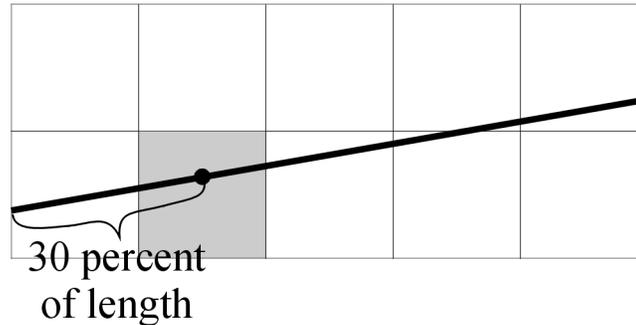


Figure 20. FractionOfObjectLength returns 0.30.

ObjectArea returns the two-dimensional area of an object. (It does not take into account the areas of any other objects that might be inside it.)

ObjectCurrentVertexX is intended for use with points and polyline objects. If the object being evaluated does not intersect the cell or element being evaluated, **ObjectCurrentVertexX** returns zero. If one of the vertices of an object is in the element or cell, **ObjectCurrentVertexX** returns the X coordinate of that vertex. Otherwise, **ObjectCurrentVertexX** returns the X coordinate of the first place where the object intersects the cell or element. For objects drawn on the side view of the model, **ObjectCurrentVertexX** returns zero.

ObjectCurrentVertexY is intended for use with points and polyline objects. If the object being evaluated does not intersect the cell or element being evaluated, **ObjectCurrentVertexY** returns zero. If one of the vertices of an object is in the element or cell, **ObjectCurrentVertexY** returns the Y coordinate of that vertex. Otherwise, **ObjectCurrentVertexY** returns the Y coordinate of the first place where the object intersects the cell or element. For objects drawn on the front view of the model, **ObjectCurrentVertexY** returns zero.

ObjectCurrentVertexZ is intended for use with points and polyline objects. If the object being evaluated does not intersect the cell or element being evaluated, **ObjectCurrentVertexZ** returns zero. If one of the vertices of an object is in the element or cell, **ObjectCurrentVertexZ** returns the Z coordinate of that vertex. Otherwise, **ObjectCurrentVertexZ** returns the Z coordinate of the first place where the object intersects the cell or element. For objects drawn on the top view of the model, **ObjectCurrentVertexZ** returns zero.

ObjectCurrentSegmentLength returns the length of the segment that intersects the cell or element. If the object being evaluated does not intersect the cell or element being evaluated, **ObjectCurrentSegmentLength** returns zero. If two or more segments of the same object intersect the cell or element, **ObjectCurrentSegmentLength** returns the length of the last one to intersect the cell or element.

ObjectIntersectArea({Column, Row, Layer}) returns the two-dimensional area of intersection between a cell or element and an object. The function has three optional arguments: Column, Row, and Layer. If these arguments are provided, they specify the cell or element for which the area should be calculated. If they are not provided, the function uses the column, row, and layer of the node or element for which the formula is being calculated. If any of the arguments has an invalid value, the function returns zero. If the object being evaluated intersects the cell or element being evaluated more than once, **ObjectIntersectArea** returns the sum of all the individual areas of intersection.

Formulas: Object

ObjectIntersectLength({Column, Row, Layer}) returns the length of intersection between a cell or element and a 2D projection of the object. The function has three optional arguments: Column, Row, and Layer. If these arguments are provided, they specify the cell for which the length should be calculated. If they are not provided, the function uses the column, row, and layer of the node or element for which the formula is being calculated. If any of the arguments has an invalid value, the function returns zero. If the object being evaluated intersects the cell or element being evaluated more than once, ObjectIntersectLength returns the sum of all the individual lengths of intersection.

ObjectLength returns the length of an object in the 2D projection in which it is created and edited. Formulas for the third dimension of an object are not taken into consideration when computing ObjectLength.

ObjectName returns the name of the object that is currently being evaluated. ObjectName returns text.

ObjectVertexCount returns the number of vertices in the object.

ObjectVertexDistance(VertexIndex) returns the distance along the length of the object from the beginning of the object to the vertex indicated by VertexIndex. Formulas for the third dimension of an object are not taken into consideration when computing ObjectVertexDistance.

ObjectVertexX(VertexIndex) returns the X coordinate of the vertex in the object indicated by VertexIndex. For objects drawn on the side view, ObjectVertexX returns zero.

ObjectVertexY(VertexIndex) returns the Y coordinate of the vertex in the object indicated by VertexIndex. For objects drawn on the front view, ObjectVertexY returns zero.

ObjectVertexZ(VertexIndex) returns the Z coordinate of the vertex in the object indicated by VertexIndex. For objects drawn on the top view, ObjectVertexZ returns zero.

VertexInterpolate(Value1, Value2, ...) is intended for use with objects that are polylines rather than points or polygons. If the object that is being evaluated does not intersect the cell or element that is being evaluated, VertexInterpolate returns zero. If the object that is being evaluated does intersect the cell or element that is being evaluated, VertexInterpolate assigns Value1 to ValueN to vertices 1 to N respectively, of the object where N is the smaller of the number of arguments in VertexInterpolate and the number of vertices in the object. If the number of vertices in the object is greater than the number of arguments, the value of the last argument will be assigned to each of the vertices in the object that would not otherwise have an associated value. If a vertex of the object is in an element or cell, the associated value will be assigned to the element or cell. Otherwise, the values will be interpolated from the end points of the line segment that intersects the cell or element using linear interpolation based on the distance from the center point of the line segment within the cell or element to the adjacent vertices in the object (fig. 21). If more than one vertex of an object is in a cell or element or the object intersects a cell or element more than once, the value applied is the value for the last vertex or segment to intersect the cell or element. VertexInterpolate returns a real number.

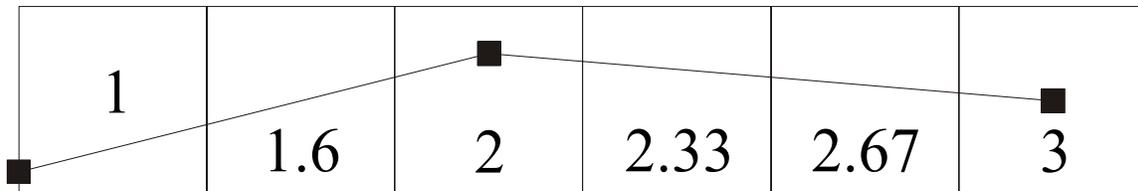


Figure 21. VertexInterpolate(1,2,3) returns the values shown for each element.

Formulas: Text

9.2.6 Text

The Text functions are used for manipulating text. One way they can be used is to control which shapes from a Shapefile are imported. See “Import Shapefile Dialog Box” on p. 33.

Copy(Text_Value, StartIndex, Count) returns a portion of Text_Value starting at the character indicated by StartIndex and extending for either Count characters or until the end of Text_Value is reached, whichever is smaller.

FloatToText(Value) converts the real number Value to its text representation.

IntToText(Value) converts the integer number Value to its text representation.

Length(Text_Value) returns the number of characters in Text_Value.

LowerCase(Text_Value) returns Text_Value with all its characters converted to lower case. See also: UpperCase.

Pos(SubText, Text_Value) returns the position of the first instance of SubText within Text_Value. If SubText does not occur within Text_Value, Pos returns zero.

PosEx(SubText, Text_Value, Offset) returns the position of the first instance of SubText within Text_Value that starts on or after Offset. If SubText does not occur within Text_Value, on or after Offset, PosEx returns zero. If Offset equals one, PosEx is equivalent to Pos.

TextToFloat(Text_Value) converts Text_Value to a real number. If Text_Value cannot be converted, TextToFloat causes an error.

TextToFloatDef(Text_Value, DefaultResult) converts Text_Value to a real number. If Text_Value cannot be converted, DefaultResult is returned instead.

TextToInt(Text_Value) converts Text_Value to an integer. If Text_Value cannot be converted, TextToInt causes an error.

TextToIntDef(Text_Value, DefaultResult) converts Text_Value to an integer. If Text_Value cannot be converted, DefaultResult is returned instead.

Trim(Text_Value) removes spaces from the beginning and end of Text_Value.

UpperCase(Text_Value) returns Text_Value with all its characters converted to upper case. See also LowerCase.

9.2.7 Trig

The trig functions are used for trigonometric operations. All angles in the functions are expressed in radians unless otherwise noted.

ArcCos(Value) returns the inverse cosine of Value. The return value is in the range from zero to Pi.

ArcCosh(Value) returns the inverse hyperbolic cosine of Value.

ArcSin(Value) returns the inverse sine of Value. The return value is in the range from $-\pi/2$ to $+\pi/2$.

ArcSinh(Value) returns the inverse hyperbolic sine of Value.

ArcTan2(Y, X) returns the inverse tangent of Y/X in the correct quadrant. The return value is in the range from $-\pi$ to $+\pi$.

ArcTanh(Value) returns the inverse hyperbolic tangent of Value.

Cos(Value) returns the cosine of Value.

Cosh(Value) returns the hyperbolic cosine of Value.

Formulas: Trig

DegToRad(Value) converts Value from degrees to radians. See also RadToDeg.

RadToDeg(Value) converts Value from radians to degrees. See also DegToRad.

Sin(Value) returns the sine of Value.

Sinh(Value) returns the hyperbolic sine of Value.

Tan(Value) returns the tangent of Value.

Tanh(Value) returns the hyperbolic tangent of Value.

10. Creating, Selecting, and Editing Objects in GoPhast

There are five types of objects in GoPhast. These are:

- Points,
-  Polylines,
-  Polygons,
-  Straight-Lines, and
-  Rectangles.

Each object consists of one or more vertices and has properties associated with it. The properties of an object determine how it is used to specify spatial properties of the model. Each object is associated with one of the three views of the model (top, front, or side).

10.1 Creating Objects

Objects are created by drawing them on the top, front or side **Working Areas** (p.10). The following sections describe how to create each type of object.

10.1.1 Points

Point objects have only a single vertex. To create a point object, the user does the following: (1) The user either selects **Object|Create Point** or clicks on the **Point** button. • (2) The user moves the cursor to the location on one of the views of the model where a point object is desired. (3) The user clicks the mouse button. A point object will be created at the cursor location. The **Object Properties** dialog box (p. 49) will appear. The **Object Properties** dialog box is used to specify the properties of the object.

Typical uses for point objects are to define the elevations of the tops or bottoms of geologic units, point values for hydraulic properties that will be defined using interpolation, or well boundary conditions.

10.1.2 Polylines

Polyline objects have two or more vertices. To create a polyline object, the user does the following: (1) The user either selects **Object|Create Line** or clicks on the **Polyline** button.  (2) The user moves the cursor to the location on one of the views of the model where the first vertex of the polyline object is desired. (3) The user clicks the left mouse button. The first vertex

Creating, Selecting, and Editing Objects in GoPhast

of the polyline object will be created at the cursor location. (4) To create additional vertices, the user continues clicking on the same view of the model. (5) When all the desired vertices have been created, the user double-clicks at the last vertex or presses the “Enter” key on the keyboard to complete the polyline. Pressing the escape or delete key while creating an object deletes the last created vertex of that object. As with points, the **Object Properties** dialog box (p. 49) is used to specify the properties of the object.

Typical uses for polylines are to define linear features, such as rivers and boundary conditions at the edges of the model.

10.1.3 Polygons

Polygon objects have four or more vertices. The last vertex is always at the same location as the first vertex, so a polygon with four vertices is a triangle. To create a polygon object, the user does the following: (1) The user either selects **Object|Create Polygon** or clicks on the **Polygon** button.  (2) The user continues adding vertices as described with Polylines. (3) When the polygon is complete, a final vertex will be added at the location of the first vertex to close the polygon. Pressing the escape or delete key while creating an object deletes the last created vertex of that object. As with points, the **Object Properties** dialog box (p. 49) is used to specify the properties of the object.

Typical uses for polygons are to define zones with differing media properties.

10.1.4 Straight-Lines

Straight-line objects are a special case of polylines in which all the line segments in the polyline are parallel to one of the edges of the grid. To create a Straight-line object, the user does the following: (1) The user either selects **Object|Create Straight Line** or clicks on the **Straight-line** button.  (2) The user continues adding vertices as described with Polylines. Pressing the escape or delete key while creating an object deletes the last created vertex of that object. As with points, the **Object Properties** dialog box (p. 49) is used to specify the properties of the object.

Typical uses of straight-line objects are the same as for polylines, that is to define linear features, such as rivers and boundary conditions at the edges of the model.

10.1.5 Rectangles

Rectangles are a special case of polygons that have four edges that are parallel to the grid. To create a rectangle, the user does the following: (1) The user either selects **Object|Create Rectangle** or clicks on the **Rectangle** button.  (2) The user moves the cursor to the location on one of the views of the model where the first vertex of the rectangle object is desired. (3) The user clicks the mouse button again at the opposite corner of the rectangle. As with points, the **Object Properties** dialog box (p. 49) is used to specify the properties of the object.

Typical uses of rectangle objects are the same as for polygons, that is to define zones with differing media properties.

10.2 Selecting Objects

To edit, move, or delete an object, the object must first be selected. Selected objects can be distinguished from objects that are not selected, because the lines used to draw the selected objects are thicker and the vertices of the selected objects are shown as squares. However, point objects are also shown as squares even if they are not selected. Selected point objects are shown as solid squares whereas point objects that are not selected are shown as hollow squares. In other types of objects, the vertices are shown as solid squares when the whole object is selected. If an individual vertex is selected, it is shown as a hollow square. The object in figure 22A is selected; the object in figure 22B is not. The object in figure 22C has one of its vertices selected.

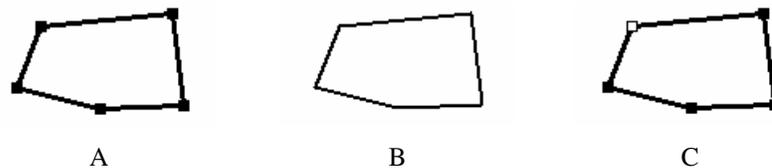


Figure 22. Appearance of (A) selected object, (B) non-selected object, and (C) an object with a selected vertex.

There are several ways to select objects. One way is to click on the **Select objects** button  and then click on the object. Another way is instead of clicking on an object, click and hold the left mouse button down somewhere on one view of the model that is not on any object and then drag the mouse. A rectangle will be drawn starting where the mouse was clicked down. When the mouse button is released, any objects that are entirely inside the rectangle will be selected. Another option is to click on the **Lasso** button . Then the user clicks down on one view of the model and moves the mouse. A line will follow the mouse. When the user releases the mouse, any objects that are entirely inside the line will be selected.

Usually, selecting one object causes any object that was previously selected to become non-selected; however, if the Shift key is held down while selecting an object, then the objects that would normally be selected are toggled between selected and non-selected and other objects remain selected.

The Ctrl key also modifies how selection occurs when the **Select objects**  button is down but not when the **Lasso**  button is down. The user can use the Ctrl key to select objects beneath another object. If several objects are on top of one another, the user can click on the objects with the Ctrl key down and if none of the objects is selected, the uppermost one will be selected. If the user clicks again with the Ctrl key down, the top object will be deselected and the next one down will be selected. If the user clicks again with the Ctrl key down, the object below that will be selected. The Shift and Ctrl key can be combined.

Individual vertices of an object can be selected as well as whole objects. To select individual vertices, the user first selects an object and then clicks on the **Select vertices** button . Next, the user clicks on the desired vertex to select it. To select additional vertices, the user clicks on them while holding down the Shift key. Vertices can only be selected on objects that are selected. The user can also click down away from any vertices of a selected object, drag the mouse, and then release it to select vertices that are inside the rectangle defined by the locations

where the user clicked down with the mouse button and where the user released it. All the vertices outside the rectangle will become non-selected (unless the Shift key is down). If the user holds down the Shift key while clicking on a vertex, the vertex will be toggled from selected to non-selected or the reverse.

A number of dialog boxes also allow the user to select objects. See “Search for Objects Dialog Box” on p. 53, “Show or Hide Objects Dialog Box” on p. 53, “Select Objects by Name Dialog Box” on p. 54, and “Go To Dialog Box” on p. 56.

10.3 Editing Objects

There are a number of ways to edit objects. Objects can be deleted or moved. Individual vertices in objects can be inserted, moved, or deleted. Edges of objects can be deleted. The order of the objects can be changed. Finally, the properties of objects can be changed.

To delete an object, select it and press the delete key on the keyboard. To delete individual vertices, select the vertices and press the delete key. To delete an edge of an object, click on the **Delete segment** button . Then click on an edge of an object to delete that edge. If deleting an edge will split the object into two separate pieces, one of the pieces will be a new object with the same properties as the original object except for its name.

One way to move objects or vertices is to select them, hold down the mouse button with the mouse cursor on or inside the object, and move the mouse before releasing the mouse button. Another way to move an object or individual vertices is to double click on the object. Then on the tab labeled **Vertices** in the **Object Properties** dialog box, type in new values for the coordinates of the vertices.

To insert a vertex, first click on the **Insert vertex** button . Then click on the edge of an object to insert a vertex at the position where the mouse was clicked. If any object is selected, this procedure will only insert a vertex in the selected object. If no object is selected, this procedure will insert a vertex into whichever object on which the user clicks.

To change the order of objects, select one or more objects and right-click on them. Select one of the options in the pop-up menu to change the order of the objects. It is also possible to select **Object|Rearrange Objects...** The **Rearrange Objects** dialog box (p. 49) will appear. In it, the user can drag objects to new positions.

To edit the properties of one or more objects, select them and then double-click on one of them. The **Object Properties** dialog box (p. 49) will appear, and the properties can be edited. The user can also display the **Object Properties** dialog box to edit the properties of a single object by displaying the **Show or Hide Objects** dialog box (p. 53) and double-clicking on the name of the object.

11. Main Menu and Buttons

The options in the following sections are provided in the GoPhast main menu. Each section starts with a table listing that briefly explains the menu items in the section. The buttons can be used to provide quick access to some of the menu items. In such cases, the picture on the button is shown next to the menu item both in the table and in the program.

All of the menu items in GoPhast have menu accelerators associated with them. Menu accelerators allow the user to navigate the menu without using the mouse. An underlined letter in the name of a menu item indicates the menu accelerator for that menu item. Some menu items also

Main Menu and Buttons

have shortcuts. A shortcut is indicated by a key sequence following the menu item. Shortcuts call a particular menu item directly without displaying the menu. For example, the **Edit|Undo** menu item has a menu accelerator of U (because the U in **Undo** is underlined) and a shortcut of Ctrl+Z (because “Ctrl+Z” follows **Undo** in the menu). A menu item can be activated by holding down the Alt key and pressing the key on the keyboard corresponding to the menu accelerator. Menu items beneath the main menu can then be selected by typing the keys on the keyboard corresponding to their menu accelerators or using the arrow keys. For example, to use the menu accelerator for **Edit|Undo**, the user would hold down the Alt key while pressing to E key to activate the **Edit** main menu item and then would press the U key to activate **Undo**. To use the shortcut for **Edit|Undo**, the user would hold down the Ctrl key while pressing the Z key. This would call the Undo menu item but unlike an accelerator, the menu would never be displayed.

For menu items or accelerators to work, the GoPhast window must have the input focus. On Linux, the method whereby a particular window can gain the focus can be set by the user. Some of these methods may be unfamiliar to users of other operating systems. For instance, a window may gain the focus when the mouse pointer is passed over it. In the KDE window manager on Linux, the method for setting the input focus can be changed by selecting **System|Desktop Settings Wizard**. In the Gnome window manager on Linux, the method for setting the input focus can be changed by selecting **Programs|Settings|Sawfish window manager|Focus behavior**. Clicking on a window with the mouse will generally give that window the focus on either Windows or Linux.

11.1 File

The menu items under **File** are listed in table 3. Many of the choices under **File|Import** refer to features of data sets and objects that are described under “Data Sets Dialog Box” (p. 42) and “Object Properties Dialog Box” (p. 49).

Table 3. File Menu

Menu Item	Explanation
 New	Creates a new model.
 Open	Opens an existing model.
 Save	Saves the current model to disk using the current file name.
Save As	Saves the current model to disk using a new file name.
Import Shapefile...	Import shapes from a Shapefile into GoPhast. See “Import Shapefile Dialog Box” on p. 33.
Import DXF File...	Import a DXF file. See “Import DXF File Dialog Box” on p. 34.
Import Points...	Import point data into GoPhast. See “Import Points Dialog Box” on p. 35.
Import Distributed Data by Zone...	Import a PHAST zone into GoPhast. See “Import Distributed Data by Zone Dialog Box” on p. 35.
Import Bitmap...	Import a background image into GoPhast. See “Import/Edit Bitmap Dialog Box” on p. 35.
Export PHAST Input File <filename>	Creates the transport data file for PHAST. The names of the four most recently opened files are displayed. Selecting one of them will open that file.
Exit	Closes GoPhast.

11.1.1 Import Shapefile Dialog Box

The **Import Shapefile** dialog box is used to import Shapefiles into GoPhast. To display the **Import Shapefile** dialog box, select **File|Import|Shapefile...**

The Shapefile format (Environmental Systems Research Institute, Inc, 1998) is a commonly used file format in Geographic Information Systems. The Shapefile is imported as a series of objects on the top view of the model. These objects will set the values of data sets as specified by the user. The names of the imported objects are based on the name of the file from which the objects are imported. The “Select Objects by Name Dialog Box” (p. 54) can be used to select all these objects at a later time.

After selecting the Shapefile to import, the attributes of the shapes are displayed in the Import Shapefile dialog box. The user chooses which attributes to import by checking the checkbox next to the name of the attribute. The user can then decide whether to create a new data set for each attribute that is imported or to assign values to existing, compatible data sets. Only data sets with an orientation of "2D Top" can be used for the imported shapes. If a new data set will be used, the user can choose an interpolation method for the new data set. (See “Interpolation Methods” on p. 16.) The user also decides whether to evaluate the objects at element or nodes and whether to set the values of enclosed elements or nodes, intersected elements or nodes, or to set values or elements or nodes by interpolation.

Some Shapefiles store the coordinates of points as latitudes and longitudes. On the **Coordinate Conversion** tab, the user can choose to convert those coordinates to Universal Transverse Mercator (UTM) coordinates. If all the points in the Shapefile belong in the same UTM zone, that zone will be picked automatically. Otherwise, the user must specify the appropriate zone number in an edit box. The user also must specify the ellipsoid used as a basis for the conversion. Normally, the default ellipsoid is appropriate. More information about coordinate conversions and map projections can be found in Snyder (1987).

Shapes in Shapefiles can contain holes inside polygons. GoPhast does not have a method of representing holes so such shapes are skipped when importing into GoPhast.

