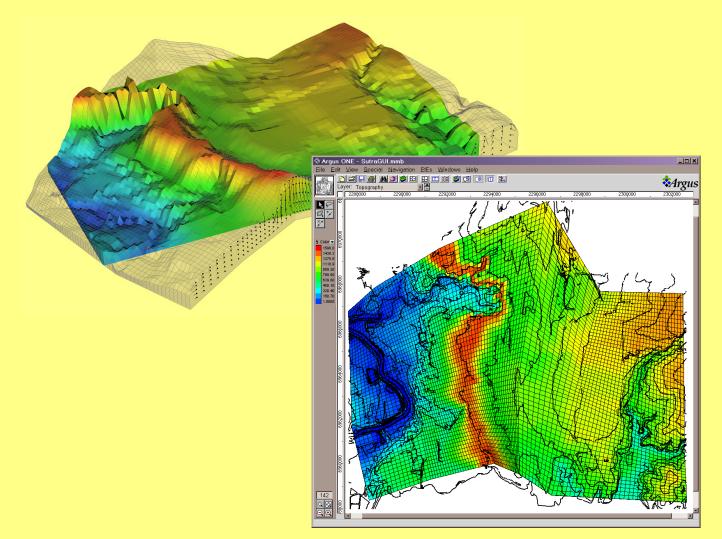
# **SutraGUI**

## A Graphical User Interface for SUTRA, a Model for Ground-Water Flow with Solute or Energy Transport



#### **Open-File Report 03-285**

Version of January 30, 2004 Latest version available at http://water.usgs.gov/nrp/gwsoftware



**Cover:** The cover image illustrates the use of **SutraGUI** to generate a three-dimensional (3D) SUTRA model. The Argus ONE<sup>TM</sup> window contains a view of elevation contours of the top of the water-table aquifer together with the map view of the 3D model domain and 3D finite-element mesh. The finite elements on the top of the mesh are colored by their elevation. The 3D illustration behind the Argus ONE window was prepared with Model Viewer (Hsieh and Winston, 2002). The model has an irregular top surface and the 3D mesh can be seen on this surface and on the vertical model sides. Fluid velocities resulting from a SUTRA simulation are shown along one vertical side and the colors represent hydraulic head in a selected part of the aquifer.

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

# SutraGUI A Graphical User Interface for SUTRA, A Model for Ground-Water Flow with Solute or Energy Transport

By Richard B. Winston and Clifford I. Voss

**Open-File Report 03-285** Version of January 30, 2004

Reston, Virginia 2004

#### **U.S. DEPARTMENT OF THE INTERIOR**

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#### **U.S. GEOLOGICAL SURVEY**

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# PREFACE

The computer program described in this report is designed to aid in the preparation of input data for the U.S. Geological Survey's (USGS) SUTRA ground-water flow and transport model. Although the program, called **SutraGUI**, has been tested and used by the USGS, no warranty, expressed or implied is made by the USGS or the United States Government as to the accuracy and performance of the program and related material. The code and report may be updated and revised periodically.

Users are requested to notify the USGS if errors are found in the report or in the computer program. Correspondence regarding the report or program should be sent to:

SUTRA Support U.S. Geological Survey 431 National Center Reston, VA 20192 USA

The computer code is available for downloading from the Internet from the USGS software repository at *http://water.usgs.gov/nrp/gwsoftware*. Any updates to or new versions of this code and report will be made available for downloading from this site.

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# **SutraGUI** A Graphical-User Interface for SUTRA, a Model for Ground-Water Flow with Solute or Energy Transport

Richard B. Winston and Clifford I. Voss

## Abstract

This report describes **SutraGUI**, a flexible graphical user-interface (GUI) that supports twodimensional (2D) and three-dimensional (3D) simulation with the U.S. Geological Survey (USGS) SUTRA ground-water-flow and transport model (Voss and Provost, 2002). **SutraGUI** allows the user to create SUTRA ground-water models graphically. **SutraGUI** provides all of the graphical functionality required for setting up and running SUTRA simulations that range from basic to sophisticated, but it is also possible for advanced users to apply programmable features within Argus ONE to meet the unique demands of particular ground-water modeling projects.