In some cases, the user may not wish to import all the shapes in a Shapefile. The **Import criterion** can be used to determine which shapes are imported. The user can enter a formula which will be evaluated for each shape. Only those shapes for which the formula evaluates to True will be imported. The user can click the **Edit F()...** button to edit the formula for the import criterion using the **Formula Editor** (p. 44). The following example shows how coordinate conversions and the **Import criterion** can be used to advantage.

In this example, only the shapes from Oklahoma will be imported from a Shapefile containing shapes for rivers throughout the United States. Oklahoma was selected for this example because example 4 from the PHAST documentation is set in Oklahoma.

1. The National Atlas of the United States (<http://nationalatlas.gov/atlasftp.html#hydrogm>) has a Shapefile that represents the major streams and water bodies in the United States. Download the Shapefile version of that data (hydrogm020.tar.gz) and extract its contents.
2. In GoPhast, select **File|Import|Shapefile...** and then select hydrogl020.shp which was extracted from hydrogm020.tar.gz.
3. After the Shape geometry file has been read, the **Import Shapefile** dialog box will be displayed. Go to the **Coordinate Conversion** tab and check the checkbox labeled **Convert coordinates from decimal degrees to UTM**. Change the **UTM zone number** to 14. This is the appropriate UTM zone for Oklahoma.

Main Menu and Buttons: File

4. Go to the **Data** tab and change the **Import criterion** to `Pos("OK", UpperCase(STATE)) > 0`. STATE is one of the attributes of the Shapefile. It holds abbreviations for the state or states in which each water body is present. This formula evaluates to true if the water body is in the state of Oklahoma (abbreviation = "OK"). Select any of the attributes you wish to import in the dialog box at the top of the **Data** tab and click the **OK** button. For an explanation of the attributes in the Shapefile, see the file hydrogm020.txt that came with the Shapefile.
5. After the shapes have been imported, select **View|Go To...** and select the first imported shape. Then zoom out to see all the imported water bodies. Only shapes that are at least partially in Oklahoma will have been imported, and their coordinates will have been converted to UTM coordinates (fig. 23).

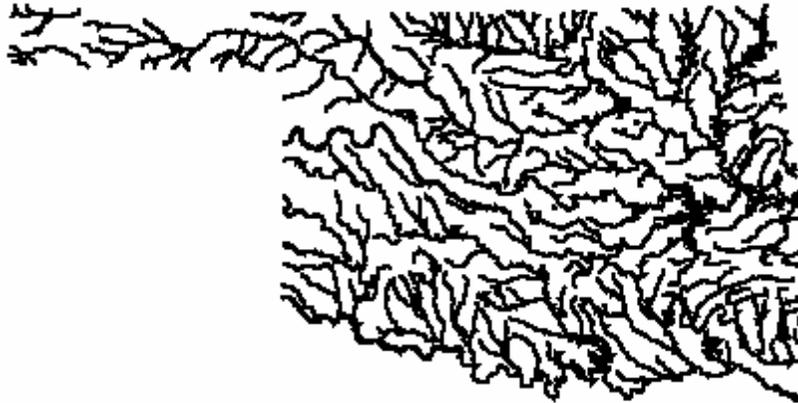


Figure 23. Imported Oklahoma water bodies.

11.1.2 Import DXF File Dialog Box

The Drawing Exchange Format (DXF) (Autodesk, Inc., accessed July 21, 2005) is a commonly used file format for Computer Aided Design (CAD) programs. The **Import DXF File** dialog box is used to import DXF files into GoPhast as a series of objects on the top view of the model. The dialog box is displayed by selecting **File|Import|DXF File...** The DXF file is then read, and the **Import DXF File** dialog box is displayed.

Objects in DXF files can contain a Z coordinate. The value of this coordinate is assigned to a data set. The data set can be either a new or an existing one; however, the orientation of the data set must be "2D Top." The user can determine whether the objects that are imported will set the values of enclosed or intersected cells or set values by interpolation. If the data are being used with a new data set, the user can choose an interpolation method for the new data set. (See "Interpolation Methods" on p. 16.) The names of the imported objects will be based on the name of the file from which the objects are imported. The **Select Objects by Name** dialog box (p. 54) can be used to select all these objects at a later time.

Objects in DXF files may cross themselves. Such objects are invalid in GoPhast so such objects are skipped when importing into GoPhast.

11.1.3 Import Points Dialog Box

A common format for data are as a series of points with associated data. To import such data, the user selects **File|Import|Import Points...** to display the **Import Points** dialog box. The dialog box has two tabs: **Controls** and **Data**. Typically, the user sets the values on the **Controls** tab before switching to the **Data** tab to specify the data that will be imported. At the top of the **Controls** tab is a list of data sets for which data can be imported. The data sets that are listed depend on where the data will be **Evaluated at** (elements or nodes), their **View direction** (top, front, or side) and the number of **Associated third-dimension formulas**. These three choices are specified with radio buttons below the list of data sets. The user also specifies whether the imported objects **Set values of intersected nodes or elements** or **Set values of nodes or elements by interpolation**. The names of the imported objects will be based on the **Root name** specified by the user. These options are explained in greater detail in the explanation of the **Object Properties** dialog box (p. 49).

Once the user is satisfied with the **Controls** tab, the data to be imported are specified in the **Data** tab. The **Data** tab has a table in which the data to be specified are entered. The first two to four columns of the table are reserved for the coordinates of the data points. The remaining columns are used for the data to be imported. The columns for the imported data can be rearranged by clicking down on a column header and dragging the column to a new position. The user can enter the required data into the table manually. When entering data manually, the user specifies the number of rows in the table in the edit box near the bottom of the **Data** tab. Another way to enter the data is to read them from a tab-delimited file or to paste them from the clipboard. In a tab-delimited file, each value is separated from the next value by a tab character. Each line in the file represents a separate data point. To read the data from a tab-delimited file, the user clicks the **Open File** button and selects the file from which the data are to be imported. To paste the data from the clipboard, put the data in a spreadsheet program, select the cells that hold the data, and copy them to the clipboard. Then the user goes back to the **Import Points** dialog box and selects the cell in the upper left corner of the space where the data belong. Pressing Ctrl-V on the keyboard will paste the data. If required, the number of rows in the table will be increased to accommodate the data that are pasted from the clipboard. Once the data have been entered into the table, the user presses the **OK** button to import the data. Each row in the table will be imported as a separate point object in GoPhast.

11.1.4 Import Distributed Data by Zone Dialog Box

PHAST has an option whereby a different value is specified for each node or element in a zone. The zone is defined by a pair of lower and higher coordinates in each of the three coordinate directions. The **Import Distributed Data by Zone** dialog box is used to import such data into GoPhast. It is displayed by selecting **File|Import|Distributed Data by Zone...**

Importing data by zone is a good method for importing data when the data already exist in a zone format and when it is known that the grid will not be changed. If the grid will be changed or if the data are not already in a zone format, other methods such as importing point data are better because the data are specified in a grid-independent fashion. (See “Import Points Dialog Box” on p. 35.)

The user specifies the boundaries of the zones and the names of files containing the data to be imported. The user can either type in the path or use the **Browse** button to select the file. The dialog box can be resized if needed to display the full path name of a data file. When the user

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clicks the **OK** button, the files will be read and the data will be imported. The format of the file is the same as that used by PHAST – a text file containing a list of data values. The values must be arranged so that all the values from lower layers precede values from high layers. Within the data for a layer, all values for lower rows precede values from higher rows. Within the data for a row, all values for lower columns precede values from higher columns. The data will be imported as a rectangular object with a formula for each data set for which the object sets the values. The formula will specify the value to apply to each node or element contained in the object. The coordinate system of the grid is used when specifying the coordinates. If the grid angle is not zero, the coordinate system of the grid is rotated relative to the global coordinate system. The user must select the view of the model to which the data will be imported (Top, Front, or Side).

The user must not change the grid or move the imported objects once the data have been imported because the data read from the file must have the correct number of values for all the nodes or elements in the zone. If the grid is changed or the object is moved, the number of values may no longer be correct or the values may no longer be in the correct locations. If the grid must be changed, it is best to delete the imported objects and then import a new set of values that is correct for the modified grid.

11.1.5 Import/Edit Bitmap Dialog Box

It is often useful to display a bitmap in the background when working with a model. To import a bitmap, the user first selects **File|Import|Bitmap...** The same dialog box can be displayed by selecting **Edit|Edit Bitmaps...** The **Import/Edit Bitmap** dialog box will be displayed. The user clicks the **Select Image** button to select the bitmap to import. If a World (*.wld) file with the same file name as the selected bitmap exists, it will be read and used to specify the location of the bitmap. The user may also click the **Import World File** button to select a World file to read. The format of world files is described at the following URL:

<http://support.esri.com/index.cfm?fa=knowledgebase.techarticles.articleShow&d=16106>

The user can also specify the location of the bitmap without using a World file. To specify the location of the bitmap, the user clicks on the bitmap two or more times. For each point the user clicks, a dialog box will appear in which the user must specify the real world locations of the pixels that were clicked. The data will be entered in the table to the left of the image. To delete one of these points, delete one or more of the values for the point. If any of the values for a point is missing, the point will be ignored. The user must enter at least two points before the bitmap can be imported. The user also must specify a name for the image and whether the image will be visible from the top, front, or side of the model. By default, the image will be visible; however, the user can hide it by unchecking the **Visible** checkbox.

Bitmaps can be in bmp, jpeg, or png formats; however, on computers using the Windows-2000 operating system, GDI+ must be installed to use jpeg images. GDI+ is not required on Windows XP or Linux because support for jpegs is built into the operating system on those platforms. GDI+ can be downloaded from the following Microsoft web site:

<http://www.microsoft.com/downloads/details.aspx?familyid=6A63AB9C-DF12-4D41-933C-BE590FEAA05A>

GDI+ is distributed as a self-extracting compressed file. The dll it contains needs to be put in a location where GoPhast can find it before starting the program. The location where GoPhast is installed is a good place to put it.

See also: “Show or Hide Bitmaps Dialog Box” on page 37.

11.2 Edit

The menu items under **Edit** are listed in table 4.

Table 4. Edit Menu

Menu Item	Explanation
 Undo	Reverses the last action.
 Redo	Cancels undo.
Edit Bitmaps...	Allows the user to edit data related to bitmaps that have been imported into GoPhast. See “Import/Edit Bitmap Dialog Box” on p. 35.
Show or Hide Bitmaps...	Allows the user to show or hide background images. See “Show or Hide Bitmaps Dialog Box” on p. 37.

11.2.1 Show or Hide Bitmaps Dialog Box

The **Show or Hide Bitmaps** dialog box provides a quick way to show or hide the bitmaps that have been imported. It is displayed by selecting **Edit|Show or Hide Bitmaps...** Each bitmap is listed next to a checkbox. If the checkbox next to a bitmap is checked, the bitmap will be visible; otherwise, the bitmap will be hidden. Clicking the **Show all** and **Show none** buttons will show or hide all of the bitmaps. Clicking the **Toggle** button will show all the bitmaps that are hidden and hide all those that are visible.

See also “Import/Edit Bitmap Dialog Box” on p. 36.

11.3 Grid

The menu items under **Grid** are listed in table 5.

Table 5. Grid Menu

Menu Item	Explanation
 Delete Grid Line	Click on a grid line to delete it. See “Editing the Grid” on p. 38.
 Move Grid Line	Click and drag a grid line to move it. See “Editing the Grid” on p. 38.
 Add Vertical Grid Line	Click to add a vertical grid line. See “Editing the Grid” on p. 38.
 Add Horizontal Grid Line	Click to add a horizontal grid line. See “Editing the Grid” on p. 38.
 Subdivide Grid Elements	Click and drag to select elements to subdivide. See “Subdivide Columns, Rows, and Layers Dialog Box” on p. 39.
 Set Width	Set the width of grid elements. See “Set Widths of Columns, Rows, and Layers Dialog Box” on p. 39.
 Drag to Rotate	Click and drag to rotate the grid. See “Editing the Grid” on p. 38.
Specify Grid Angle...	Specify a precise grid angle. See “Grid Angle Dialog Box” on p. 39.
 Generate Grid...	Create a grid using objects. See “Using Objects to Specify the Grid” on p. 12 and “Generate Grid Dialog Box” on p. 40.
Specify Grid Lines...	Specify precise grid coordinates. See “Grid Spacing Dialog Box” on p. 40.
Smooth Grid...	Adjust the grid spacing. See “Using Objects to Specify the Grid” on p. 12 and “Smooth Grid Dialog Box” on p. 41.
Set Selected Col, Row, Layer...	Choose which column, row, or layer is selected. See “Select Column, Row, and Layer Dialog Box” on p. 41.

11.3.1 Editing the Grid

Methods for editing the grid include deleting grid lines, moving grid lines, adding grid lines, subdividing elements, changing the grid angle, and “smoothing” the grid.

To delete a grid line, the user selects **Grid|Delete Grid Line** or clicks the **Delete grid line** button . Then the user moves the cursor over the grid line to be deleted. When the cursor is over a grid line, it will change from an arrow to an X. If the mouse button is clicked at that point, the grid line will be deleted.

To move grid lines, the user first selects **Grid|Move Grid Line** or clicks on the **Move grid line** button . The user next moves the cursor over one of the views of the model. When the cursor is over a grid line, the cursor will change shape so that it resembles the picture on the **Move grid line** button . Then the user clicks down the mouse button, moves the cursor, and releases the mouse button. The grid line that was under the cursor when the mouse button was pressed will be moved to the location where the mouse button was released.

To add a grid line, the user selects either **Grid|Add Vertical Grid Line** or **Grid|Add Horizontal Grid Line** or clicks on the **Add vertical grid line**  or **Add horizontal grid line**  buttons. Then the user moves the cursor over one of the views of the model. The cursor will

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change to a line parallel to one of the edges of the grid. When the user clicks the mouse, a new grid line will be added at the position where the mouse was clicked.

The grid angle can be changed in two ways. First, the user can choose **Grid|Specify Grid Angle...** The **Grid Angle** dialog box (p. 39) will appear in which the user can specify the grid angle. Another way is to choose **Grid|Drag to Rotate** or click on the **Drag to rotate grid** button . Then the user clicks down on the top view of the model and moves the cursor before releasing the mouse button.

Additional methods of editing the grid are described in “Subdivide Columns, Rows, and Layers Dialog Box” (p. 39), “Set Widths of Columns, Rows, and Layers Dialog Box” (p. 39), “Grid Angle Dialog Box” (p. 39), “Generate Grid Dialog Box” (p. 40), “Smooth Grid Dialog Box” (p. 41), and “Grid Spacing Dialog Box” (p. 40).

11.3.2 Subdivide Columns, Rows, and Layers Dialog Box

The **Subdivide Columns, Rows, and Layers** dialog box is used to split columns, rows, and layers into two or more parts. The dialog box is shown by first selecting **Grid|Subdivide Grid Elements** or clicking the **Subdivide grid elements** button . Then the user clicks and drags on the grid with the mouse to select a range of elements. The elements over which the mouse moved with the mouse button pressed will be selected and shown in a gray color. When the mouse button is released, the **Subdivide Rows, Columns, and Layers** dialog box appears. In the dialog box, the rows columns and layers selected by the user are displayed. If desired, the user can edit the range of columns, rows and layers displayed. The user specifies how many columns, rows, and layers each selected column, row, and layer should be divided into and clicks the **OK** button to subdivide them. Each selected column, row, or layer will be split into the specified number of parts. The parts making up each former element will have a uniform width, and the total width of the parts will be equal to the total width of the selected columns, rows, or layers before they were subdivided.

11.3.3 Set Widths of Columns, Rows, and Layers Dialog Box

The **Set Widths of Columns, Rows, and Layers** dialog box is used for specifying the exact widths of columns, rows, and layers. To display the dialog box, the user selects **Grid|Set Width** or clicks the **Set width** button . Next the user clicks and drags with the mouse to select one or more columns, rows, or layers on the top, front, or side view of the model. When the mouse is released, the dialog box will appear. The average width of the elements will be displayed. The user should decide whether to edit the columns, rows, or layers and check the corresponding checkboxes. The user may then edit the range of columns, rows, or layers to be edited and set the desired width. Clicking the **OK** button will cause the element size of the selected columns, rows, and layers to be changed.

11.3.4 Grid Angle Dialog Box

The **Grid Angle** dialog box is used to change the angle of the grid. It is displayed by selecting **Grid|Specify Grid Angle...** The user then enters an angle (in degrees) in the edit box and clicks the **OK** button to change the angle of the grid as viewed from the top. The grid will be

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rotated around its center. The grid angle is measured counterclockwise from the X-axis. The axis of rotation is always vertical.

See also: “Specifying a Grid with Numbers” on p. 11 and “Editing the Grid” on p. 38.

11.3.5 Generate Grid Dialog Box

The **Generate Grid** dialog box is used to help control the generation of a grid using objects (p. 12). It is displayed by selecting **Grid|Generate Grid...** or clicking the **Generate Grid** button . Before it can be used, there must be at least one polygon on the top view of the model for which **Use to set element grid size** is true and at least one polyline or polygon on the front or side views of the model for which **Use to set element grid size** is true. (See “Object Properties Dialog Box” on p. 49.) The **Calculate grid angle automatically** checkbox determines whether or not GoPhast will calculate a grid angle or use an angle supplied by the user. If GoPhast calculates the angle automatically, it will specify the angle so that the area of the grid is minimized. If it is not calculated automatically, the user must specify the grid angle (in degrees) in the **Grid angle** edit box.

Some ground-water-modeling programs benefit from keeping the contrast in the width of adjacent cells less than a value of 1.5 (Anderson and Woessner, 1991). This can be achieved by checking the **Smooth grid** checkbox in the **Generate Grid** dialog box. If it is checked, the checkboxes for rows, columns, and layers determine whether grid smoothing will be applied in those directions. The **Grid smoothing criterion** determines the maximum ratio allowed between adjacent elements.

11.3.6 Grid Spacing Dialog Box

The **Grid Spacing** dialog box is used to specify the precise locations of grid lines. The **Grid Spacing** dialog box is displayed by selecting **Grid|Specify Grid Lines...** The dialog box has three tabs labeled **Columns**, **Rows**, and **Layers**. Each tab has a table with the positions of the relevant grid lines and an edit box that can be used to change the number of grid lines. The numbers in the tables represent the distance in the X', Y', or Z directions from the origin of the coordinate system. X' and Y' represent distances in a coordinate system aligned with the grid. If the grid angle is zero, X' = X and Y' = Y. The user can type new values in the table or copy them from a spreadsheet to the operating system clipboard and then paste them in the table. (Pressing the Ctrl and V keys simultaneously will paste the contents of the clipboard into the selected cell in the table and overwrite the existing contents.) The grid-line positions do not need to be in order; they will be sorted into the correct order when the user clicks on the **OK** button. The cells in the table can be dragged to different positions in the table by clicking-down in the area of the table where the row number is displayed and moving the mouse to a new position before releasing the mouse.

The easiest way to delete a particular grid line in this dialog box is to make the cell where it is specified blank. The grid line will be deleted when the **OK** button is clicked.

To add new grid lines, increase the number of nodes to the desired number. Each new grid line will be added at a position that is equal to the number in **Default spacing** further than the previous line in the grid. For example, if the last grid line is at 100 m and the default spacing is 20 m, the next new grid line will be at a position of 120 m.

11.3.7 Smooth Grid Dialog Box

Some ground-water-modeling programs, benefit from keeping the contrast in the width of adjacent cells less than a value of 1.5 (Anderson and Woessner, 1991). The **Grid|Smooth Grid...** menu item is designed to facilitate creating grids that meet this criterion. In PHAST, contrasts in element size are not an issue, but it still can be useful to have an area with a refined grid where results need to be more accurate. When the user selects this menu item, the **Smooth Grid** dialog box will appear in which the user can specify whether to adjust the row, column, or layer spacing to meet the criterion. The **Grid smoothing criterion** is the maximum ratio between adjacent rows, columns, or layers that will be accepted. The default value is 1.2, which is well below the usual limit. After making the desired selections, the user can click the **OK** button to adjust the grid spacing. Column, row, or layer boundaries will be moved to meet the grid smoothing criterion but no new columns, rows, or layers will be created.

11.3.8 Select Column, Row, and Layer Dialog Box

The **Select Column, Row, and Layer** dialog box can be used to change the selected column row or layer. To display the **Select Column, Row, and Layer** dialog box, select **Grid|Set Selected Col, Row, Layer...** Enter the desired values in the edit boxes and click **OK** to set them.

There are two other ways to change the selected column, row, or layer that do not involve this dialog box.

1. In the corner of the top, front, and side views of the model is a **Selection Cube** (see p. 9) that displays the column, row, or layer that is selected. Clicking on the **Selection Cube** changes the selected column row or layer. For more details see “The Selection Cube” on p. 9.
2. The Page Up, Page Down, and arrow keys on the keyboard change the selected column row or layer. The left arrow key decreases the selected column by one. The right arrow key increases the selected column by one. The up arrow key increases the selected row by one. The down arrow key decreases the selected row by one. The Page Up key increases the selected layer by one. The Page Down key decreases the selected layer by one. If the “Shift” key on the keyboard is held down while pressing one of these keys, the selected column, row, or layer is changed by 10.

11.4 Data

The menu items under **Data** are listed in table 6. This section also includes descriptions of the **Formula Editor** and the **Data Type Problem** dialog boxes. Both of these are accessed from the **Data Sets** dialog box.

Table 6. Data Menu

Menu Item	Explanation
Edit Data Sets...	Edit the properties of data sets. See “Data Sets Dialog Box” on p. 42.
Color Grid...	Color the grid with the values of a data set or boundary condition. See “Color Grid Dialog Box” on p. 47.
Show Formula Errors...	Display formulas that have been set to a default value because they were invalid. See “Formula Errors Dialog Box” on p. 47.

11.4.1 Data Sets Dialog Box

Data sets are managed through the **Data Sets** dialog box. To display the **Data Sets** dialog box, select **Data|Edit Data Sets...**

Data sets have a two-dimensional or three-dimensional array of values, which correspond either to elements or to nodes in the grid or a projection of the grid in the top, front, or side views. (These values correspond to “properties” as used in section 4.2.1.3 of the PHAST manual (Parkhurst and others, 2004). In this report, “properties” do not necessarily refer to spatially distributed data.) This section describes each of the properties of a data set that the user can change.

All of the data sets required by PHAST (table 7) are displayed in the **Data Sets** dialog box along with data sets that the user has created. If a data set is sometimes required by PHAST but is not being used in the current project, it is displayed in the dialog box in italics with a light gray background. Each data set has several properties: its name, whether or not it is visible, type, orientation (top, front, side, or 3D), where it is evaluated (nodes or elements), its units, its formula, and, for 2D data sets, its interpolation method. For data sets used directly by PHAST (table 7), the name, type, orientation, and where it is evaluated cannot be changed. For data sets created by the user, these properties can be changed. For some data sets that are used directly by PHAST, the user can use a special PHAST-style interpolation method (p. 16).

To create a new data set, click the **Add** or **Insert** button in the **Data Sets** dialog box. Clicking the **Add** button, adds a new data set at the end of the table. Clicking the **Insert** button, inserts a new data set above the currently selected row in the table. To delete a data set, select the row in the table containing the data set and then click on the **Delete** button. (Users cannot delete data sets that are used directly by PHAST.)

The **Name** of a data set is used to identify it in formulas for other data sets and when exporting the corresponding PHAST data set (if there is one). A name must begin with either the underscore character or one of the letters A through Z in either upper- or lower-case characters. Subsequent characters must be the underscore character, the letters A through Z in either upper- or lower-case characters, or the digits 0 through 9. Spaces are not allowed in the names of data sets. Data Set names are case insensitive. Thus, “A_NAME”, “a_name”, and “A_Name” are all equivalent.

Each data set must have a **Type** that indicates what kind of data are stored in it. Valid types are "Real", "Integer", "Boolean", and "Text." These types represent real numbers, integers, true/false values, and text, respectively. Most of the data sets built into GoPhast are "Real" or "Integer." The "Active" data set is "True/False." No built-in data sets are "Text."

The **Orientation** of a data set determines the shape of a data set. The possible choices are **2D Top**, **2D Front**, **2D Side**, and **3D**. Most data sets have an **Orientation** of **3D**. A data set with a **2D Top** orientation has a single layer but multiple columns and rows. A data set with a **2D Front** orientation has a single row but multiple columns and layers. A data set with a **2D Side** orientation has a single column but multiple rows and layers. A data set with a **3D** orientation has multiple columns, rows, and layers.

If **Evaluated at** (the evaluation location) is set to **Elements**, then the values in the data set correspond to elements in the model grid and are evaluated at the centers of elements. If **Evaluated at** is set to **Nodes** then the values in the data set correspond to nodes in the model grid. For orientations of **2D Top**, the data set values correspond to the elements or nodes in a 2D projection of the model grid from above. Similarly for **2D Front** and **2D Side**, the data set values

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correspond to the elements or nodes in a 2D projection of the model grid from the front or side, respectively.

The **Units** of a data set are meant to serve as a reminder to the user. The units do not affect how values are computed.

The **Default formula** of a data set is a mathematical expression that defines the value that will be applied to each location in a data set unless a value for that location is specified in some other way (such as being set by objects). A formula may be a simple numerical value or it can express much more complex relationships. See the section on “Formulas” for more information. (See p. 17.)

If a data set is a two-dimensional data set, it can use one of the 2D **Interpolation** methods in conjunction with one or more objects to define the values of a data set. If an interpolation method is being used with a data set, the **Anisotropy** edit box related to that interpolation method becomes enabled in the bottom part of the dialog box when the data set is selected. Three interpolation algorithms are available in GoPhast: **Nearest**, **Inv. Dist. Sq.** (Inverse Distance Squared), and **Nearest Point**. See the section on “Interpolation Methods” for more information (p. 16.)

If the data set is one of the PHAST data sets with which **PHAST-style interpolation** can be used, the **Use PHAST-style interpolation for all cells** checkbox will be enabled when the data set is selected. If the user checks this checkbox, the other controls related to PHAST-style interpolation will become enabled. See “PHAST-Style Interpolation” on p. 16.

In a new GoPhast project, the only data sets present are those required by PHAST (table 7). However, the user can create additional data sets for his or her own purposes. One reason to create a data set would be to use it in a formula for one of the data sets required by PHAST. For example, the user could create a **2D Top** data set that represented the hydraulic conductivity of a particular geologic unit. It could then be used to assign Kx for just those elements that were part of that geologic unit. The Biscayne Bay aquifer example (p. 87) illustrates this process.

Table 7. Data Sets required by PHAST

Data Set	Description	PHAST equivalent	When used
Active	Specifies whether an element in PHAST is active or not.	MEDIA, active	always
Kx	Specifies the hydraulic conductivity in the X direction.	MEDIA, Kx	always
Ky	Specifies the hydraulic conductivity in the Y direction.	MEDIA, Ky	always
Kz	Specifies the hydraulic conductivity in the Z direction.	MEDIA, Kz	always
Porosity	Specifies the porosity.	MEDIA, porosity	always
Specific_Storage	Specifies the specific storage.	MEDIA, specific_storage	always
Longitudinal_Dispersivity	Specifies the longitudinal dispersivity.	MEDIA, longitudinal_dispersivity	Use solute transport checked in Chemistry Options Dialog Box
Horizontal_Transverse_Dispersivity	Specifies the horizontal transverse dispersivity.	MEDIA, horizontal_dispersivity	Use solute transport checked in Chemistry Options Dialog Box

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Table 7: continued

Data Set	Description	PHAST equivalent	When used
Vertical_Transverse_- Dispersivity	Specifies the vertical transverse dispersivity.	MEDIA, vertical_dispersivity	Use solute transport checked in Chemistry Options Dialog Box
Initial_Head	Specifies the initial head.	HEAD_IC, head	Neither Use free surface nor Use water table for initial condition checked in Free Surface Dialog Box
Initial_Water_Table	Specifies the initial water table.	HEAD_IC, water_table	Use free surface and Use water table for initial condition checked in Free Surface Dialog Box
Chemistry_Initial_- Solution	Specifies the initial solution.	CHEMISTRY_IC, solution	Use solute transport in Chemistry Options Dialog Box
Chemistry_Initial_- Equilibrium_Phases	Specifies the initial equilibrium phases.	CHEMISTRY_IC, equilibrium_phases	Use solute transport and Use equilibrium phases checked in Chemistry Options Dialog Box
Chemistry_Initial_Surface	Specifies the initial surface properties.	CHEMISTRY_IC, surface	Use solute transport and Use surface assemblages checked in Chemistry Options Dialog Box
Chemistry_Initial_- Exchange	Specifies the initial exchange properties.	CHEMISTRY_IC, exchange	Use solute transport and Use exchange checked in Chemistry Options Dialog Box
Chemistry_Initial_Gas_- Phase	Specifies the initial gas phase properties.	CHEMISTRY_IC, gas_phase	Use solute transport and Use gas phases checked in Chemistry Options Dialog Box
Chemistry_Initial_Solid_- Solutions	Specifies the initial solid-solution properties.	CHEMISTRY_IC, solid_solution	Use solute transport and Use solid solution checked in Chemistry Options Dialog Box
Chemistry_Initial_- Kinetics	Specifies the initial kinetic properties.	CHEMISTRY_IC, kinetics	Use solute transport and Use kinetics checked in Chemistry Options Dialog Box
Print_Chemistry	Specifies the "Print Chemistry" distribution.	PRINT_LOCATIONS, chemistry	Use solute transport checked in Chemistry Options Dialog Box
Print_XYZ_Chemistry	Specifies the "Print XYZ Chemistry" distribution.	PRINT_LOCATIONS, xyz_chemistry	Use solute transport checked in Chemistry Options Dialog Box

11.4.2 Formula Editor Dialog Box

The **Formula Editor** dialog box is used to edit formulas (see p. 17). It can be displayed by clicking a button next to a formula in the **Data Sets** dialog box (p. 41), the **Object Properties** dialog box (p. 49), or the **Import Shapefile** dialog box (p. 33). The **Formula Editor** dialog box has four main parts (fig. 24):

- the **formula text box** in the upper left where the formula is composed,
- the **buttons** in the lower left where numbers, operators, and dividers can be selected,
- the **list of data sets and functions** on the right where data sets and functions can be selected (**Data Sets** is replaced by **Attributes** when the **Formula Editor** is used to edit the **Import criterion** in the **Import Shapefile** dialog box), and

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- the **Select Matching Parenthesis**, **Function Help**, and other buttons at the bottom of the dialog box.

The relative size of the formula text box and the list of data sets and functions can be adjusted by clicking on the boundary between them and dragging with the mouse button held down.

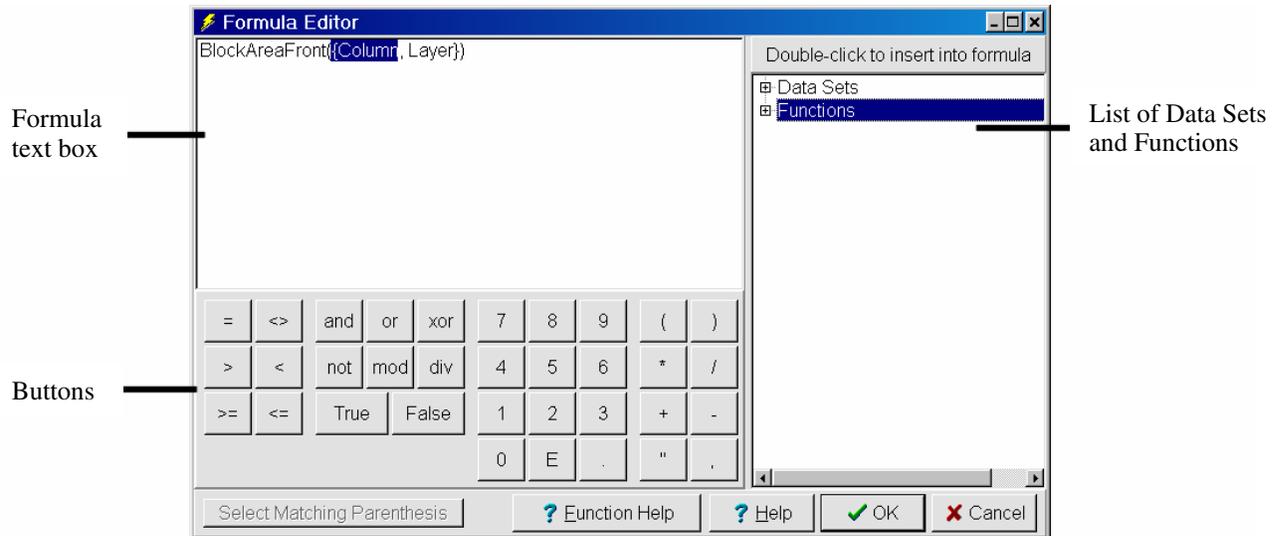


Figure 24. Formula Editor.

11.4.2.1 The Formula Text Box

The formula text box is used to compose the formula. Three methods can be used to create the formula: (1) The formula can be typed in the formula text box directly; (2) the number and operator buttons can be used to insert items into the formula; or (3) the list of data sets and functions can be used to insert items into the formula. When the formula is complete, the user clicks the **OK** button. If the formula is valid, the formula will be accepted, and the **Formula Editor** will close. If it is invalid, an error message will be displayed, and the **Formula Editor** will remain open.

11.4.2.2 Number and Operator Buttons

The number and operator buttons all work the same way: when the user clicks one of the buttons, the text displayed on the button will be inserted in the **Formula text box** at the position of the cursor. If any text in the formula is selected, it will be replaced. See “Operators” on p. 18 for more information on the meanings of the operators.

11.4.2.3 List of Data Sets and Functions

The data sets and functions that can be included in a formula are listed in the **List of Data Sets and Functions** on the right in the **Formula Editor**. For compactness, they are shown in a tree view. To see the available data sets or functions click the plus (+) sign to the left of **Data Sets** or **Functions** to expand the list. Within functions, there are additional lists that can be expanded by clicking the plus sign to their left. When the terminal branches of the tree are visible, the user can

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double click on one of them to insert it into the formula at the location of the cursor. If any text in the formula is selected, it will be replaced by the data set or formula. See “Functions” on p. 19 for more information on the meanings of the functions.

Not all data sets will be listed in the data set list, because not all data sets can be included in a formula for all other data sets. For instance, a formula for a data set cannot include a reference to itself either directly or indirectly. For example, if the formula for **Ky** is "Kx", the formula for **Kx** could not include **Ky** because that would make the formula for **Kx** depend on itself. Another example of a circular reference that is not allowed is to set the formula for **Ky** to "Kx", the formula for **Kz** to "Ky", and the formula for **Kx** to "Kz". Because **Kx** ultimately refers back to itself, this circular reference is not allowed.

Another requirement for a data set to be included in a formula is that the data set used in the formula must be evaluated at the same locations as the data set or object for which the formula is being set up. For example, **Kz** can include a reference to **Kx** because both **Kx** and **Kz** are evaluated at elements; however, **Kz** cannot include a reference to **Initial_Head** because **Kz** is evaluated at elements and **Initial_Head** is evaluated at nodes.

Finally, the formula for a two-dimensional data set can only include a reference to two-dimensional data sets with the same orientation; however, the formula for three-dimensional data sets can include a reference to a two-dimensional data set of any orientation.

11.4.2.4 Select Matching Parenthesis Button

The **Select Matching Parenthesis** button helps the user determine which parenthesis in a formula goes with which other parenthesis. If an opening or closing parenthesis is selected in the formula, the button becomes enabled. Then if the button is clicked, the matching parenthesis will become selected. For example suppose the formula is $((A + B) * C)$ and the opening parenthesis just before "A" is selected. If the **Select Matching Parenthesis** button were clicked, the closing parenthesis just after B would be selected. The large, bold text in the two formulas below indicates what was selected before and after clicking the button.

$((A + B) * C)$

$((A + B) * C)$

11.4.2.5 Function Help Button

The **Function Help** button is used to obtain help on a particular function. If a function is selected in the **List of Data Sets and Functions**, the **Function Help** button will become enabled. Clicking the button will bring up a description of the function that was selected. The functions are also described in this report in “Functions” on p. 19.

11.4.3 Data Type Problem Dialog Box

The **Data Type Problem** dialog box appears when the user has entered a formula in the **Data Sets** dialog box (p. 41) whose result is of the wrong type for the data set in question. For user-created data sets, there are two ways of handling this.

1. The type of the data set can be changed to match the type returned by the formula. For example, if the type of the data set is an integer, and the formula is "0.5", the type of the data set could be changed to real.

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2. The formula could be adjusted to match the type of the data. For example, if the type of the data set is an integer, and the formula is "0.5", the formula could be changed to "Round(0.5)." (In this case, "Round(0.5)" would then be converted to "0" because Round(0.5) is a constant.)

The built-in data sets for GoPhast cannot have their type changed because the type must match the type of the corresponding data set in PHAST. Thus, for these data sets, only the second option is available.

11.4.4 Color Grid Dialog Box

The **Color Grid** dialog box is used to color the grid according to the value of a data set or boundary condition. It is displayed by selecting **Data|Color Grid...**

The user chooses the data set or boundary condition used to color the grid in the combo box at the top of the dialog box. If the item chosen, such as **Specified_Head**, can vary with time, the user should also select the time in the edit box labeled **Time**.

The user can select the range to be colored by checking the checkboxes labeled **Lower limit** and **Upper limit** and then entering the desired limit in the edit box to the right of the corresponding checkbox.

Different color schemes can be used to associate a given value of the data set or boundary condition with a color. The desired color scheme is selected in the combo box near the bottom of the dialog box. The range of colors in the selected color scheme is displayed below the combo box.

To cycle through the range of colors for a color scheme more than one time, change the value in the edit box labeled **Cycles**.

See Light and Bartlein (2004, 2005), and Stephenson (2005) for more information about color schemes.

11.4.5 Formula Errors Dialog Box

If the user has entered a formula that is invalid, the formula will be reset to a default value when an attempt is made to evaluate it. The **Formula Errors** dialog box shows what formulas have been reset. The **Formula Errors** dialog box is displayed by selecting **Data>Show Formula Errors...** It is also shown automatically if an invalid formula is detected.

Normally, GoPhast prevents the user from entering an invalid formula; however, a formula that was valid can become invalid if the data type or evaluation location of a data set that is included in the formula is changed, or if the GoPhast project file is edited outside of GoPhast.

11.5 Object

The menu items under **Object** are listed in table 8.

Table 8. Object Menu

Menu Item	Explanation
 Select Objects	Click or drag to select objects. See “Selecting Objects” on p. 30. Double click to edit objects. See the “Object Properties Dialog Box” on p. 49.
 Select Vertices	Click or drag to select individual vertices. See “Selecting Objects” on p. 30.
 Select With Lasso	Drag to select objects. See “Selecting Objects” on p. 30.
Edit Selected Object(s)	Edit the properties of the selected objects. See the “Object Properties Dialog Box” on p. 49.
 Create Point	Create a point object. See “Points” on p. 28 and the “Object Properties Dialog Box” on p. 49.
 Create Line	Create a polyline object. See “Polylines” on p. 28 and the “Object Properties Dialog Box” on p. 49.
 Create Polygon	Create a polygon object. See “Polygons” on p. 29 and the “Object Properties Dialog Box” on p. 49.
 Create Straight Line	Create a polyline object whose segments are parallel to the grid. See “Straight-Lines” on p. 29 and the “Object Properties Dialog Box” on p. 49.
 Create Rectangle	Create a rectangular polygon object. See “Rectangles” on p. 29 and the “Object Properties Dialog Box” on p. 49.
 Insert Vertex	Insert a new vertex into the selected object by clicking the location on the object where a new vertex is desired. See “Editing Objects” on p. 31.
 Delete Segment	Delete a segment from an object by clicking on it. See “Editing Objects” on p. 31.
Rearrange Objects...	Change the order of the objects. See “Rearrange Objects Dialog Box” on p. 53.
Search For Object...	Search for objects based on the data sets or boundary conditions they affect. See “Search for Objects Dialog Box” on p. 53.
Show Selected Objects...	Display the Selected Objects dialog box which shows which objects are selected. See “Selected Objects Dialog Box” on p. 53.
 Show or Hide Objects...	Show or hide objects based on the data sets or boundary conditions they affect or individually. See “Show or Hide Objects Dialog Box” on p. 53.
Select Objects by Name...	Select objects based on their names. See “Select Objects by Name Dialog Box” on p. 54.

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11.5.1 Object Properties Dialog Box

To create an object, see “Creating, Selecting, and Editing Objects in GoPhast” (p. 28). When the object is complete, the **Object Properties** dialog box will appear (fig. 25). The **Object Properties** dialog box is also used to edit the properties of existing objects by double clicking on them or selecting **Object|Edit Selected Object(s)** or by using the **Show or Hide Objects** dialog box (p. 53).

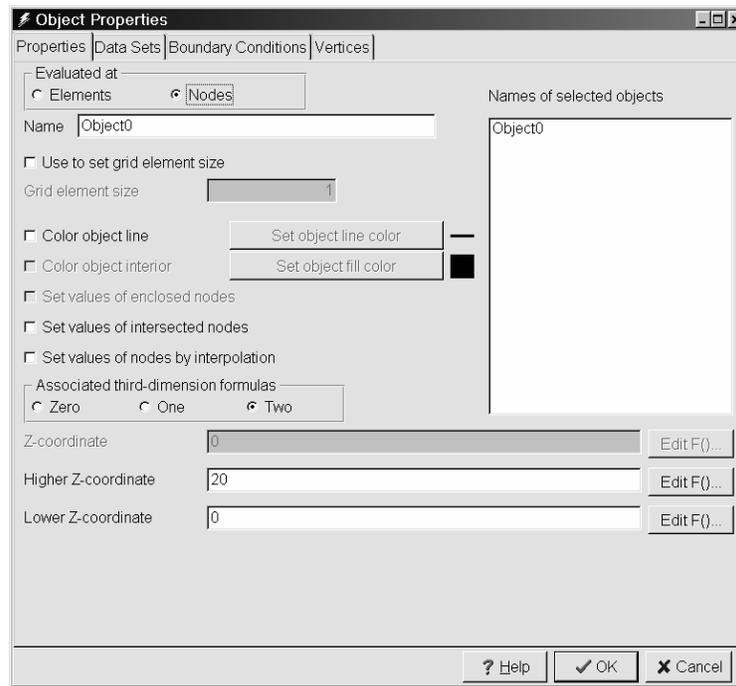


Figure 25. Object Properties dialog box.

The **Object Properties** dialog box is a tabbed dialog box with 2 to 4 visible tabs. The **Properties** and **Data Sets** tabs are visible for all objects. If the object in question is evaluated at nodes and only one object is being edited, an additional tab, **Boundary Conditions**, is visible. If only one object is being edited, the **Vertices** tab will be visible.

11.5.1.1 Properties Tab

Evaluated at: When objects are used to assign values to data sets, the formula for the object can be evaluated either at the grid nodes or at the element centers. The choice partially determines for which data sets the object can set values. If an object is evaluated at elements, it can be used to set the values of a data set that is evaluated at elements. If an object is evaluated at nodes, it can be used to set the values of a data set that is evaluated at nodes.

Name: Each object is assigned a name. By default, when an object is created, it is assigned a unique name; however, object names are not required to be unique. The user can edit the name of an object if only one object is being edited. Object names are useful for identifying particular objects. For example, The **View|Go To...** menu item (p. 55) allows the user to move the view of

the model so that a particular object is visible in the field of view by selecting the name of the object.

Names of selected objects: This displays the names of all the objects that are being edited. The names cannot be edited in the list. The list is only present if two or more objects are being edited simultaneously.

Use to set grid element size and Grid element size: If the **Use to set grid element size** checkbox is checked, the value in the **Grid element size** edit box is used to help define the extent and node spacing of the grid. See “Using Objects to Specify the Grid” on p. 12 for more information.

Color object line, Color object interior, Set object line color, and Set object fill color: If desired, the lines and interiors of objects can be colored. These checkboxes and buttons allow the user to specify how the object will be colored. If one of the checkboxes is checked, the corresponding button becomes enabled. The user can then click the button to select the color used for the boundary line or interior of the object.

Set values of enclosed elements\nodes, Set values of intersected elements\nodes, and Set values of elements\nodes by interpolation: An object can be used to assign the values to a data set in any of the three ways indicated by these three checkboxes. If none of these checkboxes is checked and the **Use to set grid element size** checkbox is also not checked, the object cannot affect the model in any way. The user is warned of this problem when clicking the **OK** button and given a chance to check one of the checkboxes.

The **Set values of enclosed elements\nodes** checkbox is used to specify that the object will be used to set the values of data sets or boundary conditions of nodes or of elements whose centers are inside the object. In the case of objects with a single associated third-dimension formula, a node or element is considered to be in the interior of the object if its center is inside the plan view of the object and the cell around the node or the element is intersected by the object in the third dimension (fig. 26).