**SutraGUI** is a public-domain computer program designed to run with the proprietary Argus ONE<sup>TM</sup> package, which provides 2D Geographic Information System (GIS) and meshing support. For 3D simulation, GIS and meshing support is provided by programming contained within **SutraGUI**. When preparing a 3D SUTRA model, the model and all of its features are viewed within Argus 1 in 2D projection. For 2D models, **SutraGUI** is only slightly changed in functionality from the previous 2D-only version (Voss and others, 1997) and it provides visualization of simulation results. In 3D, only model preparation is supported by **SutraGUI**, and 3D simulation results may be viewed in SutraPlot (Souza, 1999) or Model Viewer (Hsieh and Winston, 2002). A comprehensive online Help system is included in **SutraGUI**.

For 3D SUTRA models, the 3D model domain is conceptualized as bounded on the top and bottom by 2D surfaces. The 3D domain may also contain internal surfaces extending across the model that divide the domain into tabular units, which can represent hydrogeologic strata or other features intended by the user. These surfaces can be non-planar and non-horizontal. The 3D mesh is defined by one or more 2D meshes at different elevations that coincide with these surfaces. If the nodes in the 3D mesh are vertically aligned, only a single 2D mesh is needed. For nonaligned meshes, two or more 2D meshes of similar connectivity are used. Between each set of 2D meshes (and model surfaces), the vertical space in the 3D mesh is evenly divided into a user-specified number of layers of finite elements.

Boundary conditions may be specified for 3D models in **SutraGUI** using a variety of geometric shapes that may be located freely within the 3D model domain. These shapes include points, lines, sheets, and solids. These are represented by 2D contours (within the vertically-projected Argus ONE view) with user-defined elevations. In addition, boundary conditions may be specified for 3D models as points, lines, and areas that are located exactly within the surfaces that define the model top and the bottoms of the tabular units. Aquifer properties may be specified separately for each tabular unit. If the aquifer properties vary vertically within a unit, **SutraGUI** provides the **Sutra\_Z** function that can be used to specify such variation.

## Introduction

Note: Some sections of this document, particularly those dealing with two-dimensional models are extracted from Voss and others (1997) and are presented here with only minor modifications.

The numerical model is a modern tool of the hydrologist involved in practical or theoretical evaluation of subsurface flow and transport processes. Numerical models cannot be considered as exact representations of the real world because the complexity of natural hydrogeologic systems is not easily captured in a discrete model representation. The strongest application of numerical modeling is to test hypotheses concerning the major hydrogeologic controls on subsurface system behavior. The most popular use of numerical models is to predict the response of subsurface systems to applied stresses. Both of these uses often are time consuming because numerical models have complex data requirements, and it is rarely practical for hydrologists to carry out thorough analyses. Application of numerical models and the modeling process itself can be facilitated by the development and use of graphical user interfaces (GUIs) that can manage and synthesize geospatial information and simulation control parameters, create meshes and other formatted input data for the numerical models, and display the simulation results.

This report describes a GUI developed for SUTRA, a U.S. Geological Survey (USGS) twodimensional (2D) and three-dimensional (3D) finite-element model for saturated-unsaturated, variable-density ground-water flow with solute or energy transport (Voss and Provost, 2002). This GUI for SUTRA, **SutraGUI**, was developed using commercially available software developed by Argus Interware. The Argus Interware product, known as Argus Open Numerical Environments (Argus ONE<sup>TM</sup>), is a model-independent, programmable system with geographic information system (GIS) functionality that includes automated gridding and meshing capabilities for synthesizing geospatial information and linking it with finite-difference and finite-element discretizations. The programmable nature of Argus ONE allows geospatial information and simulation control parameters to be exported to ASCII files that can be read by a numerical model, which in this case is SUTRA.

Attributes of Argus ONE make it particularly flexible for model developers. Argus ONE allows externally developed Plug-In Extensions (PIEs) (executable codes loaded into the memory of Argus ONE at run time) that appear as an integral part of the Argus ONE user environment. PIEs may be developed independently by users (Argus Interware, 1997) and are similar in use to user-programmed macros for common spreadsheet and word-processing software. For example, PIEs can be developed for purposes such as spatial interpolation, grid and mesh generation, geostatistics, and control of model pre- and post-processing. In addition, Argus ONE allows users to import geospatial information from other GIS-type applications to provide compatibility with existing user projects. For **SutraGUI**, the PIE provides, among other utilities, a dialog box for entry of certain input data and a means of using the 2D Argus ONE technology to generate input data for both 2D and 3D SUTRA models.

**SutraGUI** consists of a public domain, freely available PIE that must be used in conjunction with the Argus ONE commercial package. Together, these codes provide a fully functioning graphical pre- and post-processor for 2D simulation, and a preprocessor for 3D simulation. Other software provides post-processing for 3D models (Souza, 1999; Hsieh and Winston,

2002). These codes significantly reduce the time and effort required to use SUTRA as a hydrologic tool. In addition, the advanced user may apply programmable features within Argus ONE to extend or modify **SutraGUI** to meet the unique demands of any modeling project.

This report is a description of the use of **SutraGUI** and is not intended as a description of the programming used to develop the PIE. It is assumed herein that the reader has knowledge of the basic data requirements and underlying principles for using the USGS SUTRA code. Voss and Provost (2002) provide thorough discussions of the principles underlying SUTRA and its application to hydrologic problems. Moreover, it is assumed that the reader has knowledge of the general attributes and use of Argus ONE. Information about Argus ONE can be obtained from the Argus ONE User's Guide (Argus Interware, 1997) and the World-Wide Web site for Argus Interware (http://www.argusint.com), from which a demonstration version and documentation may be downloaded.

Note: Users should familiarize themselves with the Argus ONE User's Guide (Argus Interware, 1997) before attempting to use **SutraGUI**. In particular, users should be familiar with chapters 2 and 3, pages 91-162.

#### Conventions

Menu items, dialog boxes, and other features that are part of Argus ONE rather than a plug-in extension (PIE) are shown in *italics*. Menu items, dialog boxes, and other features that are part of **SutraGUI**, the **Utility PIE** (Winston, 2001), **GW\_Chart** (Winston, 2000), or **Model Viewer** (Hsieh and Winston, 2002) are shown in **bold**. If there are a series of menu and submenu items that must be chosen in succession, each menu item is separated from the next by a vertical line (]). For example, choosing the **Quit** submenu item from the **File** menu is shown as **File**[**Quit**.

In Argus ONE, "Layers" are a series of GIS coverages or maps. Layers can have "Parameters" that represent the type of data that is specified in the Layer. Layer names and parameter names are shown in **bold**. If part of a layer name is sometimes absent, the part that is sometimes absent is included in parentheses. If there are two different versions of a layer name, the two different versions are separated by a slash (/) mark. If a layer name has a number after it to designate a particular unit, the number is included in square brackets.

An example of a layer including all these options is (**Top/Bottom**) **Sources of Solute / Energy** (**Unit[i]**). For two-dimensional (2D) models using solute transport, the name of this layer would be **Sources of Solute**. In two-dimensional models using energy transport, it would be called **Sources of Energy**. In three-dimensional (3D) models, the name of the layer is followed by **Unit[i]**, where i represents the number of the unit. For the second unit, i=2, and the name of the unit would be followed by **Unit2**. In the uppermost unit, there can be one such layer for the top of the unit and another for the bottom of the unit. These two layers would be **Top Sources of Solute Unit1** and **Bottom Sources of Solute Unit1**, respectively.

#### Installation

Before installing **SutraGUI**, Argus ONE must be installed. (Argus ONE may be obtained from http://www.argusint.com/.) To install **SutraGUI** manually, download the zip file that contains **SutraGUI** and extract its contents into the Argus Interware\ArgusPIE directory, maintaining the directory structure in the zip file. To install **SutraGUI** with the automatic installer, download

the installer and extract its contents into an empty directory. Run Setup.exe and follow the prompts on the screen.

#### Basic Description of Software Use for Two-Dimensional Models

This section provides a brief description of how the Argus ONE environment with **SutraGUI** is used to create and evaluate 2D numerical simulations with SUTRA. More detail on each step may be found in subsequent sections of this report.