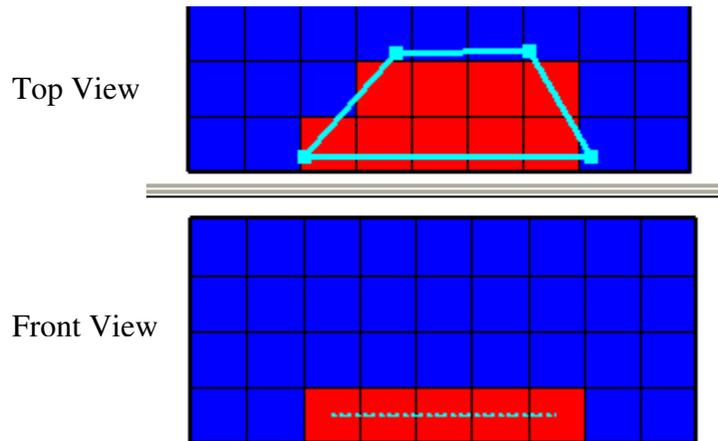


Figure 26. Elements affected by object with **Set values of enclosed elements** checkbox (shown in red) in top and front views.

The **Set values of intersected elements\nodes** checkbox is used to specify that the object will be used to set the values of data sets or boundary conditions of elements intersected by the object or of nodes whose cells are intersected by the object.

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The **Set values of elements\nodes by interpolation** checkbox is used to specify that the object will be used to set the values of data sets (but not boundary conditions, p. 52) of elements or nodes by interpolation. The interpolation method is specified in the Data Sets dialog box (see p. 41). Interpolation only applies to two-dimensional data sets.

Associated third-dimension formulas: An object can have zero, one, or two associated third-dimension formulas. If an object has zero associated third-dimension formulas, it is a 2D object and can only be used to set the values of 2D data sets. If it has one or two associated third-dimension formulas, it is a 3D object and can be used to set the values of both 2D and 3D data sets. The third-dimension formulas set the position of the object in the dimension perpendicular to the one in which the object has been drawn. For example, if an object is drawn on the top view of the model, its third-dimension formula(s) set its position on the Z axis. An example of using the third-dimension formula for defining the properties of a geologic unit with an irregular upper and lower surface has been presented earlier in “Assigning Values to Data Sets” on p. 5.

X-, Y-, or Z-coordinate: The **Z-coordinate** formula sets the Z coordinate of the object as a function of position for objects that have one associated third-dimension formula. For objects drawn on the side and front views of the model, the corresponding formula sets the X or Y coordinate respectively.

Higher X-, Y-, or Z-coordinate and Lower X-, Y-, or Z-coordinate: The **Higher Z-coordinate** and **Lower Z-coordinate** formulas sets the Z coordinates of the object as a function of position for objects that have two associated third-dimension formula. For objects drawn on the side and front views of the model, the corresponding formulas set the X or Y coordinates respectively.

11.5.1.2 Data Sets Tab

The **Data Sets** tab is used to specify which data sets will be affected by an object and the formulas used to set the value for each data set. Alternatively, the interpolation mechanism built into PHAST can be used to specify the values that will be assigned for a particular object.

The main part of the **Data Sets** tab is made up of a table with three columns: **Name**, **Affects**, and **Formula**. Each row of the table represents a separate data set. If a data set is not being used in the current model, its name is written in italics and a light gray background is used for its cells. Under the **Affects** column, there is a checkbox for each data set. Only those data sets whose values can be set by the current object have their checkboxes enabled. The user can change which data sets can have their values set by changing their choices for **Evaluated At** and **Associated third-dimension formulas** on the **Properties** tab. Once the user has checked the checkbox for a data set under the **Affects** column, the user can enter a formula for the object or check the checkbox near the bottom of the tab labeled **Use PHAST-style interpolation**. *PHAST-style interpolation is only applied to cells or elements enclosed or intersected by an object, not to cells or elements that are assigned by interpolation among objects.* When interpolating among objects, the formula for the object is always used even if PHAST style interpolation is used when assigning values to enclosed or intersected cells. This is because only two values can be used for PHAST-style interpolation. That limitation prevents PHAST-style interpolation from being used when interpolating among several objects. The only Data Set for which both the GoPhast interpolation methods and the PHAST-style interpolation methods can be used is **Initial_Water_Table**. See “PHAST-Style Interpolation” (p. 16) for more information.

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11.5.1.3 Boundary Conditions Tab

The **Boundary Conditions** tab is used to assign boundary conditions with an object. Because all the boundary conditions in PHAST are assigned at nodes, the **Boundary Conditions** tab is only visible when the object is evaluated at nodes. In addition, the **Boundary Conditions** tab is only visible if a single object is being edited. To apply a boundary condition using an object, select the type of boundary condition to apply from the list of radio buttons. The choices are **None**, **Specified head**, **Flux boundary**, **Leaky boundary**, **River boundary**, and **Well boundary**. **River** and **Well** boundary conditions can only be used with objects drawn on the top view of the model. In addition **Rivers** can only be used with polyline objects and **Wells** can only be used with point objects. If the boundary applies to only one face of a cell such as a flux boundary, it will be applied to the face of the cell on which the object is drawn. For example, if an object was drawn on the top view of the model, any boundaries associated with that object will be on a horizontal cell surface.

All of the different types of boundary conditions include a table that specifies how the boundary varies with time. For each boundary, the user specifies the number of times that the boundary condition values are specified in the edit box labeled **Number of times**. On the right side of the dialog box, the user can specify data related to the type of boundary condition that is being specified. One of the columns in the table specifies when the boundary condition changes. The first time is required to be zero so it cannot be edited. The user must specify each of the other times when the boundary condition changes. The times that are specified do not need to be the same as those specified elsewhere in GoPhast. GoPhast synthesizes all the times throughout the model and combines them to create the PHAST input file.

All of the boundary conditions have parameters that may vary with time. These time-varying parameters are specified in the table. The user can specify a formula for any of these parameters. If PHAST allows PHAST-style interpolation (see p. 16) to be used with the a parameter, a column of checkboxes will be next to the parameter in the table with a heading indicating that the parameter can be interpolated. To use PHAST-style interpolation, check the checkbox for PHAST-style interpolation for the parameter and specify the interpolation direction distances and values using the radio buttons and edit boxes on the left side of the dialog box. If a boundary condition has more than one parameter that varies with time and the parameters do not change at the same times, the user may leave some values blank. A value may be left blank if PHAST-style interpolation is not used and the parameter has been specified at an earlier time. A time-varying parameter must always be specified for time zero.

For **Leaky**, **River**, and **Well** boundaries, additional non-time-varying information is required by PHAST. This information is specified on the right side of the dialog box. For a **Leaky** boundary, **Hydraulic conductivity** and **Thickness** must be specified. For a **River** boundary, a **River name**, **Hydraulic conductivity**, **Width**, **Depth**, and **Bed thickness** must be specified. For a **Well**, a **Name**, **Diameter**, the open intervals in the well, and the method of allocating pumpage among the open intervals must be specified. In addition, if the open intervals are specified by using depths rather than elevations, a **Land surface datum** must be specified. Some of these data can be specified by using formulas. If so, a button (labeled **Edit F()...**) is provided next to the edit box in which the formula is specified. Clicking the button will call up the **Formula Editor** (see p. 44).

11.5.1.4 Vertices Tab

If only one object is being edited, the **Vertices** tab will be visible. On it, the user can adjust the positions of vertices of the object by entering new values for their X and Y coordinates. If the

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coordinates that are entered in the **Vertices** tab are invalid in some way, all changes to the vertex coordinates will be ignored. The coordinates are invalid if they cause the object to cross itself. It is impossible to add or delete vertices on the **Vertices** tab. Tools described in the section entitled “Editing Objects” on p. 31 allow the user to add and delete vertices.

11.5.2 Rearrange Objects Dialog Box

When values are assigned to a data set, each object overwrites any previous values so the last object that sets the value at any particular location is the one that determines the value at that location. (See “Assigning Values to Data Sets” on p. 5.) The **Rearrange Objects** dialog box can be used to change the order of the objects. To display the **Rearrange Objects** dialog box, select **Object|Rearrange Objects...** All of the objects will be listed in order in the table in the dialog box. The objects that are selected will be shown in bold type. To change the order of the objects, click to the left of an object and drag with the mouse to move the object to a new position in the table. Objects can be renamed in this dialog box too. To rename an object, type its new name in the table.

The order of the objects can also be changed without using the **Rearrange Objects** dialog box. The user can select one or more objects in the main window, right click and select **To Front**, **To Back**, **Forward One**, or **Back One** from the popup menu.

11.5.3 Search for Objects Dialog Box

The **Search for Objects** dialog box is used to select objects based on which data sets they affect. To display the dialog box, select **Object|Search for Objects...** Next the user checks the checkboxes next to the data sets and clicks the **OK** button. If any objects set that data set directly by specifying a formula for it, they will be selected.

See also: “Selected Objects Dialog Box” on p. 53 and “Show or Hide Objects Dialog Box” on p. 53.

11.5.4 Selected Objects Dialog Box

The **Selected Objects** dialog box displays a list of the objects that are currently selected. The user can continue to work with the model while this dialog box is visible. To display the **Selected Objects** dialog box, select **Object|Show Selected Objects...**

11.5.5 Show or Hide Objects Dialog Box

The purpose of the **Show or Hide Objects** dialog box is to allow the user to change which objects (points, lines, and polygons) are visible in the main Working Area. It can also be used to select and edit objects. The **Show or Hide Objects** dialog box is displayed by selecting **Object|Show or Hide Objects...** or by clicking on the **Show or Hide Objects** button . The user can continue to work with the model while this dialog box is visible. The names of the objects are displayed on the terminal branches of a tree control. Before the name of each object is a checkbox. The checkbox will be checked if the object is visible and unchecked if the object is hidden. The user can check or uncheck a checkbox next to an object’s name to show or hide that object.

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Hiding objects does not deactivate them; it just makes the **Working Area** less cluttered. A typical reason to show some objects but not others would be to display only the objects that affect a particular data set. For example, to display only the objects that affect the **Kx** data set, the user would uncheck the checkbox next to **All Objects** to hide all the objects and then check the checkbox for **Kx** under **Data Sets** to show all the objects that directly affect **Kx**.

In addition to a checkbox, the main branches of the tree also have a plus or minus sign. The symbol will be a plus if the branch is open to display its subbranches or a minus if the branch is closed so that its sub branches are hidden. If the user clicks on this symbol, the branch will switch between the opened and closed state.

The checkboxes before the main branches will either be checked, unchecked or grayed. A checkbox will be checked if all the branches beneath it are checked. It will be unchecked if all the branches beneath it are unchecked. It will be grayed if some of the branches beneath it are checked and others are unchecked. If the user checks or unchecks the checkbox for one of the main branches, it will show or hide respectively all of the objects for the branches beneath it. If all of the objects beneath it are already visible, they all will be hidden. If any of the objects beneath it are hidden, they all will be made visible.

The main branches are labeled

- All Objects,
- Set Grid Cell Size,
- Data Sets,
- Boundary Conditions, and
- Unused Objects.

All the objects are listed under **All Objects**. All the objects used to set the size of the grid cells are listed under **Set Grid Cell Size**. In addition, the value the user has specified for the cell size will be displayed in parentheses after the name of the object. All the data sets are listed under **Data Sets**. Beneath each data set in **Data Sets** are listed all the objects that directly set the values of the data set. The formula used for each data set will be displayed in parentheses after the name of the object. All the boundary conditions are listed under **Boundary Conditions**. Beneath each boundary condition in **Boundary Conditions** are listed all the objects that directly set the values of that boundary condition. Any objects that are not used to set the size of grid cells, or to set the value of one or more data sets or boundary conditions are listed under **Unused Objects**.

The user can select or edit objects by right-clicking on the name of the object and selecting **Select** or **Edit** from the popup menu. The user can also edit an object by double-clicking on its name. When the user selects **Select**, the object will become selected in the main GoPhast window and all other objects will be deselected. If the user selects **Edit** or double-clicks on an object's name, the **Object Properties** dialog box (p. 49) will be displayed so the user can edit the object.

See also: "Select Objects by Name Dialog Box" on p. 54 and "Search for Objects Dialog Box" on p. 53.

11.5.6 Select Objects by Name Dialog Box

The **Select Objects by Name** dialog box is used to select objects by their names. To show the **Select Objects by Name** dialog box, select **Object|Select Objects by Name...** The dialog box has three tabs; one each for the top, front, and side views of the model. If a particular model has no objects on a particular view of the model, the tab for that view of the model will be hidden. All the objects on each view of the model will be listed in their respective tabs including hidden objects. To suppress the listing of hidden objects, uncheck the **Include hidden objects** checkbox.

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To select objects, check the checkboxes next to their names and then click the **OK** button. Only objects on one view of the model can be selected at a time. The **Select All**, **Select None**, and **Toggle** buttons can be used to change which checkboxes are checked. Clicking the **Select Names Containing:** button will check all the boxes for objects contain the search term in the edit box next to the **Select Names Containing:** button.

See also: “Search for Objects Dialog Box” on p. 53 and “Show or Hide Objects Dialog Box” on p. 53.

11.6 View

The menu items under **View** are listed in table 9.

Table 9. View Menu

Menu Item	Explanation
 Zoom	Drag to zoom in to a specific area. See “Changing the Magnification” on p. 55 for more information.
 Zoom In	Zoom in by a factor of two. See “Changing the Magnification” on p. 55 for more information.
 Zoom Out	Zoom out by a factor of two. See “Changing the Magnification” on p. 55 for more information.
 Pan	Move the displayed area that is shown on the top, front, or side view of the model by clicking with the mouse and dragging while holding the mouse down.
Go To...	Go to a location, element, or object. See “Go To Dialog Box” on p. 56.
Vertical Exaggeration...	Change the vertical exaggeration. See “Vertical Exaggeration Dialog Box” on p. 57.
 Show Grid Shell	Show or hide the grid shell in the 3D view of the model.
 Show Top Grid	Show or hide the grid lines for a horizontal cross section of the model in the 3D view of the model. The selected layer determines where the grid lines are drawn.
 Show Front Grid	Show or hide the grid lines for a vertical cross section parallel to the front view of the model in the 3D view of the model. The selected row determines where the grid lines are drawn.
 Show Side Grid	Show or hide the grid lines for a vertical cross section parallel to the side view of the model in the 3D view of the model. The selected column determines where the grid lines are drawn.
 Show 3D Colored Grid	Show or hide colored cells or elements in the 3D grid. This control is disabled, if the grid is not being colored.
 Show 3D Objects	Show or hide objects in the 3D view of the model.
Restore Default 3D View	Position the 3D view of the model so that it is viewed from above at a default magnification and without rotation.
3D Lighting...	Change the lighting for the 3D view. See “3D Lighting Controls Dialog Box” on p. 57.

11.6.1 Changing the Magnification

The magnification of the top, front, and side views of the model can be changed in several ways. To zoom in by a factor of two, select **View|Zoom In** or click on the **Zoom In** button . While the cursor is over the model, it will change to a magnification glass with a plus sign in the

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middle if the magnification can be increased. The user then clicks at the location that is desired to be directly under the cursor after zooming in.

To zoom out by a factor of two, select **View|Zoom Out** or click on the **Zoom Out** button . While the cursor is over the model, it will change to a magnification glass with a minus sign in the middle if the magnification can be decreased. The user then clicks at the location that is desired to be directly under the cursor after zooming out.

To zoom in to a specific region select **View|Zoom** or click on the **Zoom** button . While the cursor is over the model, it will change to a magnification glass if the magnification can be increased. The user clicks down on one corner of the desired region, moves the mouse to the other corner and releases the mouse button. The selected region will be displayed at a higher magnification.

To change the magnification of the 3D view of the model, hold down the right mouse button. Then click on the 3D view and move the mouse either up or down. Moving it up will increase the magnification. Moving it down will decrease the magnification.

11.6.2 Go To Dialog Box

The **Go To** dialog box is used to change one or more of the views of the model so that a particular location, element, or object is visible. It can also be used to select a particular object. To show the **Go To** dialog box, select **View|Go To...**

The **Go To** dialog box has three tabs. However, some of those tabs are hidden when they cannot be used. The three tabs are

- The Position Tab,
- The Element Tab, and
- The Object Tab.

The user selects one of the tabs, chooses what is to be made visible and clicks on the **OK** button to change what is visible.

11.6.2.1 The Position Tab

The **Position** tab is always visible. In it, the user specifies the coordinates of the location to be made visible. The user also specifies the views of the model to be changed. Depending on which view of the model the user selects, some of the edit boxes in which the coordinates are specified will be enabled or disabled.

11.6.2.2 The Element Tab

The **Element** tab is visible when a grid has been created. In it, the user specifies the column, row, and layer number to be made visible. The user also specifies the views of the model to be changed. Depending on which views of the model the user selects, some of the edit boxes in which the column, row, and layer numbers are specified will be enabled or disabled.

11.6.2.3 The Object Tab

The **Object** tab is visible when one or more objects have been created. In it, the user selects the object to be displayed on the screen. Because objects are associated with particular views of the

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model, the user does not specify the view of the model to be changed. If the user checks the **Select object** checkbox, the object will become selected as well as being brought into view when the **OK** button is clicked.

11.6.3 Vertical Exaggeration Dialog Box

The **Vertical Exaggeration** dialog box is used to change the ratio of the horizontal to the vertical scale as displayed on the screen. The vertical exaggeration only affects how the model is displayed. It does not change the model itself. The **Vertical Exaggeration** dialog box is displayed by selecting **View|Vertical Exaggeration...** The front, side, and 3D views of the model are affected by the vertical exaggeration.

11.6.4 3D Lighting Controls Dialog Box

The **3D Lighting Controls** dialog box helps control the appearance of the 3D image of the model in the lower right corner of the Working Area. The **3D Lighting Controls** dialog box is displayed by selecting **View|3D Lighting...** There are six controls in the dialog box. The three controls on the left set the position of the light. The other three set different aspects of the light intensity.

11.6.4.1 Light Position

The coordinate system for the light has its origin in the center of the screen. X increases to the right. Y increases toward the top of the screen. Z increases out from the screen toward the viewer. The units of the coordinate system are arbitrary. They merely control the direction of the light.

11.6.4.2 Light Intensity

The light is considered to have three components: Ambient light, Diffuse light and Specular light. Ambient light is light that does not come from any particular direction. For instance, light from the sky would be considered ambient light. Diffuse light comes from a particular direction but is reflected evenly off a surface. However, surfaces directed at the light will receive more light than those directed away from the light. Specular light, like diffuse light is directional. However, it causes a bright spot on the surface on which it is shining.

11.7 Customize

The menu items under **Customize** are listed in table 10.

Table 10. Customize Menu

Menu Item	Explanation
Font...	Change the font used throughout GoPhast.
Color...	Change the background color of the windows used throughout GoPhast.
Hint Display Time...	Change how long “hints” are displayed. See “Hint Display Time Dialog Box” on p. 58.
Ruler Format...	Change the numeric format of the Rulers. See “Ruler Format Dialog Box” on p. 58.
Change Style...	Change the style used for controls. See “Choose Style Dialog Box” on p. 58.

11.7.1 Hint Display Time Dialog Box

When the mouse is held over a control in the GoPhast main window, a small "hint" box will appear in which the purpose of that control is briefly described. A longer hint will also appear on the status bar. The **Hint Display Time** dialog box is used to specify how long the small "hint" box is displayed (in seconds). By default, the hint box is displayed for 2.5 seconds. To display the **Hint Display Time** dialog box, select **Customize|Hint Display Time...**

11.7.2 Ruler Format Dialog Box

The top, front, and side views of the model each have a pair of **Rulers** (see p. 9) that show the coordinates of the model. If the numbers to be displayed on these **Rulers** become too large or too small, numbers might not be displayed with enough precision. The **Ruler Format** dialog box can be used to change the number of digits displayed on the **Rulers**. To display the **Ruler Format** dialog box, either double-click on a **Ruler** or select **Customize|Ruler Format...** To change the precision of a particular **Ruler**, change to the tab for that **Ruler** and change the precision in the edit box. To see what effect this will have, type a number in the **Sample number** edit box and see how it is displayed in the preview area.

11.7.3 Choose Style Dialog Box

GoPhast allows the user to configure its appearance in a number of different styles. Each style will affect the appearance of different controls such as checkboxes and radio buttons. To choose a style, select **Customize|Choose Style...** and the **Choose Style** dialog box will appear. When the user chooses a style in the **Choose Style** dialog box, the dialog box will display a preview of the changed appearance of the controls. Preview controls can be tested but have no other effect.

11.8 PHAST Options

The menu items under **PHAST Options** are listed in table 11.

Table 11. PHAST Options Menu

Menu Item	Explanation
Title and Units...	Display the “Title and Units Dialog Box” (p. 59).
Grid Options...	Display the “Grid Options Dialog Box” (p. 59).
Chemistry Options...	Display the “Chemistry Options Dialog Box” (p. 59).
Solution Method...	Display the “Solution Method Dialog Box” (p. 60).
Steady Flow...	Display the “Steady Flow Dialog Box” (p. 60).
Time Control...	Display the “Time Control Dialog Box” (p. 61).
Free Surface...	Display the “Free Surface Dialog Box” (p. 61).
Print Initial...	Display the “Print Initial Conditions Dialog Box” (p. 61).
Print Frequency...	Display the “Print Frequency Dialog Box” (p. 62).

11.8.1 Title and Units Dialog Box

The **Title and Units** dialog box is used to specify the title and the default units for the model. It is displayed by selecting **PHAST Options|Title and Units...** The entire title will be included in the input, but PHAST only prints the first two lines of the title in the “*.o” output file.

11.8.2 Grid Options Dialog Box

The **Grid Options** dialog box is used to change certain options related to the grid in PHAST. To display the dialog box, select **PHAST Options|Grid Options...**

If the model is logically a one- or two-dimensional model, the user can use the **Chemistry dimensions** checkboxes to choose which dimensions should be used for the chemistry calculations.

If the model is a vertical cross sectional model, the user may wish to have the output from the model printed in the “*.o” output file in XZ orientation rather than the default XY orientation. The user can make that selection in the **Grid Options** dialog box.

11.8.3 Chemistry Options Dialog Box

The purpose of the **Chemistry Options** dialog box is to specify whether solute transport will be used and, if so, which reactants will be used as well as the diffusivity. The **Chemistry Options** dialog box is displayed by selecting **PHAST Options|Chemistry Options...** The options that are available are

- Use solute transport,
- Use equilibrium phases,
- Use surface assemblages,
- Use exchange,
- Use gas phases,
- Use solid solution, and
- Use kinetics.

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To use solute transport in a model, the checkbox labeled **Use solute transport** must be checked. If it is checked, the other options become enabled. A particular reactant will be used in the model if the checkbox next to it is checked. Note however, that even if a checkbox is unchecked, data sets related to that option still will be present in the **Data Sets** dialog box. (See p. 41.) However, the data sets that are not used directly in the model will be shown in italics and with a light gray background. Data sets that are not used directly in the model can still be used in the formulas for other data sets and thus may still have an influence on the model. The user must define the reactants to be used in the chemistry data file and define their initial conditions in the appropriate data set for each type of reaction.

The diffusivity in the model is specified in the edit box labeled **Diffusivity**.

11.8.4 Solution Method Dialog Box

The **Solution Method** dialog box is used to control which solver is used and to set the parameters for the solver. The **Solution Method** dialog box is displayed by selecting **PHAST Options|Solution Method...**

The user can select either the direct or iterative solver. For large problems, the iterative solver is more efficient.

The user can choose to include cross dispersion terms by checking the appropriate checkbox. For problems where there is flow at an angle to the grid, including the cross-dispersion terms can lead to a more accurate solution at the cost of an increased execution time. However, the cross-dispersion terms can also lead to negative concentrations. These will be set to zero in the chemical calculations, which leads to global mass-balance errors.

Edit boxes are available to set the space-differencing and time-differencing weighting. Space-differencing weighting and time-differencing weighting are important parameters because they help control the oscillation and numerical dispersion in the numerical solution. In general, centered-in-space and centered-in-time weightings (when both parameters are 0.5) reduces numerical dispersion, but can lead to oscillation of the solution. Upstream-in-space (space differencing = 0) and backwards-in-time (time differencing = 1) does not produce oscillations, but has more numerical dispersion (Parkhurst and others, 2004).

If the iterative solver is used, a tolerance must be specified in the related edit box. The tolerance determines when the solver has converged to a solution to the difference equations. The tolerance must be sufficiently small to obtain an accurate solution.

If the iterative solver is used, the number of search directions to be saved (Save Directions) between restarts of the iterative solver must be specified in the **Save directions** edit box.

Sometimes iterative solvers cannot converge for a particular problem. The user specifies the maximum number of iterations that will be allowed before the solver quits in the **Maximum iterations** edit box.

11.8.5 Steady Flow Dialog Box

Some aquifer systems can be treated as being at steady state with regard to flow. In modeling such systems, a single flow-only simulation is performed at the beginning of the simulation and the flows from that simulation are used for all the transport simulations. The **Steady Flow** dialog box is used to specify this option and its associated parameters as listed below. The dialog box is shown by selecting **PHAST Options|Steady Flow...**

- The steady-flow option is selected by checking the **Steady flow** checkbox.

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- The user also specifies the **Head tolerance** in the **Steady Flow** dialog box. The Head tolerance is the maximum change in head for determining when flow is at steady state.
- The user also specifies the **Flow balance tolerance**. The fractional flow balance must be less than the flow balance tolerance for the flow system to be at steady state. The fractional flow balance is the difference between the inflow and outflow rates divided by the average of the inflow and outflow rates for the current time step.
- In the **Iterations** edit box, the user specifies the maximum number of time steps that will be used in attempting to attain a steady-flow condition.
- The user also specifies the **Minimum time step size**. It is the initial time step used in calculating steady-state flow and also is the minimum time step allowed for automatic time stepping in the steady-state flow calculation. The default is the time-step length defined in the **Time Control** dialog box (see p. 61) divided by 1,000.
- The user specifies the **Maximum time step size** in the related edit box. The maximum time step is the maximum time step used in the steady-state flow calculation. The default value is the time-step length defined in the **Time Control** dialog box (see p. 61) times 1,000.
- The user specifies the **Head change target** in the related edit box. The head change target is the amount by which it is desired that the head will change during a single time step in the steady-flow calculation. The time step will be decreased or increased during the steady-flow calculation to try to achieve head changes of target over each time step. The default value is 0.3 times the thickness of the grid region.

11.8.6 Time Control Dialog Box

The **Time Control** dialog box is used to specify how the time step size varies period-by-period during the simulation. The **Time Control** dialog box is displayed by selecting **PHAST Options|Time Control...** The user species a **Time step length** and the **Ending time** when the time step length changes to another value or the simulation ends. The times entered in the **Time Control** dialog box do not need to be the same as the times entered in other parts of the model. GoPhast synthesizes all the times throughout the model and combines them to create the PHAST input file.

11.8.7 Free Surface Dialog Box

The **Free Surface** dialog box is used to specify whether or not a free surface (water table) is used in the model. The **Free Surface** dialog box is displayed by selecting **PHAST Options|Free Surface...** If a free surface will be used, the user can check the **Use free surface** checkbox to use the water table to define the initial head. If the free surface is used and the water table is used to define the initial head, the **Initial_Water_Table** data set is used to define the initial head. If a free surface is not used or if the water table is not used to define the initial head, the **Initial_Head** data set is used to define the head at each node.

11.8.8 Print Initial Conditions Dialog Box

The **Print Initial Conditions** dialog box is used to control printing of initial condition data to various output files. It is displayed by selecting **PHAST Options|Print Initial...** The data corresponding to each checkbox will be printed if the checkbox is checked. The files to which the

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data will be saved are the same ones in which the corresponding data in the **Print Frequency** dialog box (see “Print Frequency Dialog Box” on p. 62) are saved except for the following items that have no corresponding items in the **Print Frequency** dialog box.

- The **Echo input** data are saved in the *.log file. (This option writes data from the flow and transport input file to the *.log file as each line is processed.)
- The **Fluid properties** data are saved in the *.O.probdef file.
- The **Media properties** data are saved in the *.O.probdef file.
- The **Solution method** data are saved in the *.O.probdef file.

11.8.9 Print Frequency Dialog Box

The **Print Frequency** dialog box is used to specify the simulation times at which PHAST will generate output. To display the **Print Frequency** dialog box, select **PHAST Options|Print Frequency...**

The main part of the dialog box is occupied by a table listing the items that can be printed, the files to which they are printed, and the frequency with which they are printed. The **Add**, **Insert**, and **Delete** buttons are used to add, insert, or delete columns in the table. The **Add** button adds a new column at the end of the table. The **Insert** button inserts a new column before the selected column. The **Delete** button deletes the selected column. When a column is added to the table, the values in the new column will be the same as in the preceding column. When a column is inserted into the table, the values in the new column will be the same as in the column before which it was inserted.

To enter a frequency, the user selects one of the choices for units from the drop down list of units for each type of output at each time. One of the choices for units is **default**. If that choice is selected, the units on the **Title and Units** dialog box (p. 59) will be used. If the units are set to **end**, the data will be saved at the end of the simulation period and no numeric value can be entered for time. If a numeric value is required, it is entered in the edit box before the units.

At the bottom of the dialog box is the **Save final heads** checkbox. If this checkbox is checked, heads will be saved to the file *.head.dat at the end of the simulation. The file *.head.dat is an ASCII file that can be used for initial head conditions in subsequent simulations. Initial heads can be imported into GoPhast from the file using the **File|Import|Distributed Data by Zone...** menu item (p. 35).

The items specified in each row of the table are as follows.

- **Time** represents the simulation time at which the remaining items in the column take effect. No units are specified for time. It is not required that a time match the times specified in other parts of the model. All the specified times in all parts of the model will be combined properly when preparing the PHAST input file.
- **Flow rates in boundary condition cells** determines the frequency with which flow rates in boundary conditions cells are save to the *.O.bcf file. By default, they are not saved.
- **Components** determines the frequency with which total chemical element (component) data for each cell are written to the *.O.comps file.
- **Conductance** determines the frequency with which static fluid and transient solute dispersive conductances for each cell face are written to the *.O.kd file.
- **Flow balance** determines the frequency with which flow-balance information is written to the *.O.bal file.

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- **Force chemistry print** determines the frequency with which detailed chemical descriptions of the composition of the solution and all reactants for each cell are written to the *.O.chem file. **Warning:** this file could exceed file-size limits of the operating system because a long description of the chemistry in each cell is written for each selected time step. Writing this information may be useful for debugging, for small problems, or if the **Print_Chemistry** data set is used to limit the set of cells for which data are written. Data written to the file *.O.chem also can be limited by the options of the PRINT data block of the chemistry data file.
- **HDF chemistry** determines the frequency with which chemistry data are written to the *.h5 file. Chemistry data to be written to the file *.h5 are defined in the SELECTED_OUTPUT and USER_PUNCH data blocks of the chemistry data file. The *.h5 file is used by Model Viewer (Hsieh and Winston, 2002) when displaying data from PHAST models.
- **HDF heads** determines the frequency with which heads are written to the *.h5 file. The *.h5 file is used by Model Viewer when displaying data from PHAST models.
- **HDF velocities** determines the frequency with which X, Y, and Z velocities are written to the *.h5 file. The *.h5 file is used by Model Viewer when displaying data from PHAST models.
- **Heads** determines the frequency with which potentiometric heads are written to the *.O.head file.
- **Progress statistics** determines the frequency with which solver statistics, including solution-method information, number of iterations, and maximum changes in head and component concentrations (due to transport) are written to the *.log file and to the screen.
- **Velocities** determines the frequency with which interstitial velocities at cell boundaries and interpolated velocities at nodes are written to the *.O.vel file.
- **Wells** determines the frequency with which transient well information, including fluid and solute flow rates, cumulative fluid and solute flow amounts, and solute concentrations, are written to the *.O.wel file. Data are written in the order of the well sequence numbers.
- **XYZ chemistry** determines the frequency with which selected chemical data are written to the *.xyz.chem file. The SELECTED_OUTPUT and USER_PUNCH data blocks of the chemistry data file are used to select data that are written to the file prefix.xyz.chem. Cells for which results are to be written can be restricted with the **Print_XYZ_Chemistry** data set.
- **XYZ components** determines the frequency with which component (chemical element) concentrations are written to the *.xyz.comps file.
- **XYZ heads** determines the frequency with which heads are written to the *.xyz.head file.
- **XYZ velocities** determines the frequency with which interpolated velocities at cell nodes are written to the *.xyz.vel file.
- **XYZ wells** determines the frequency with which a time-series of concentrations for each well are written to the *.xyz.wel.
- **Boundary conditions** determines whether heads, component concentrations, fluxes, and other boundary-condition information are written to the *.O.probdef file. The *.O.probdef file can be used to document the boundary conditions in a way that is easier for humans to read than are the model input files.

See also: "Print Initial Conditions Dialog Box" on p. 61.

11.9 Help

The menu items under **Help** are listed in table 12.

Table 12. Help Menu

Menu Item	Explanation
Contents	Show the contents page of the help system for GoPhast.
Help On Main Window	Show help for the main window of GoPhast.
Topic Search	Search for a word in the GoPhast help.
Examples	Show instructions for recreating examples.
About...	Shows the About box for GoPhast.

12. Examples

The PHAST documentation (Parkhurst and others, 2004) includes four examples. This section describes how to create the transport input files for all but the third of those examples. This section also includes an example not represented among the examples distributed with PHAST. (The third example from the PHAST documentation does not show any features of GoPhast not illustrated with the other examples.) The complete GoPhast project files for the examples are included with GoPhast. In addition other GoPhast files are included. These example project files can be used to create the transport input files for the other examples included with PHAST.

Some users may choose to use this manual by starting with this section. Such users would benefit from reading the “Basic Concepts” section on p. 3 first.

12.1 Example 1

Example 1 is described beginning on p. 85 of the PHAST documentation (Parkhurst and others, 2004). The flow and transport data file itself begins on p. 88. If PHAST is installed on a Windows computer at the default location, this file can be found at C:\Program Files\USGS\phast-1.2\examples\ex1\ex1.trans.dat. To follow this example, the user should open this file in a text editor. For the most part, the various data sets will be specified in the same order in which they appear in the original input file. The one exception will be the grid. It will be specified before anything else.

The goals of this example are to:

1. Create a simple model using GoPhast.
2. Introduce setting default formulas for Data Sets in the **Data Sets** dialog box.
3. Introduce creating objects.
4. Introduce using objects to specifying boundary conditions.
5. Introduce zooming in and out.
6. Introduce visualizing data.

Examples: Example 1

12.1.1 Creating the Grid

1. Start GoPhast by double-clicking on its icon. The **Start-Up** dialog box shown in figure 27 will appear. If it is not already selected, select **Create new model**. Then click the **Next** button.

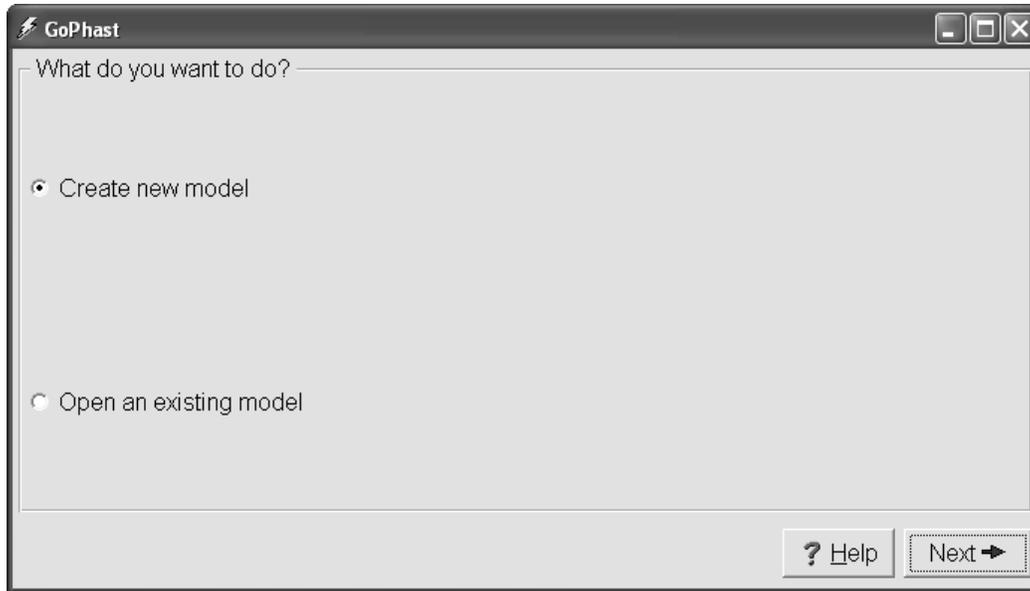


Figure 27. GoPhast Start-Up dialog box.

2. The **Initial Grid** dialog box will appear. Fill it in as illustrated in figure 28 and click the **Finish** button. This will create the grid illustrated in the GoPhast main window (fig. 29).

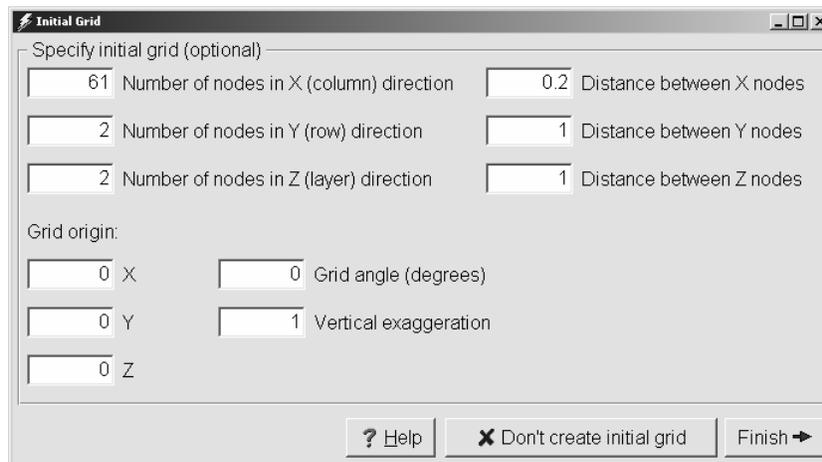


Figure 28. Initial Grid dialog box.

Examples: Example 1

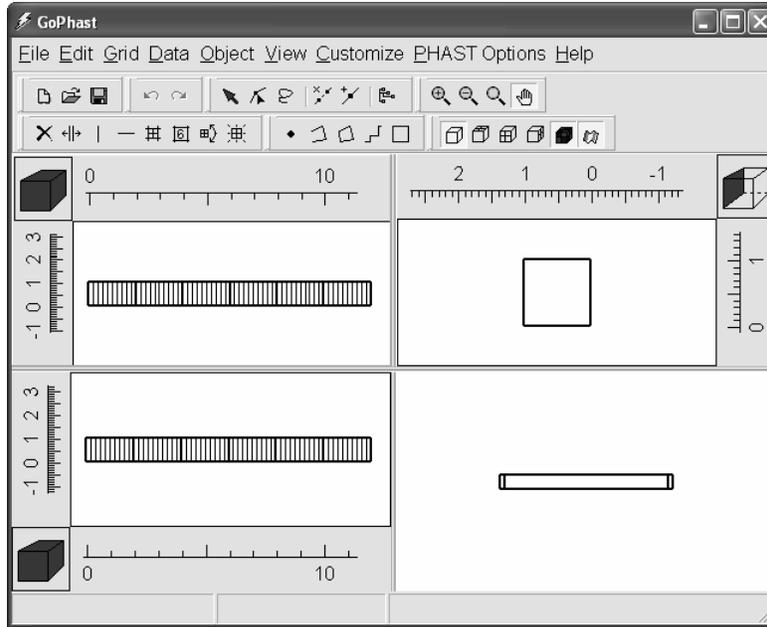


Figure 29. Initial appearance of GoPhast main window in Example 1.

12.1.2 Phast Options

- Next, select **PHAST Options|Title and Units...** With ex1.trans.dat in a text editor, copy the title section to the clipboard and paste it into the **Title** section of the **Title and Units** dialog box (fig. 30). The title can be edited to remove the blank spaces, “#” and quote characters at the beginnings of the lines. If desired, a different title of the user’s choice can be specified. The dialog box can be resized so that more of the title is visible. Click **OK** to close the dialog box.

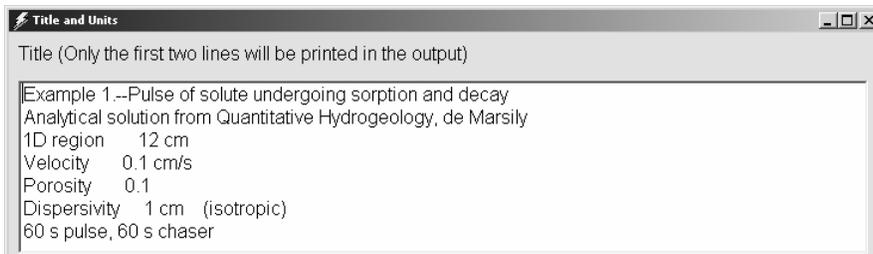


Figure 30. Top section of the **Title and Units** dialog box showing the title for example 1.

- The next steps are to activate steady flow and solute transport. To do so, select **PHAST Options|Steady Flow...** and check the **Steady flow** checkbox. Then click **OK** and select **PHAST Options|Chemistry Options...** and check the **Use solute transport** checkbox. Click **OK** to close the dialog box.

Examples: Example 1

5. Next change some of the default units. Select **PHAST Options|Title and Units...** again and this time specify the units as follows. (Those that are not listed can be ignored.) Click **OK** to close the dialog box.

Item	Units
Time units	sec
Horizontal grid units	cm
Vertical grid units	cm
Head units	cm
Hydraulic conductivity units	cm/s
Specific storage units	1/cm
Dispersivity units	cm

6. The grid is one-dimensional so the model will be more efficient if the chemistry dimension is specified as X. Select **PHAST Options|Grid Options...** and change the chemistry dimensions to just X (fig. 31). Click **OK** to close the dialog box.

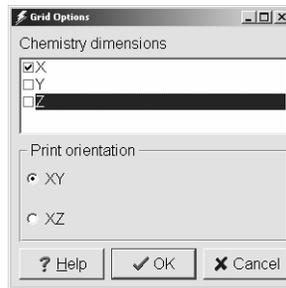


Figure 31. Grid Options dialog box showing selection of just the X Chemistry dimensions.

12.1.3 Data Sets

7. The aquifer properties are constant so it is possible to use the default formulas for the data sets to specify those properties (fig. 32). Select **Data|Edit Data Sets...** to edit the data sets. Click the **Help** button and read about this dialog box. The default formulas should be as follows. When they have been entered, click **OK** to close the dialog box.

Data Set	Default Formula
Kx	0.12
Ky	0.12
Kz	0.12
Porosity	0.1
Specific_Storage	0
Longitudinal_Dispersivity	0.1
Horizontal_Transverse_Dispersivity	0.1
Vertical_Transverse_Dispersivity	0.1

Examples: Example 1

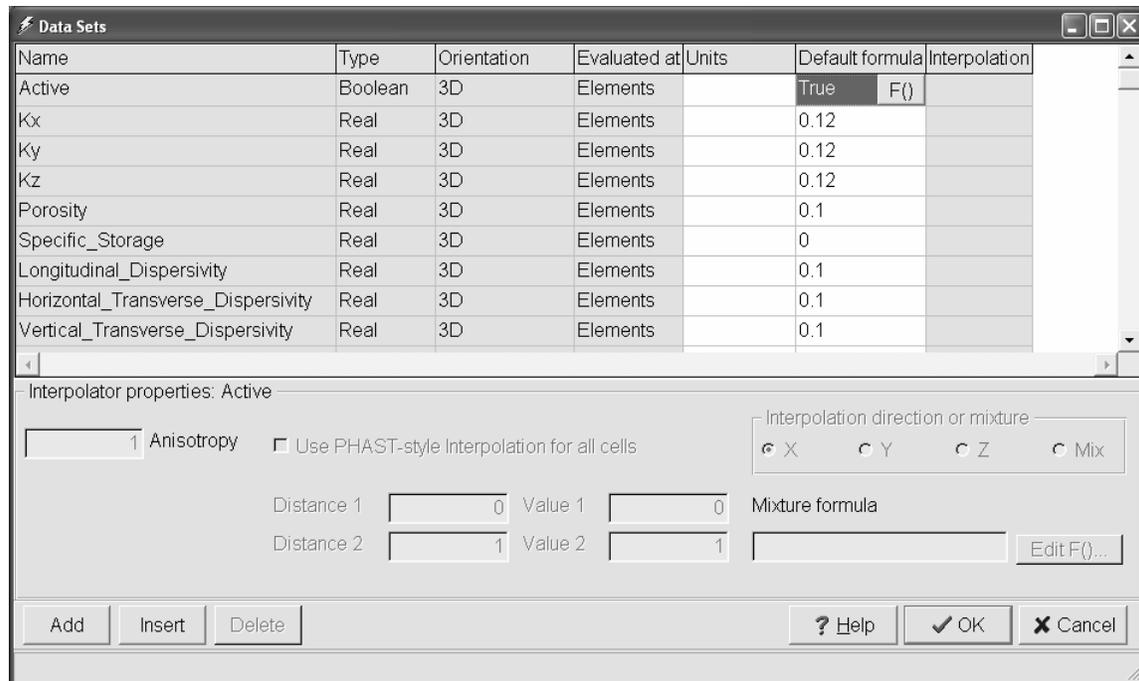


Figure 32. Data Sets dialog box showing specifications of the aquifer properties.