- 1. After starting Argus ONE, the Argus ONE Window appears and the user begins preprocessing for SUTRA by selecting **PIEs**|**New SUTRA Project**. This causes the **SUTRA Project Information** dialog box to appear.
- 2. The user then chooses the desired type of simulation problem, such as areal solute transport, cross- sectional variable-density flow with solute transport, saturated-unsaturated flow with energy transport, or other available types. This choice determines the kinds of geospatial coverages (*Information* layers) required for such a SUTRA simulation and automatically makes them available to the user for data entry and manipulation.
- 3. Next, the user may enter simulation control parameters (those that are not spatiallydependent in other words, 'nonspatial information', such as time-step size) in other parts of the **SUTRA Project Information** dialog box that appears on the computer screen. Individual panes in the dialog box are selected by selecting the names of the panes on the left side of the dialog box. Upon completing data entry or editing of these values, the user closes the dialog box and returns to the Argus ONE window.
- 4. The user should then modify the default information in any geospatial *Information* layer, by manually drawing closed or open contours, or points to represent the desired spatial distributions of hydrogeologic and hydrologic parameters, sources, sinks, boundary conditions, and a desired distribution of finite-element mesh density. As an alternative to drawing, any of these spatial distributions may be directly imported from other applications that can generate text files, DXF (AutoCAD<sup>TM</sup> format) files, or Shape (ArcView<sup>TM</sup> format) files.
- 5. Next, the user creates the finite-element mesh using commands built into Argus ONE or provided by the SutraGUI. Two mesh types are available, a general irregularly-connected mesh of quadrilaterals (normally provided in Argus ONE), and a "fishnet mesh" of regularly connected quadrilaterals (provided by SutraGUI). Before finally proceeding to run SUTRA, the user may modify any of the spatial or nonspatial information that has already been input.
- 6. The user then selects the **SUTRA Mesh** layer, and from the menu *PIEs*, proceeds to export the geospatial and nonspatial information, at which time Argus ONE writes out the standard input- data files for SUTRA to the selected directory and runs the SUTRA simulation. When the simulation is complete, the user may choose to plot any of the simulation results within Argus ONE in a post-processing step provided by **SutraGUI** for 2D problems, or the plot is done externally for 3D problems using **SutraPlot** (Souza, 1999) or **Model Viewer** (Hsieh and Winston, 2002).

The power of the GUI approach in hydrogeologic hypothesis testing and practical modeling should be apparent to any experienced modeler at this point. The user can return to any type of spatial information already input to the SUTRA-Argus ONE environment, make major modifications to it or the finite- element mesh, re-export from Argus ONE, run SUTRA, and graphically evaluate results of new simulations. Each cycle of changing information, running SUTRA, and inspecting results, can take as little as a few minutes depending on the number of model nodes and the speed of the computer.

### Starting Argus ONE and Starting a New SUTRA Project

To start Argus ONE, do any of the following:

- 1. Double-click on the Argus ONE shortcut on the desktop.
- 2. Click on the "Start" button. Select "Programs," then "Argus ONE," and then "Argus ONE" again.
- 3. In Windows Explorer, double-click on any existing Argus ONE project file ('filename'.mmb).

Argus ONE will start, load the Plug-In Extensions (PIEs), and then open either an empty generic project (options 1 or 2) or the project that was selected (option 3). To start a new SUTRA project, select **PIEs**|**New SUTRA Project**. The **SUTRA Project Information** dialog box will appear. The user specifies nonspatial information about the project in the **SUTRA Project Information** dialog box. When the **OK** button is clicked, the **SUTRA Project Information** dialog box will close and the layer structure for the SUTRA project will be established. The Argus ONE layer structure is where all spatial data in the model are entered.

## Accessing Online Help

The online help is the primary documentation for **SutraGUI**. The online help for **SutraGUI** can be accessed in several ways.

- 1. Locate the file SutraGUI.hlp in the directory in which **SutraGUI** is installed and doubleclick on it inside Windows Explorer.
- 2. Start Argus ONE, start a new SUTRA project, and select the **PIEs**|SUTRA Help menu item.
- 3. In most dialog boxes provided by **SutraGUI**, there is a button labeled **Help**. Click on such buttons to access the online help.
- 4. In many dialog boxes provided by **SutraGUI**, there will be a "?" icon in the upper righthand corner. The online help can be accessed by clicking on the icon and then clicking on one of the controls in the dialog box.
- 5. In dialog boxes provided by **SutraGUI**, select a control and press the F1 button on the keyboard.