- This model does not use a free surface. Select **PHAST Options|Free Surface...** and verify that a free surface is not used. Click **OK** to close the dialog box.

12.1.4 Boundary Conditions

There are two specified head boundaries. One is on the left end of the model and the other is on the right. The one on the left has a head of 1 and an associated solution with an index of 2 from time 0 to time 60. For the rest of the duration of the model, it has an associated solution with an index of 1. The boundary on the right side has a head of 0.0 and an associated solution of 1.

- First zoom in on the left side of the model by selecting **View|Zoom In** and then clicking on the left side of the top view of the model (fig. 33).

Examples: Example 1

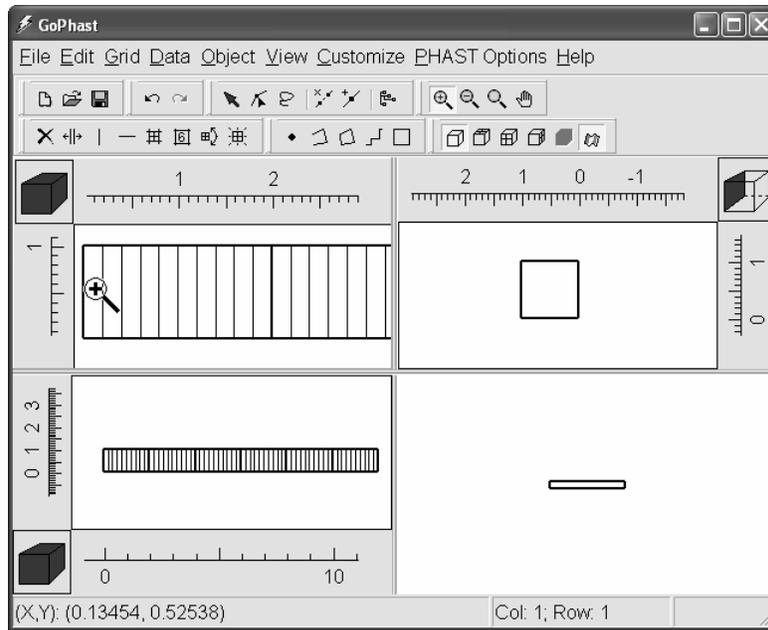


Figure 33. Appearance of model in example 1 after zooming in on the left side of the top view of the model.

10. The next step is to create the boundary condition on the left side of the model. Select **Object|Create Straight Line**. Click on the top view of the model and then click again to draw a line near the left end of the model (fig. 34). Double-click or push the Enter key on the keyboard to finish drawing the line.

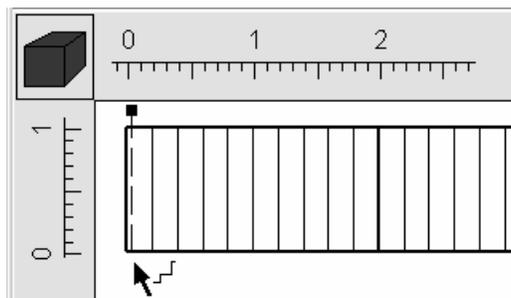


Figure 34. Drawing a line near the left side of the top view of the model.

11. At this point the **Object Properties** dialog box will appear. Click the **Help** button and read about this dialog box. On the **Properties** tab, check the **Nodes** radio button. Then change to the **Boundary Conditions** tab and select the **Specified head** radio button. Change the **Number of times** (near the bottom left) to 2. Then fill in the table for the specified head boundary condition as illustrated in figure 35. This specified head boundary will have a **Head** of 1 for the duration of the model but its **Associated solution** will change from 2 to 1 after 60 seconds. The value for **Head** only needs to be specified once.

Examples: Example 1

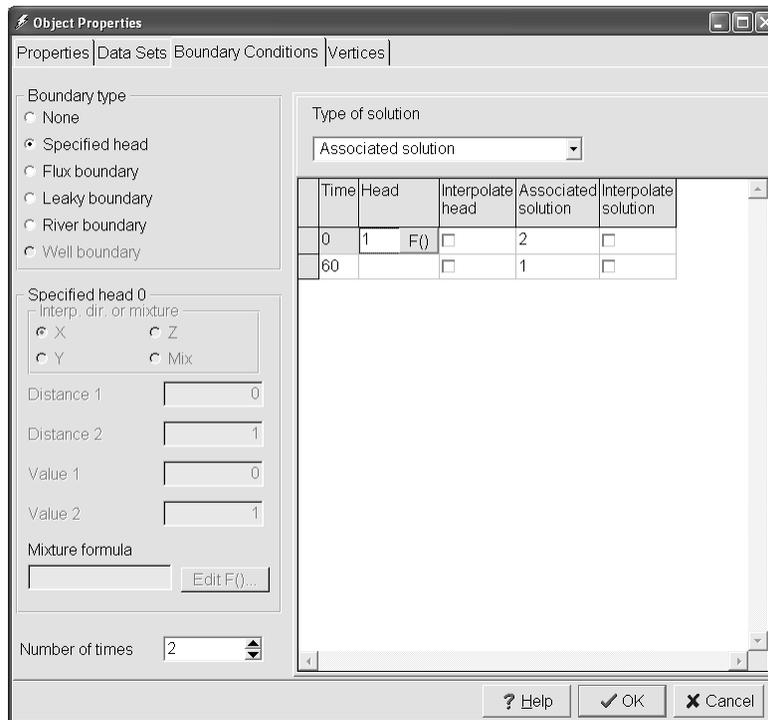


Figure 35. Object Properties dialog box showing how to set up the specified head boundary for the left side of the model.

- Click the **OK** button. A warning message will appear. Read the message and click the **No** button. Then on the **Properties** tab, check the **Set values of intersected nodes** checkbox. Also check that the **Higher Z-coordinate** is 1 and the **Lower Z coordinate** is 0. This means that the line is a vertical surface with a top of 1 and a bottom of 0. Click the **OK** button again. That completes setting up the specified head boundary for the left side of the model.
- Click with the mouse on the 3D view of the model and drag with the mouse button held down to rotate the 3D view. Note that on the left side there is a black rectangle representing the 3D vertical surface (fig. 36).



Figure 36. Three dimensional view of model showing object on left side of model.

- The next step is to create the specified head boundary on the right side of the model (fig. 37). Select **View|GoTo...** and change to the **Element** tab. Uncheck the checkboxes for **Front** and **Side**. Change **Column** to 60 and click the **OK** button. The right end of the model should now be visible in the top view of the model. Again select **Object|Create Straight Line** and draw a

Examples: Example 1

line on the right side of the top view of the model. Again select the **Nodes** radio button and check the **Set values of intersected nodes** checkbox. On the **Boundary Conditions** tab, select a **Specified head** boundary and set the **Head** to 0 for time 0 and the **Associated solution** to 1. Click the **OK** button. This **Specified head** boundary will have a **Head** of 0 for the duration of the model and an **Associated solution** of 1.

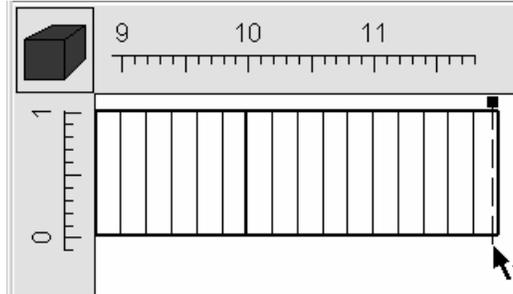


Figure 37. Drawing a line to represent a specified head boundary on the right side of the top view of the model.

12.1.5 Initial Head

15. The next step is to set the initial heads. The heads will vary uniformly from 1 on the left to 0 on the right. Select **Data|Edit Data Sets...** Select the row for **Initial_Head**. Note that the **Use PHAST-style interpolation for all cells** checkbox becomes enabled. Check this checkbox. Leave the **Interpolation direction** set to X. Set **Distance 1** and **Distance 2** to 0 and 12 respectively. Set **Value 1** to 1 and **Value 2** to 0 (fig. 38).

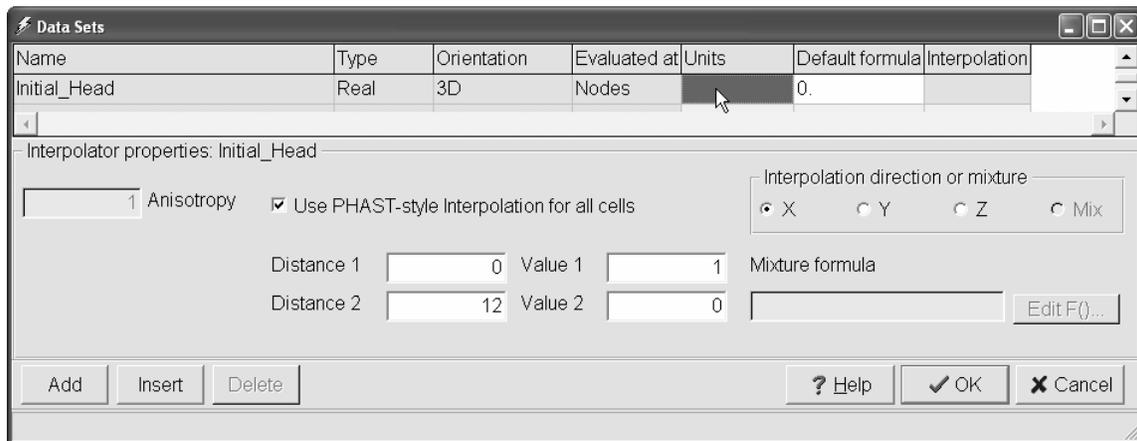


Figure 38. Data Sets dialog box showing how to set up a gradient in initial head.

16. The next step is to set the initial conditions for chemistry. The solution, surface and kinetics will all have an initial index of 1. With the **Data Sets** dialog box still visible, set the formula for **Chemistry_Initial_Solution**, **Chemistry_Initial_Surface**, and **Chemistry_Initial_Kinetics** each to 1. Click the **OK** button.

12.1.6 More PHAST Options

17. To deactivate the other chemistry options, select **PHAST Options|Chemistry Options...** and uncheck the checkboxes for **Use equilibrium phases**, **Use exchange**, **Use gas phases**, and **Use solid solution**. Leave the other three checkboxes checked. Click **OK** to close the dialog box. Then select **Data|Edit Data Sets...** again. Note that the data for **Chemistry_Initial_Equilibrium_Phases**, **Chemistry_Initial_Exchange**, **Chemistry_Initial_Gas_Phase**, and **Chemistry_Initial_Solid_Solutions** are all now in italics with a light gray background indicating that they are not being used. Click **OK** to close the dialog box.
18. The next step is to set up the solution method. Select **PHAST Options|Solution Method...** Click the **Direct** radio button and set the **Space differencing** and **Time differencing** both to 0.5 (fig. 39). Click **OK** to close the dialog box.

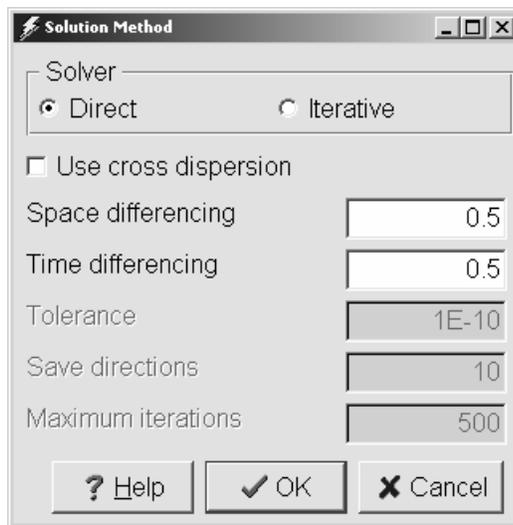


Figure 39. Solution Method dialog boxes showing how to set up the solution method for example 1.

19. The model has a duration of 120 seconds with time steps lasting 0.4 seconds. Select **PHAST Options|Time Control...** and set the **Time step length** to 0.4 and the **Ending time** to 120 (fig. 40). Click **OK** to close the dialog box.

Examples: Example 1

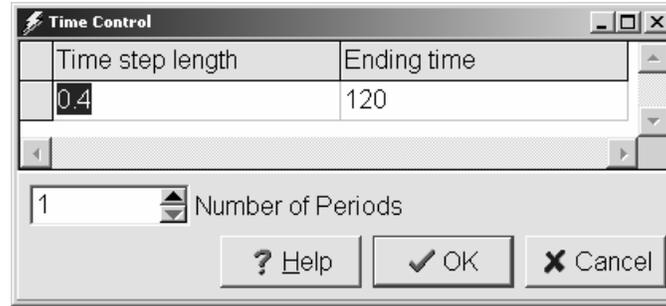


Figure 40. Time Control dialog box showing how to set up the time control for example 1.

20. The final step in setting up the model is to set up the print frequency. Select **PHAST Options|Print Frequency...** The units of all the items that will be changed are seconds. For time 0 set **HDF chemistry** to 10 seconds and **XYZ chemistry** to 0 seconds. (The frequency edit box for **HDF chemistry** is initially disabled because the default unit is **end**. Changing the units to seconds will enable the frequency edit box.) Click the **Add** button to add another time at which to specify the print frequency. Resize the dialog box to completely show the new column. In the new column set the time to 60. Also set **Force chemistry print** to 60 seconds, **Velocities** to 60 seconds and **XYZ chemistry** to 60 seconds. Note that **HDF chemistry** for time = 60 has a value of 10 seconds. This value was copied from the previous time when the **Add** button was clicked. Click **OK** to close the dialog box. Select **File|Save** to save the model.

12.1.7 Visualizing Data

21. The model is now ready to run. However, before running it, it is worthwhile to color the grid with some of the data sets to make sure the data have been applied properly. Select **Data|Color Grid...** and select the **Initial_Head** data set. Click the **OK** button. The model should appear similar to figure 41. Try using the **Selection Cube** for the side view of the model to change the selected column progressively from 1 to 61. The color displayed on the side view should change from red to blue. (See “The Selection Cube” on p. 9.) If the mouse cursor is over a colored cell or element on the top view of the model, the value of the data set for the colored element or cell will be displayed in the third panel of the status bar along with an explanation of how the value was assigned. It is possible to color the grid using the **Specified_Head_Solution** data set at time 0 and time 60.

Examples: Example 1

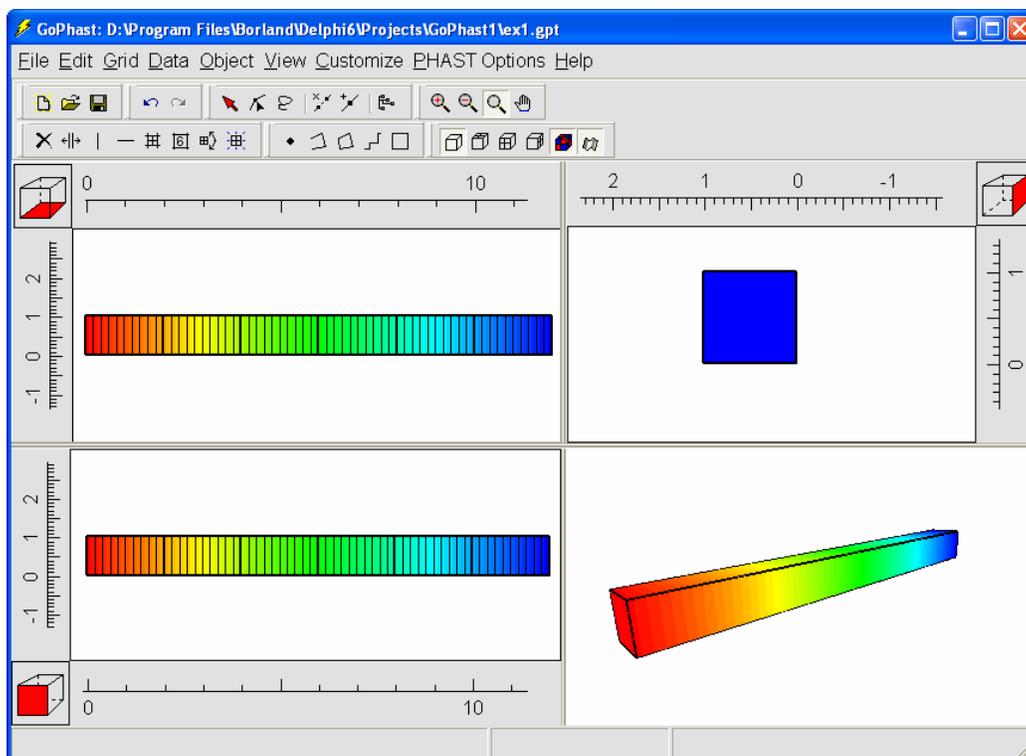


Figure 41. Main window showing the grid being colored by the **Initial_Head** data set.

22. Now that the model has been set up, it is possible to run it. Select **File|Export PHAST Input File**. In the **Save File** dialog box, save the file as **ex1.trans.dat**. Then copy **phast.dat** and **ex1.chem.dat** from the examples distributed with PHAST to the location where **ex1.trans.dat** was saved. Open up a command prompt and change the directory to the location where **ex1.trans.dat** was saved. (On Windows, an easy way to do this is to type “**cd**” in the command prompt window and then drag the directory from Windows Explorer. The directory name will be copied into the command prompt window. Then push the Enter button on the keyboard.) Run PHAST by typing “**Phast ex1**” in the command prompt window. When it is finished running, Model Viewer (Hsieh and Winston, 2002) can be used to display the results. (The capability of displaying PHAST results in Model Viewer was added by Scott R. Charlton.)

12.2 Example 2

Example 2 is described beginning on p. 91 of the PHAST documentation (Parkhurst and others, 2004). The flow and transport data file itself is reproduced beginning on p. 94. If PHAST is installed on a Windows computer at the default location, this file can be found at **C:\Program Files\USGS\phast-1.2\examples\ex2\ex2.trans.dat**.

The goals of this example are to:

1. Introduce using objects to define the grid.
2. Introduce PHAST-style interpolation.
3. Introduce showing and hiding objects to reduce clutter.

12.2.1 Initial Set Up

1. Start GoPhast by double-clicking its icon. The **Start-Up** dialog box will appear. If it is not already selected, select **Create new model**. Click the **Next** button.
2. The **Initial Grid** dialog box will appear. The grid in this example is too complex to create through **Initial Grid** dialog box so click the **Do not create initial grid** button. The grid will be created in a different way.
3. In the main GoPhast window select **PHAST Options|Title and Units...** Copy the title from ex2.trans.dat to the clipboard and paste it in the title section or enter an appropriate title. Assign the following units. Then click the **OK** button to close the dialog box.

Data Set	Units
Time units	days
Horizontal grid units	meters
Vertical grid units	meters
Head units	meters
Hydraulic conductivity units	meters/day
Specific storage units	1/meters
Dispersivity units	meters

4. Activate solute transport by selecting **PHAST Options|Chemistry Options...** and checking the **Use solute transport** checkbox. Uncheck all the other checkboxes except for **Use kinetics** and click the **OK** button.

12.2.2 Create the Grid with Objects

The next step is to define the grid. In this case, objects will be used to define where the grid should be and the grid element sizes. (See “Using Objects to Specify the Grid” on p. 12.) The grid should be 100 m long in the X direction, 20.5 m wide in the Y, direction and 12.5 m high in the Z direction. The elements will be 4 m long in the X direction. The first row of elements will be 0.5 m wide in the Y direction. The rest will be 1 m wide in the Y direction. The first layer will be 0.5 m high in the Z direction. The rest will be 1 m high in the Z direction.

The default view of the top view is zoomed out too far to draw an object of this size conveniently. Therefore select **View|Zoom In** and click on the top view until the size of the top view is appropriate. It is possible to use the menu items **View|Go To...** or **View|Pan** to position the top view so that the origin is included in the top view.

Examples: Example 2

5. Select **Object|Create Rectangle** and click twice on the top view of the model to create a rectangle whose opposite corners are close to (0, 0) and (100, 20.5) (fig. 42). The locations do not need to be precise because they will be edited later.

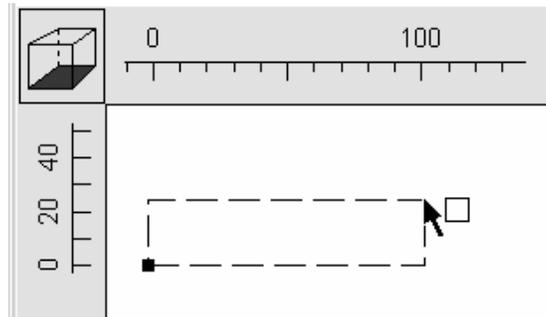


Figure 42. Creating a rectangle object in GoPhast.

6. Change the **Name** of the object to “Domain_Outline” in the **Object Properties** dialog box (p. 49), check the **Use to set grid element size** checkbox, set the **Grid element size** to 4. Switch to the **Vertices** tab. On the **Vertices** tab, set the corners of the rectangle to be at (0, 0), (100, 0), (100, 20.5), (0, 20.5) and (0, 0). (The last vertex is a duplicate of the first one so that the object will be a closed polygon.) This object will be used to define the horizontal extent of the grid and set the size of grid elements in the X direction to 4 meters. However, more needs to be done to define the grid. Click **OK** to close the dialog box.
7. It will be easier to see the grid on the front and side views of the model if the vertical exaggeration is decreased. Change the vertical exaggeration from 20 to 1. (Select **View|Vertical Exaggeration...** and enter “1.”) Then, on the front view of the model, zoom in and draw a line object from approximately (-1, 0.5) to (-1, 12.5). In the **Object Properties** dialog box, change its name to “Z_Discretization”, check the **Use to set grid element size** checkbox, and set the **Grid element size** to 1. On the **Vertices** tab, edit the position of the vertices so that the Z-coordinates are exactly 0.5 and 12.5. This object will help define the vertical extent of the grid and set the height of the layers to 1 m. Click **OK** to close the dialog box.
8. Draw another line object on the front view from about (-2, 0) to (-2, 0.5). In the **Object Properties** dialog box, change its name to “Z_Discretization_Bot_Layer”, check the **Use to set grid element size** checkbox, and set the **Grid element size** to 0.5. On the **Vertices** tab, edit the position of the vertices so that the Z-coordinates are exactly 0 and 0.5. This object will define the position of the bottom layer of the grid. Click **OK** to close the dialog box.
9. Draw another line object on the top view. It should extend from approximately (105, 0) to (105, 0.5). In the **Object Properties** dialog box, change its name to “Y_Discretization_First_Row”, check the **Use to set grid element size** checkbox, and set the **Grid element size** to 0.5. On the **Vertices** tab, edit the position of the vertices so that the **Y-coordinates** are exactly 0 and 0.5. This object sets the width of the first row in the Y direction. Click **OK** to close the dialog box.
10. Draw another line object on the top view. It should extend from approximately (110, 0) to (110, 20.5). In the **Object Properties** dialog box, change its name to “YDensity” check the **Use to set grid element size** checkbox, set the **Grid element size** to 1. On the **Vertices** tab, edit the position of the vertices so that the Y-coordinates extend at least from 0 to 20.5. This

Examples: Example 2

object defines the width of the rows in the Y direction. Because it is not a polygon, and it is on the top view of the model, it does not define the location of the grid but only the grid element size. (Polylines on the front view of the model do define the vertical extent of the grid. This object overlaps in the Y direction with the previous object (step 9). They both set the grid element size but because the previous object sets a smaller value, the previous object wins out. Click **OK** to close the dialog box.

11. There are now a sufficient number of objects to define the desired grid. Choose **Grid|Generate Grid...** and click the **OK** button to create the grid. Note that the first row and bottom layer are smaller than the others. They are smaller than the other rows and layers because the “Z_Discretization_Bot_Layer” (step 8) and “Y_Discretization_First_Row” (step 1) objects specified smaller element sizes than the “Z_Discretization” (step 7) and “YDensity” (step 10) objects respectively. Also note that all the elements are longer in the X direction than in the Y direction. This is because the “YDensity” object (step 10) specified a smaller element size than the “Domain_Outline” (step 6) object. To check that the grid has the correct dimensions, select **Grid|Specify Grid Lines...** and compare the grid line positions to what they should be based on the description at the start of this section.

12.2.3 Data Sets

12. Select **Data|Edit Data Sets...** and enter the follow for the default formulas. Leave the **Data Sets** dialog box (p. 42) open.

Data Set	Default Formula
Kx	2
Ky	2
Kz	2
Porosity	0.1
Specific_Storage	0
Longitudinal_Dispersivity	1.5
Horizontal_Transverse_Dispersivity	0.45
Vertical_Transverse_Dispersivity	0.15
Chemistry_Initial_Solution	1
Chemistry_Initial_Kinetics	1

13. The next step is to set the initial heads. The heads will vary uniformly from 1 on the left to 0 on the right. Select the row for **Initial_Head**. Note that the **Use PHAST-style interpolation for all cells** checkbox becomes enabled. Check this checkbox. Leave the **Interpolation direction** set to X. Set **Distance 1** and **Distance 2** to 0 and 100 respectively. Set **Value 1** to 1 and **Value 2** to 0. Click **OK** to close the dialog box.

12.2.4 Boundary Conditions

14. The next step is to define the specified head boundaries. On the side view of the model, draw a polygon completely surrounding the grid. In the **Object Properties** dialog box, select the **Nodes** radio button. Set the **Name** of the object to “Left_Specified_Head_Boundary”, and check the **Set values of intersected nodes** checkbox. Set **Associated third dimension formulas** to **One**. Leave **X-coordinate** set at 0. On the **Boundary Conditions** tab, select a **Specified head** boundary. Change the **Type of solution** to **Specified solution**. In the table

Examples: Example 2

enter a value of 1 for both **Head** and **Specified solution** (fig. 43). Click **OK** to close the dialog box.

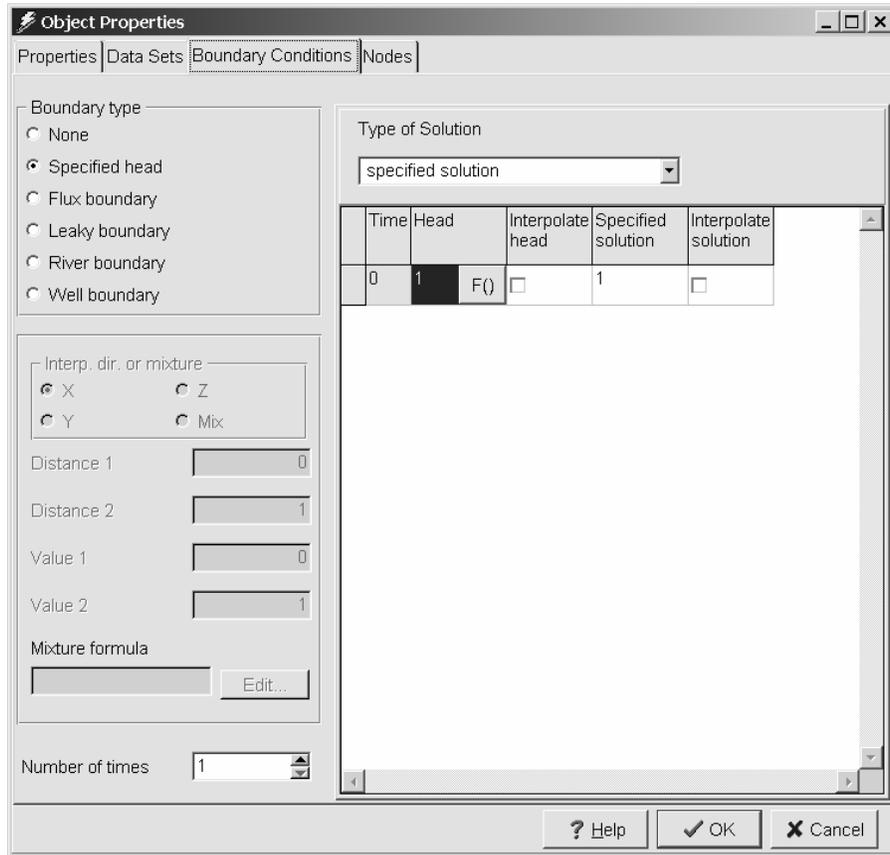


Figure 43. Object Properties dialog box. Specified head boundary condition.

15. Now color the grid (**Data|Color Grid...**) with the specified head. The left end of the model should be specified head cells.
16. Right-click on the side view of the model and select **Hide** from the popup menu to hide the previous object. (The object must be selected.) Hiding an object does not deactivate it; it just makes the **Working Area** less cluttered. On the side view of the model, draw another polygon completely surrounding the grid. In the **Object Properties** dialog box, select the **Nodes** radio button. Set its name to "Right_Specified_Head_Boundary." Check the **Set values of intersected nodes** checkbox. Set **Associated third dimension formulas** to **One**. Set **X-coordinate** to 100. On the **Boundary Conditions** tab, select a **Specified head** boundary. Leave the **Type of solution** at **Associated solution**. In the table enter a value of 0 for **Head** and 1 for **Associated solution**. Click **OK** to close the dialog box. Now both the left and right ends of the model should be specified head boundaries.
17. Hide all the objects created so far by selecting **Object|Show or Hide Objects...** Then in the dialog box, uncheck the checkbox for **All Objects**. If desired, click **Close** to close the dialog box.
18. The next step is to create a specified concentration boundary on the left end of the model. On the side view of the model, draw another polygon. This should enclose only part of the grid. It should extend from approximately $(Y, Z) = (15, 10)$ to $(21, 13)$ (fig. 44). In the **Object**

Examples: Example 2

Properties dialog box, select the **Nodes** radio button. Set its name to “Specified_Concentration_Boundary.” Check the **Set values of enclosed nodes** checkbox. Set **Associated third dimension formulas** to **One**. Leave the **X-coordinate** set to 0. On the **Boundary Conditions** tab, select a **Specified head** boundary. Change the type of solution to **Specified solution**. In the table enter a value of 1 for **Head** and 2 for **Specified solution**. Click **OK** to close the dialog box. Now color the grid with the **Specified_Head_Solution** (fig. 44). The left end of the model should be specified head cells. The cells with a specified head solution of 1 will be colored red and those with a specified head solution of 0 will be colored blue.

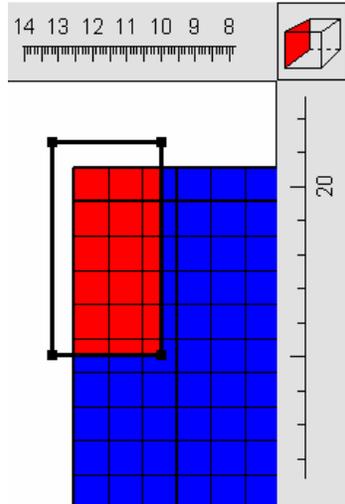


Figure 44. Location of the specified concentration boundary. The grid has been colored by the specified head solution.

12.2.5 PHAST Options

19. Set the following options for the solution method (**PHAST Options|Solution Method...**).

Solution Option	State
Solver	Iterative
Use cross dispersion	unchecked
Space Differencing	0.5
Time Differencing	0.5
Tolerance	1e-14

20. Set the following options for print frequency (**PHAST Options|Print Frequency...**).

Print Frequency Option	Value
HDF chemistry	400 days
Velocities	400 days
XYZ chemistry	400 days
XYZ heads	400 days
XYZ velocities	400 days

Examples: Example 2

21. Set the time control to a time step size of 10 and ending time of 400 (**PHAST Options|Time Control...**).
22. Save the project by selecting **File|Save**. Then run the model in the same way as in example 1 except that the file name should be ex2.trans.dat and the other files should come from the ex2 folder.

12.3 Example 3 (Example 4 in PHAST)

Example 4 in PHAST is described beginning on p. 103 of the PHAST documentation (Parkhurst and others, 2004). The flow and transport data file itself is reproduced beginning on p. 107. If PHAST is installed on a Windows computer at the default location, this file can be found at C:\Program Files\USGS\phast-1.2\examples\ex4\ex4.trans.dat.

The goals of this example are to:

1. Create a model using more complex boundary conditions including rivers and wells.
2. Introduce using objects to specify the spatial distribution of data sets.
3. Introduce the use of the **Formula Editor**.
4. Illustrate use of GoPhast for displaying the spatial distribution of values in data sets and boundary conditions.

12.3.1 Initial Set Up

1. Start GoPhast as before. In the **Initial Grid** dialog box, set the number of nodes in the X, Y, and Z directions to be 16, 9, and 5 respectively. Set the distance between nodes in the X, Y, and Z directions to be 6000, 6000, and 100 respectively. Click the **Finish** button to close the dialog box.
2. In the main GoPhast window select **PHAST Options|Title and Units...** Copy the title from ex4.trans.dat to the clipboard and paste it in the title section. Assign the following units. Then click the **OK** button.

Option	Units
Time units	years
Horizontal grid units	meters
Vertical grid units	meters
Head units	meters
Hydraulic conductivity units	meters per second
Specific storage units	1/meters
Dispersivity units	meters
Flux units	meters per year
Leaky hydraulic conductivity units	meters per second
Leaky thickness units	meters
Well diameter units	inches
Well flow rate units	liters/day
River bed hydraulic conductivity units	meters per second
River bed thickness units	meters

3. The next step is to activate the chemistry options. Select **PHAST Options|Chemistry Options...** Check the **Use solute transport** checkbox. Uncheck the **Use gas phases**, **Use solid solution**, and **Use kinetics** checkboxes. Click the **OK** button.

Examples: Example 3 (Example 4 in PHAST)

4. Set the Steady Flow options by selecting **PHAST Options|Steady Flow...** and checking the **Steady flow** checkbox. Change the **Head tolerance** to 1E-6 and click the **OK** button.
5. Select **PHAST Options|Free Surface...** and check the **Use free surface** checkbox. Click the **OK** button to close the dialog box.

12.3.2 Data Sets

6. Select **Data|Edit Data Sets...** and enter the following values for the default formulas.

Data Set	Default Formula
Kx	1.5E-5
Ky	1.5E-5
Kz	1.5E-7
Porosity	0.22
Specific_Storage	0
Longitudinal_Dispersivity	2000
Horizontal_Transverse_Dispersivity	50
Vertical_Transverse_Dispersivity	50
Initial_Head	380
Chemistry_Initial_Solution	2
Chemistry_Initial_Equilibrium_Phases	2
Chemistry_Initial_Surface	2
Chemistry_Initial_Exchange	2

7. In this example, the bottom layer to the right of an X coordinate of 48000 is inactive. To set this, first draw an object on the top view of the model enclosing this area (fig. 45). In the **Object Properties** dialog box, leave the **Elements** radio button checked, set the object's **Name** to "Inactive_Area", check the **Set values of enclosed elements** checkbox and set the **Higher Z-coordinate** to 100. On the **Data Sets** tab, check the checkbox for **Active** and set the formula to "False." After closing the **Object Properties** dialog box, color the grid with the **Active** data set and set the selected layer to the bottom layer. Check that the inactive area is restricted to the bottom layer (fig. 45). Using the mouse cursor, right click on the top view of the model and select **Hide** to hide the "Inactive_Area" object.

Examples: Example 3 (Example 4 in PHAST)

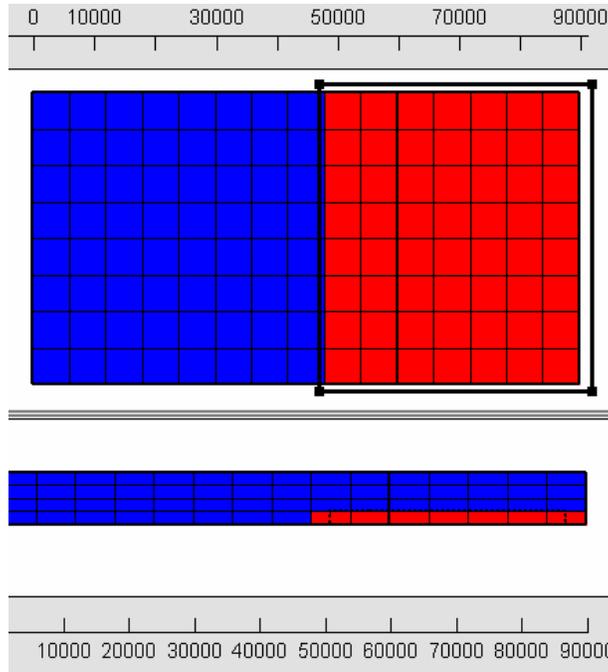


Figure 45. Active (blue) and inactive (red) areas in example.

12.3.3 Rivers

8. This model has three rivers: the Little River, the North Fork River and the North Canadian River. The Little River is defined by a polyline object with vertices at (44000., 15000.), (44000., 0.), and (90000., 0.). Draw a polyline object on the top view of the model at approximately those locations. (When drawing the object, it is possible to see the current location of the cursor in the status bar.) In the **Object Properties** dialog box, select the **Nodes** radio button. Change the **Name** of the object to “Little_River.” Check the **Set values of intersected nodes** checkbox. Then go to the **Vertices** tab and correct the locations of the vertices to be exactly correct.

On the **Boundary Conditions** tab, select a **River** boundary, and set the following properties.

River Property	Value
Name	Little River
Hydraulic Conductivity	1
Width	200
Depth	1
Bed Thickness	1

9. In the table for the river boundary set the **Associated solution** to 1. The head must vary along the length of the river. A formula can be used to accomplish this. Click on the cell in the table for head and observe the **F()** button that appears. Click it. This will open the **Formula Editor**. Click the **Help** button and read about this dialog box.
10. The head in Little River should vary from 335 at the upstream end to 275 at the downstream end. The **Interpolate** or **MultiInterpolate** functions can be used to achieve this goal. On the

Examples: Example 3 (Example 4 in PHAST)

(fig. 47). In the **Object Properties** dialog box, select the **Nodes** radio button. Set its **Name** to “Flux_Boundary.” Check the **Set values of enclosed nodes** checkbox. Set the number of **Associated third dimension formulas** to **One** and set **Z-coordinate** to 400. On the **Boundary Conditions** tab, choose a **Flux boundary**. Set the **Flux** for time 0 to -0.055 and set the **Associated solution** to 1. Click **OK** to close the dialog box. It is possible to color the grid with **Top_Flux_Boundary_Flux** to make sure the boundary condition was applied properly.

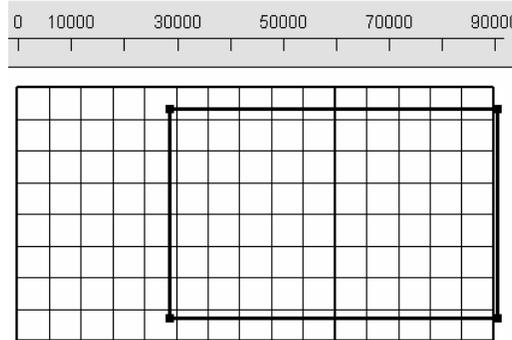


Figure 47. Polygon used to define specified flux boundary in example 3.

15. The next boundary condition is a specified head boundary (Lake Stanley Draper, figure 48). On the top view of the model, it looks like the lake only affects one node. However, it actually extends from an elevation of 300 to 400. Thus, it affects two nodes: one in the top layer and one in the layer just beneath it. Draw a polygon surrounding the node at (30,000, 18000) on the top view of the model. In the **Object Properties** dialog box, select the **Nodes** radio button. Set its **Name** to “Lake_St Stanley_Draper.” Check the **Set values of enclosed nodes** checkbox. Set the **Higher Z-coordinate** to 400 and the **Lower Z-coordinate** to 300. On the **Boundary Conditions** tab, select a **Specified head** boundary and set the **Head** to 348 and the **Associated solution** to 1. Click **OK** to close the dialog box.

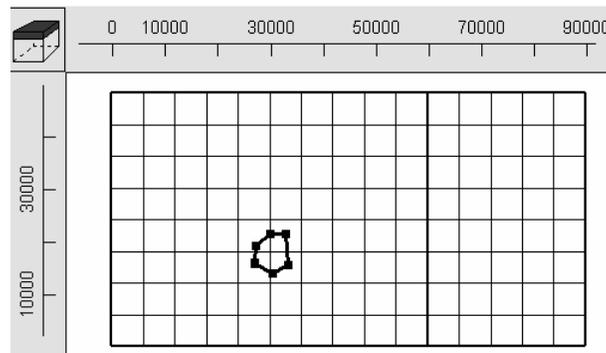


Figure 48. Polygon used to specify the specified head boundary condition in example 3.

12.3.5 Leaky Boundaries

There are two leaky boundaries in the model. Both are in the XZ plane so they are drawn on the front view of the model. One is at the front of the model and extends from the left edge of the model to an X-coordinate of 39000. The other is at the back of the model and extends from the left of the model to an X-coordinate of 29000. Both leaky boundaries extend over the whole extent of the model in the Z direction.

16. For the front boundary draw a rectangle on the front view of the model that goes from the left edge to approximately 39000 and that covers the entire height of the model (fig. 49). In the **Object Properties** dialog box, select the **Nodes** radio button. Set its **Name** to “Front_Leaky_Boundary.” Check the **Set values of enclosed nodes** checkbox. Set the **Associated third-dimension formulas** to **One**. Set the **Y-coordinate** to 0. On the **Boundary Conditions** tab, select the **Leaky boundary**, set the **Hydraulic conductivity** to $1.5e-5$, the **Thickness** to 20000, the **Head** to 320 and the **Associated solution** to 2. Click **OK** to close the dialog box.

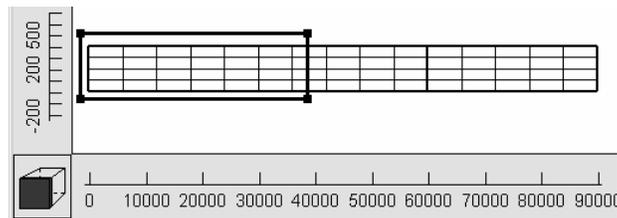


Figure 49. Polygon used to specify the leaky boundary on the front view of the model in example 3.

17. For the back boundary draw a rectangle on the front view of the model that goes from the left edge to approximately 29000 and that covers the entire height of the model. In the **Object Properties** dialog box, select the **Nodes** radio button. Set its **Name** to “Back_Leaky_Boundary.” Check the **Set values of enclosed nodes** checkbox. Set the **Associated third-dimension formulas** to **One**. Set the **Y-coordinate** to 48000. On the **Boundary Conditions** tab, select the **Leaky boundary**, set the **Hydraulic conductivity** to $1.5e-5$, the **Thickness** to 30000, the **Head** to 305, and the **Associated solution** to 1. Click **OK** to close the dialog box.

Examples: Example 3 (Example 4 in PHAST)

- The next boundary condition is a well located at $(X, Y) = (12000, 36000)$. Make a point object on the top view of the model at that location (fig. 50). In the **Object Properties** dialog box, select the **Nodes** radio button and **Name** the object “Well.” Check the **Set values of intersected nodes** checkbox. On the **Boundary Conditions** tab, select the **Well** boundary, set the **Diameter** to 2, the **First elevation** to 90, the **Second elevation** to 110, the **Pumping rate** to 1, and the **Solution** to 1. Make sure the **Allocate by pressure and mobility** checkbox is unchecked. Click **OK** to close the dialog box.

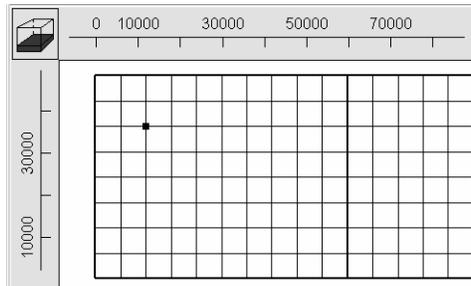


Figure 50. Point object used to specify well boundary in example 3.

12.3.6 PHAST Options

- The **Solution Method** options will be left at the default values. Select **PHAST Options|Solution Method...** Verify that an **Iterative** solver is selected, **Space differencing** is 0, **Time differencing** is 1, and the **Tolerance** is $1e-10$. Click **OK** to close the dialog box.
- Next, set the Print Initial options. Select **PHAST Options|Print Initial...** Check the **Steady flow velocities**, **XYZ heads**, and **XYZ steady flow velocities** checkboxes. Click **OK** to close the dialog box.
- Next set the Print Frequency. Select **PHAST Options|Print Frequency...** Change **XYZ chemistry** to “50000 years”, **HDF chemistry** to “2000 years”, and **XYZ wells** to “2000 years.” Change the rest to “0 default” Check the **Save final head in *.head.dat** checkbox at the lower left. Click **OK** to close the dialog box.
- To set the time control, select **PHAST Options|Time Control...** and set the **Time step length** to 2000 and the **Ending time** to 100000. Click **OK** to close the dialog box.
- The last step is to turn off the printing of the chemistry for the bottom layer. To do this, draw a polygon entirely surrounding the grid on the top view of the model. In the **Object Properties** dialog box, select the **Nodes** radio button. Set the **Name** to “Deactivate_Printing.” Check the **Set values of enclosed nodes** checkbox. Set the number of **Associated third dimension formulas** to **One** and set **Z-coordinate** to 0. On the **Data Sets** tab, check the checkbox for **Print_XYZ_Chemistry** and change the formula for it to “0.” Click **OK** to close the dialog box.