#### Acknowledgments

The authors wish to thank Allen Shapiro, Elena Abarca, and Dorothy Tepper for their extremely helpful reviews of this document and Argus Interware for the modifications they made in Argus

ONE that made this software possible. The authors also wish to thank the numerous individuals who have participated in testing this software and providing feedback on it.

# **Basic Concepts**

The hydrogeological properties of an area and their distribution in two or three dimensions are represented in Argus ONE as a set of 2D maps. These are referred to as "*Information layers*." In GIS applications, these are referred to as 'coverages'. The specific layers created by **SutraGUI** are described in the section, "Layer Descriptions." Associated with most layers is a set of one or more parameters. These parameters represent the data associated with the 2D-space associated with the layer. Each parameter has an "*Expression*" associated with it. *Expressions* in Argus ONE provide a default (or 'background') value for a parameter that may be based on mathematical operations on data stored elsewhere in the data file. A layer may contain one or more *contours* that represent the location of data. A contour may be a single point (*point contour*), a series of connected points (*open contour*) or a polygon (*closed contour*). For each contour on a layer, the user may assign a value for each parameter. The value of a parameter at any specific point will depend on the contours on the layer, the values assigned to the parameters for those contours, the default expression for the parameter, and the *Interpretation* methods as described in the Argus ONE User's Guide (Argus Interware, Inc., 1997).

As an example, consider the **Hydraulic Conductivity** layer. In 2D models, it has three parameters: **maximum**, **minimum**, and **angle\_of\_max\_to\_x\_axis**. The default *Expressions* for them are simply values, 1.0E-3, 1.0E-3, and 0, respectively. By default, the interpretation method for the layer is *Nearest*. If the interpretation method is changed to *Exact*, a closed contour is drawn, and the **maximum** parameter is assigned a value of 2.0E-3. The maximum hydraulic conductivity inside the contour will be 2.0E-3, whereas outside the contour it will be 1.0E-3.

Separation of the underlying physical information from the simulation model provides a powerful hydrogeologic tool. The GIS coverages (*Information* layers) may be used interchangeably for any simulation model coupled with Argus ONE. For example, if a Data layer is used to specify the distribution of hydraulic conductivity in the **SutraGUI**, the data points in that layer could be exported to a text file and then imported into a MODFLOW model created with the MODFLOW GUI (Winston, 2000).

In addition to *Information* layers, *Data* layers may be used to store point data. The main differences between *Data* layers and *Information* layers are that, in *Data* layers: (1) only point data can be used; (2) only real-number data, not integers or other data types, can be used; (3) *Expressions* cannot be used to set the value of a data point; and (4) only interpolation methods can be used on the point data in contrast with the Nearest and Exact methods.

The mesh for the model is stored in a *Quad Mesh* layer. Parameters on this layer, for the most part, represent the inputs to the SUTRA model as determined by an interpretation of the *Information* and *Data* layers.

#### Nodes, Elements, and Cells

In SUTRA, the region to be modeled is divided up into *elements*. These can be either 2D quadrilaterals (<u>fig. 1</u>) or 3D solids with six sides ("generalized hexahedra", <u>fig. 2</u>). (Strictly speaking, the elements are not hexahedra because the faces can be curved.) The determinant of the Jacobian matrix of all elements must be positive (Voss and Provost, 2002). For both 2D and

3D elements, this means that no node can be displaced toward the interior of the element beyond the line or plane defined by its two or three neighboring nodes in the element. The corners of elements are *nodes*. 2D elements have four nodes (fig. 1) and 3D elements have eight nodes (fig. 2). The nodes are where values for pressure, saturation, and concentration or temperature of the model are calculated by SUTRA. Each node is associated with a region termed the *cell*. The cell associated with any node is made up of portions of all the neighboring elements. Each element is divided into 4 or 8 pieces depending on whether the element is 2D (fig. 1) or 3D (fig. 2). Each piece is assigned to its corner node as part of the cell of that node.