It is now possible to export the transport data file as ex4.trans.dat, run the model and view the results as with the previous examples.

12.4 Example 4 (Biscayne Bay Aquifer)

This example is a simplified model of the Biscayne Bay aquifer in southeast Florida. An upper aquifer and a lower aquifer are included in the model:

Data for this problem are in several shape files provided with GoPhast in the Examples\Biscayne directory: InitialWaterTable.shp, LowerAquiferBottom.shp, UpperAquiferBottom.shp, and UpperAquiferTransmissivity.shp. Each of these files also has associated with it two other files with the extension .shx and .dbf. The names of the shape files reflect the data contained within them. These shape files will be imported into GoPhast and used to set the hydraulic conductivity, active area, and initial water table of the model. A specified head boundary will be specified on the coastline, and a specified flux boundary (recharge) will be specified for the entire upper surface.

The goals of this example are the following:

1. Illustrate importing data from external files.
2. Illustrate use of formulas for specifying the geometry of geologic units.
3. Illustrate use of formulas for specifying aquifer properties tied to geologic units.
4. Illustrate the effects of different interpolation methods.

12.4.1 Initial Set Up

1. Start GoPhast. Select **Create new model**. Click the **Next** button.
2. Click the **Do not create initial grid** button.
3. Select **PHAST Options|Title and Units...** Change all the units to use feet and days except for flux, which should be set to inches per year. Click **OK** to close the dialog box.
4. Select **PHAST Options|Time Control...** Change **Time step length** to 10 and **Ending time** to 3500. Click **OK** to close the dialog box.
5. Select **PHAST Options|Print Frequency...** Change **HDF Heads** to 1 step. (You must specify **step** in the right-hand column before the numeral can be specified.) Click **OK** to close the dialog box.

12.4.2 Creating New Data Sets

For this example, five user-defined data sets will be created. Four of them will be used for working with imported data. The fifth will be used for the hydraulic conductivity of the upper aquifer. This final data set will be used in conjunction with the geometry of the aquifers to help specify the hydraulic conductivity distribution.

6. Select **Data|Edit Data Sets...**
7. Click the **Add** button and name the new data set "Imported_Water_Table." Leave everything else the same.
8. Click the **Add** button and name the new data set "Upper_Aquifer_Bottom." Leave everything else the same.
9. Click the **Add** button and name the new data set "Lower_Aquifer_Bottom." Leave everything else the same.
10. Click the **Add** button and name the new data set "Upper_Aquifer_Transmissivity." Leave everything else the same.

Examples: Example 4 (Biscayne Bay Aquifer)

11. Click the **Add** button and name the new data set “Upper_Aquifer_Kx.” Leave everything else the same. Click the **OK** button to close the **Data Sets** dialog box.

12.4.3 Importing Data

12. Select **File|Import|Shapefile...** Select InitialWaterTable.shp and click the **Open** button. The **Import Shapefile** dialog box will appear. In the table at the top of the dialog box, check the checkbox next to ZVALUE and change the data set to “Imported_Water_Table.” In the lower half of the dialog box, check the **Set values of elements by interpolation** checkbox. Click the **OK** button to import the Shapefile (One object in the shapefile will not be imported because it crosses itself. When the warning message appears, click **Yes** to continue.)
13. The shapes do not appear on the screen because the area that is shown does not include them. To easiest way to move the screen area to the objects is to select **View|Go To...** In the **Go To** dialog box, select the **Object** tab, select the first object and click the **OK** button.
14. Only a small part of one object will be visible. To show more, first maximize GoPhast and then select **View|Zoom Out** and click several times on the top view of the model (figure 3 on p. 8) until all the objects are visible (fig. 51). Nothing more needs to be done with them for the time being, so hide these object (Right click on the top view of the model and select **Hide** from the pop-up menu.



Figure 51. Imported initial water table, Biscayne Bay aquifer example.

15. Select **File|Import|Shapefile...** Select LowerAquiferBottom.shp and click the **Open** button. In the table at the top of the dialog box, check the checkbox next to ZVALUE and change the data set to “Lower_Aquifer_Bottom.” In the lower half of the dialog box, check the **Set values of elements by interpolation** checkbox. Click the **OK** button to import the Shapefile. Hide these objects in the same way as before.
16. Select **File|Import|Shapefile...** Select UpperAquiferBottom.shp and click the **Open** button. In the table at the top of the dialog box, check the checkbox next to ZVALUE and change the data set to “Upper_Aquifer_Bottom.” In the lower half of the dialog box, check the **Set values of elements by interpolation** checkbox. Click the **OK** button to import the Shapefile. Hide these objects in the same way as before.
17. Select **File|Import|Shapefile...** Select UpperAquiferTransmissivity.shp and click the **Open** button. In the table at the top of the dialog box, check the checkbox next to ZVALUE and

Examples: Example 4 (Biscayne Bay Aquifer)

change the data set to “Upper_Aquifer_Transmissivity.” In the lower half of the dialog box, check the **Set values of elements by interpolation** checkbox. Click the **OK** button to import the Shapefile.

12.4.4 Generating the Grid

18. The next step is to draw a domain outline around the area to be modeled. Select **Object|Show or Hide Objects...** Check the checkbox next to **All Objects** so that all objects are visible. Select **Object|Create Polygon** and draw a polygon on the top view of the model that roughly surrounds all the objects (fig. 52). In the **Object Properties** dialog box, set the **Name** to “Domain_Outline“, check **Use to set grid element size** and set the **Grid element size** to 2500. Click **OK** to close the **Object Properties** dialog box. It is no longer necessary to see the imported objects so in the **Show or Hide Objects** dialog box, uncheck the checkbox next to **Data Sets** to hide them all. (It may be necessary to display the **Show or Hide Objects** dialog box if it is hidden behind the main GoPhast window.)

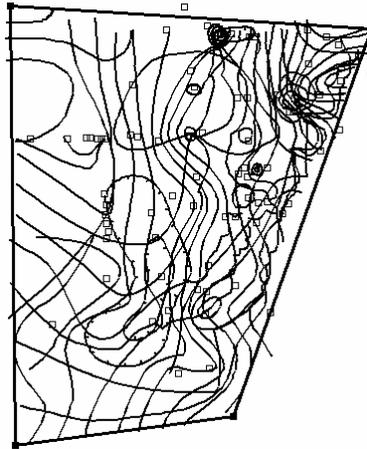


Figure 52. Domain outline for Biscayne Bay aquifer model.

19. To define the vertical extent and element size of the grid, draw a vertical line object on the front view of the model (figure 3 on p. 8) using **Object|Create Straight Line**. The model extends from 9 to -271 feet so when the **Object Properties** dialog box appears set the **Z coordinates** to 9 and -271 in the **Vertices** tab. Set the **Name** of the object to “Side_Domain_Outline.” Check **Use to set grid element size** and set the **Grid element size** to 28. Click **OK** to close the dialog box.
20. To create the grid (fig. 53), select **Grid|Generate Grid**, uncheck **Calculate grid angle automatically** and click the **OK** button.

Examples: Example 4 (Biscayne Bay Aquifer)

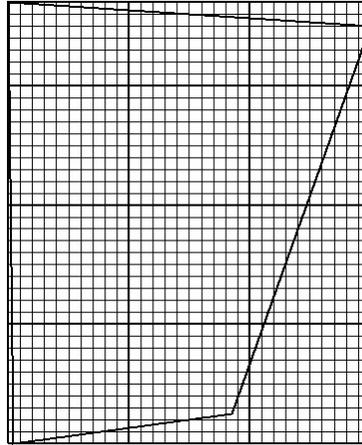


Figure 53. Grid in Biscayne Bay aquifer example.

12.4.5 Using Formulas to Define Aquifer Properties

21. Only the portion of the aquifer within the domain outline and above the bottom of the lower aquifer should be active. The first step in making the correct elements active is to make the default formula for the **Active** data set “False” for all of the elements. To do this select **Data|Edit Data Sets...** and change the formula for the **Active** data set from “True” to “False.”
22. After clicking **OK** to close the **Data Sets** dialog box, double click on the “Domain_Outline” object. In the **Object Properties** dialog box, check **Set values of enclosed elements**, and change **Higher Z-Coordinate** to 9 and **Lower Z-Coordinate** to -271. On the **Data Sets** tab, check the **Affects** checkbox for **Active** and click once in the **Formula** cell of the table for the **Active** data set. A button labeled **F()** will appear. Click it to display the **Formula Editor**. Change the formula to “ $Z > \text{Lower_Aquifer_Bottom}$.” (Z is found under **Functions|GIS** and **Lower_Aquifer_Bottom** is found under **Data Sets**.) This formula will evaluate to True for all elements whose centers are above the bottom of the lower aquifer. Click **OK** to close the **Formula Editor** and **OK** again to close the **Object Properties** dialog box. To check whether the **Active** data set is being set properly, select **Data|Color Grid...**, select the **Active** data set, and click **OK**. Click on the **Selection cube** for the top view of the model to change the selected layer and see the values of the **Active** data set in each layer (fig. 54). To view the **Active** data set in the 3D view, it is convenient to show only the elements in which **Active** is true. To do so, select **Data|Color Grid...** again, set the lower limit to “True” and click **OK**. Only the elements for which the **Active** data set is true will be colored.

Examples: Example 4 (Biscayne Bay Aquifer)

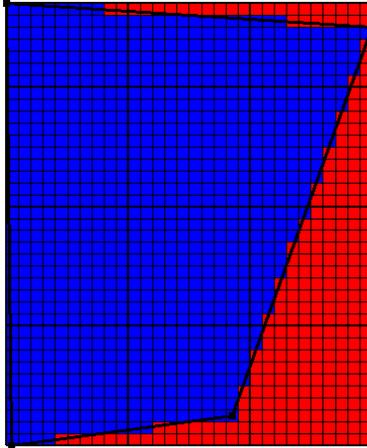


Figure 54. Active data set in the top layer of the Biscayne Bay aquifer model.

23. The next step is to define the hydraulic conductivity of the upper aquifer. This can be calculated from the data that have been imported by dividing the transmissivity by the saturated thickness. The saturated thickness is just the imported initial water table minus the bottom of the upper aquifer. To make this calculation, select **Data|Edit Data Sets...** Select the **default formula** for the **Upper_Aquifer_Kx** data set and display the **Formula Editor**. Set the formula to

$$\text{Upper_Aquifer_Transmissivity} / (\text{Imported_Water_Table} - \text{Upper_Aquifer_Bottom})$$
and click **OK**.

24. The next step is to use this hydraulic conductivity to help set the distribution of the **Kx** data set used by PHAST. Select the **default formula** for the **Kx** data set and display the **Formula Editor**. Set to formula to

$$\text{If}(Z > \text{Upper_Aquifer_Bottom}, \text{Upper_Aquifer_Kx}, 20)$$

(This formula assigns a value of 20 to the hydraulic conductivity of the lower aquifer.) **If** can be found under **Functions|Logical**. **Z** can be found under **Functions|GIS**.

“Upper_Aquifer_Bottom” and “Upper_Aquifer_Kx” can be found under **Data Sets**. Click **OK** to close the Formula Editor and click **OK** again to close the **Data Sets** dialog box. Try coloring the grid by the **Kx** data set. It may take a few seconds for the screen to be refreshed because **Kx** needs to be calculated.

25. The hydraulic conductivity in the Y direction (**Ky**) will be to the hydraulic conductivity in the X direction. The hydraulic conductivity in the Z direction (**Kz**) will be set to the hydraulic conductivity in the X direction divided by 10. To set these values, select **Data|Edit Data Sets...** Select the **default formula** for the **Ky** data set. Set its formula to “Kx” and click **OK**. Select the **default formula** for the **Kz** data set. Set its formula to “Kx / 10.” and click **OK**. Click **OK** to close the **Data Sets** dialog box.

12.4.6 Boundary Conditions

Two boundary conditions will be defined in this model: a specified head of zero on the eastern edge of the model (the ocean), and a specified flux of 4 inches per year through the top of the model (recharge).

Examples: Example 4 (Biscayne Bay Aquifer)

26. To define the specified flux boundary, select **Object|Create Rectangle** and draw a rectangle that completely encloses the top view of the model.). In the **Object Properties** dialog box, change **Evaluated At** to **Nodes**, change the **Name** to “Specified_Flux”, check **Set values of intersected nodes**, change **Associated third dimension formulas** to **One**, and change **Z-Coordinate** to “9.” On the **Boundary Conditions** tab, select **Flux boundary** and change the **Flux** for time zero to -4. (The flux is negative because it is downward. Click **OK** to close the **Object Properties** dialog box.
27. To define the specified head boundary, select **Object|Create Line** and draw a poly line on the eastern edge of the model (fig. 55). In the **Object Properties** dialog box, change **Evaluated At** to **Nodes**, change the **Name** to “Specified_Head”, and check **Set values of intersected nodes**. On the **Boundary Conditions** tab, select **Specified Head** and change the **Head** for time zero to 0. Click **OK** to close the **Object Properties** dialog box. Try coloring the grid by the two boundary conditions (**Specified_Head** and **Top_Flux_Boundary_Flux**) to make sure they are applied properly.

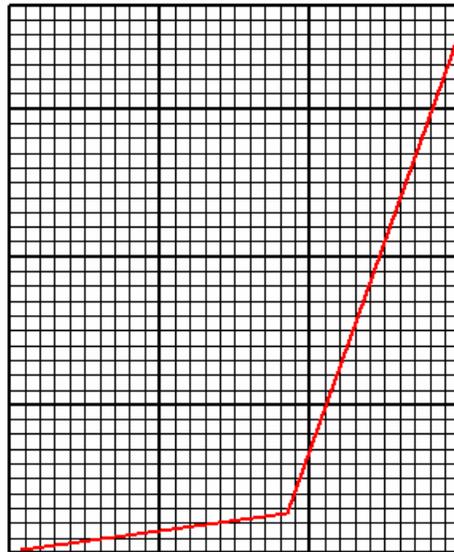


Figure 55. Object representing a specified head boundary (in red) in the Biscayne Bay aquifer model.

12.4.7 Initial Conditions

In this model the water table will be used as the initial conditions. However, the imported water table data can't be used because they applies only to elements. They must be imported a second time and applied to nodes.

28. The first step is to activate the water table. Select **PHAST Options|Free Surface...** Check both checkboxes and click **OK** to close the dialog box.
29. Because the data for the initial water table will be specified by interpolating among data points, an interpolation algorithm must be selected for the **Initial_Water_Table** data set. Select **Data|Edit Data Sets...** and select **Nearest** as the interpolation algorithm for the **Initial_Water_Table** layer. Click **OK** to close the dialog box.

Examples: Example 4 (Biscayne Bay Aquifer)

30. Select **File|Import|Shapefile...** and select “InitialWaterTable.shp.” In the **Import Shapefile** dialog box. Check the checkbox for “ZVALUE”, change **Evaluated At** to **Nodes**, and check **Set values of nodes by interpolation**. Set the **Data Set** for “ZVALUE” to **Initial_Water_Table**. (You must set **Evaluated At** first before you can set the **Data Set** for “ZVALUE.” Click **OK** to close the dialog box. When the warning message appears, click **Yes** to continue.

12.4.8 Running the Model

31. Select **File|Export PHAST Input File**. Accept the default name and click the **Save** button. Then open a command line prompt and run PHAST with the input file you just created. If you wish, use Model Viewer to display the results.

12.4.9 Variations

This example uses interpolation for several user-defined data sets. Several different interpolation algorithms are available in GoPhast. In this section, the effects of changing the interpolation algorithm will be explored. To do this, the grid will be colored using the Kx data set and then the interpolation algorithm for several user-defined data sets will be changed to see how that affects the results. The user may not get identical results to those illustrated for the **Nearest** interpolation method (fig. 56) and for the **Inv. Dist. Sq.** interpolation method (fig. 57). This is because the user most likely will not have cells in precisely the same locations as those used to generate figures 56 and 57.

32. Select **Data|Color Grid...** Select the **Kx** data set and click the **OK** button. After hiding all objects, the grid should look similar to figure 56.

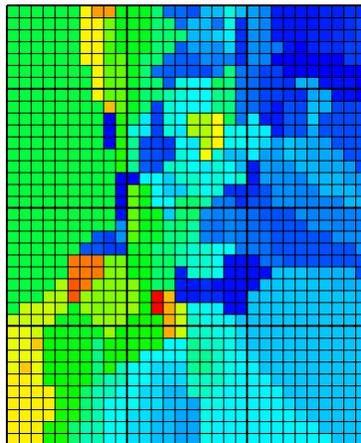


Figure 56. Distribution of Kx in the top layer of the Biscayne Bay aquifer model when the **Nearest** interpolation method is used.

33. Select **Data|Edit Data Sets...** Select the “Upper_Aquifer_Transmissivity” data set, change its **Interpolation** to **Inv. Dist. Sq.** (Inverse distance squared) and click **OK**. The grid should look similar to figure 57. The hydraulic conductivity at each element in the upper aquifer is

Examples: Example 4 (Biscayne Bay Aquifer)

calculated by dividing the interpolated transmissivity by the aquifer thickness. When the interpolation algorithm for the transmissivity is changed, K_x changes too.

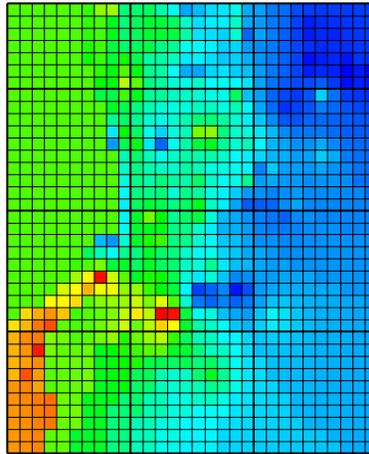


Figure 57. Distribution of K_x in the top layer of the Biscayne Bay aquifer model when the **Inv. Dist. Sq.** interpolation method is used.

34. Next change the interpolation algorithm for “Upper_Aquifer_Transmissivity” to **Nearest Point**. The appearance of the grid should go back to what it was when the interpolation algorithm was **Nearest**. This is because the data for “Upper_Aquifer_Transmissivity” consist entirely of point objects. The **Nearest Point** and **Nearest** interpolation algorithms give the same results when applied to points, although **Nearest Point** is faster. They give different results when applied to other sorts of objects.
35. Next try changing the interpolation algorithm for “Upper_Aquifer_Kx” from **Nearest** to any of the other algorithms (including **none**). Note that this has no effect on the distribution of K_x . This is because no objects directly set the values of “Upper_Aquifer_Kx.” When there are no objects to set the value of a data set, interpolation cannot be used and the default formula is used instead.

13. Summary

GoPhast provides a graphical user interface for creating the flow and transport input file for PHAST. It uses objects (points, lines, and polygons) and formulas to define the spatial distribution of aquifer properties in a convenient fashion. GoPhast can also be used to create the grid required by PHAST and to edit nonspatial data required by PHAST in the flow and transport input file. The use of formulas has several benefits: (1) objects can have a third dimension that varies; (2) complicated distributions of values in data sets can be easily specified; and (3) changes to the grid can be made without requiring the user to reenter data. Just as the spatial distribution of data is independent of the grid, the temporal distribution of data in boundary conditions is independent of the temporal discretization of the model. In addition, GoPhast combines all the times specified throughout the model to determine the proper temporal discretization of the model. GoPhast allows the user to display the spatial input graphically. This display makes it easier for the user to avoid

References Cited

and detect errors in the input, thus making the modeling process more efficient and accurate. GoPhast has built-in methods for importing data from DXF files and Shapefiles. It also has several built-in interpolation methods.

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16. Appendix 1. Tools for Programmers

During development of GoPhast, a number of tools were developed that programmers may find helpful in working with the source code.

16.1 Help Generator

Help Generator is a program for generating documentation for programs written in Object Pascal based on comments in the source code. Help Generator uses PasDoc (<http://pasdoc.sipsolutions.net/FrontPage>), an open-source Object-Pascal program and component to read the source code, extract the comments from it and format the comments as either a series of linked web pages or a LaTeX file. The LaTeX file can be easily converted into either a PostScript, Portable Document Format (PDF), or DVI file. The source code for Help Generator is available for download at the same location as GoPhast.

Most of the source code for GoPhast includes comments that can be used by Help Generator. However, GoPhast includes some source code written by others and these files do not contain comments that can be used by Help Generator. The source code for Help Generator also includes a project file that can be used to set the options used by Help Generator to create documentation for GoPhast. The project file only includes the names of source code files that include comments that can be used by Help Generator. A PDF of the source code documentation generated by Help Generator is included with GoPhast. The web page from which GoPhast can be downloaded contains a link to the web pages generated by Help Generator for GoPhast. Help Generator project files are also available for the custom components in GoPhast.

Help Generator can work in conjunction with the GraphViz “dot” program (<http://www.graphviz.org/>) to create some summary diagrams that are used in the documentation. It also works in conjunction with GNU Aspell (<http://aspell.sourceforge.net/>) which performs spell checking. The location of the Aspell program must be available in the search \$PATH.

16.2 GoPhast Testing Tool

GoPhast Testing Tool is a tool designed to run GoPhast automatically. It starts GoPhast, instructs it to read a GoPhast file and exports the transport input file for PHAST. It then compares the newly exported version to a previous version. If the two files have the same contents, GoPhast is considered to have passed the test. If the files are not identical, GoPhast is considered to have failed the test and the user is informed of the problem. The user must then determine whether the new or old version of the file is correct. If the old version of the file is correct but not the new one, a bug has been introduced into GoPhast. When the source code of GoPhast is modified, such tests should be run to ensure that the changes have not caused unexpected changes in how GoPhast works.

Only opening files and exporting the PHAST transport input file in GoPhast can be tested by the GoPhast Testing Tool. Other aspects of GoPhast must be tested manually.

16.3 WebIndexer

GoPhast uses the Tipue search engine in its help (<http://www.tipue.com/>). The search engine requires an index of the web pages it searches. WebIndexer is used to create that index. The user enters the names of the web pages for which an index is to be created, the file name for the index file to be created, and clicks the **Create Index** button to create the index. The settings can be saved to a file and reopened.

17. Appendix 2. Running GoPhast from the Command Line

It is possible to run GoPhast from the command line. This capability can be useful when testing GoPhast after making changes to the source code or using GoPhast with an automatic calibration tool such as UCODE (Poeter and Hill, 1998). When running GoPhast from the command line, the first argument must be the name of the file to be opened. The second argument on the command line can be “-e”. If present, this option causes GoPhast to export the PHAST transport input file with the default file name. The third argument on the command line can be “-c”. If present, this option causes GoPhast to close after exporting the PHAST transport input file. An example is shown below.

```
GoPhast ex1.gpt -e -c
```

This command would cause GoPhast to open ex1.gpt, export the PHAST transport data file, and then close.