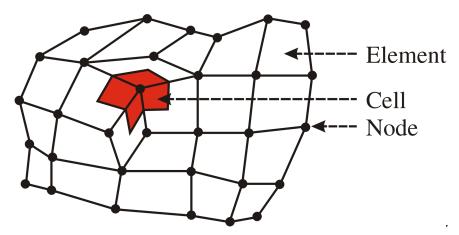


Figure 1. Nodes, elements, and a cell in a two-dimensional (2D) SUTRA mesh.

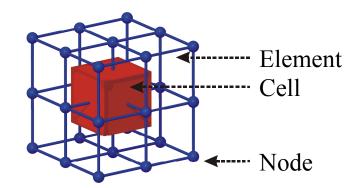


Figure 2. Nodes, elements, and a cell in a three-dimensional (3D) SUTRA mesh.

#### Two-Dimensional Domains and Meshes in SutraGUI

The model domain is the spatial region that is included in the model. A SUTRA simulation may employ either a 2D or 3D domain and mesh. For a 2D simulation, the domain is a 2D region enclosed by a single continuous boundary. Internally, there may be holes in the 2D region and each is enclosed by a continuous boundary. To create a mesh, this domain or region is divided into a set of contiguous finite elements. If a 2D mesh is used, the mesh created by Argus ONE is the same as the mesh used by SUTRA. A 2D mesh may be either an irregular mesh or a FishNet Mesh. An irregular mesh (for example, <u>fig. 1</u>) is the type of mesh normally created by Argus ONE and is described in the Argus ONE User's Guide (Argus Interware, 1997). A FishNet

Mesh (for example, <u>fig. 3</u>) consists of superblocks (large contiguous quadrilaterals) that are each subdivided into a specified number of quadrilateral finite elements, four of which are connected to each internal node. The mesh may be considered similar to a deformed finite-difference grid. FishNet meshes are created as described in the section of this report entitled "FishNet\_Mesh\_Layout."

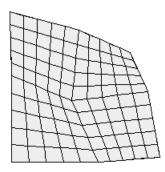


Figure 3. Example of a FishNet mesh.

#### Three-Dimensional Domains and Meshes in SutraGUI

For 3D problems, the X and Y coordinate plane, as viewed on the computer monitor, may be oriented in any direction in space. However, for most problems, it is recommended that X be directed east, Y north, and Z outward from the screen, representing elevation.

A 3D model domain is conceptualized as comprising a stack of one or more tabular units. Each tabular unit extends across the entire domain in either a subhorizontal or subvertical direction. Units may represent geologic units or any other geometric features. The top of the model domain is a curved, uneven, or flat 2D surface. A 2D surface also defines the bottom of the unit in 3D. The bottom of each unit also is the top of the unit below it.

Most often, a tabular unit will represent a hydrogeologic unit, although this is not required. If a unit represents a hydrogeologic unit, and the hydrogeologic unit pinches out within the model domain, the portion of the unit that is outside the area of the hydrogeologic unit should be considered part of a separate hydrogeologic unit and its properties should be consistent with the other unit in those locations.

Often, the user may wish to represent a unit with several layers of nodes and elements. To do so, the user needs to specify the discretization across the unit (referred to here as the 'vertical discretization' though the direction need not be vertical). The reader is referred to the section of this report entitled "Structure in Z (3D Only)" on page 29 for instructions on how to specify the vertical discretization. The vertical discretization represents the number of layers of elements represented by the unit.

Argus ONE does not provide a method for creating 3D meshes. **SutraGUI**, therefore, creates the 3D mesh in memory each time it is needed. **SutraGUI** uses one or more 2D meshes created by Argus ONE to represent the 3D mesh.

Note: At present (2003), SUTRA requires that all 3D meshes be FishNet Meshes. In a FishNet mesh for a 3D model, the nodes must be connected in such a way that the entire mesh can be deformed into a finite-difference grid.

The 3D mesh is constructed by allowing layers of nodes to follow along the top of the model domain and along the bottoms of the units. The layers of nodes that define the boundaries between the units are represented by Quad Mesh layers in Argus ONE. Between the top and bottom of each unit lie one or more layers of elements (<u>fig. 4</u>) and their nodes. **Vertical Discretization** controls the number of layers of elements for each unit.

Note: Except for the uppermost unit, each unit extends from the layer of nodes at its bottom up to but not including the layer of nodes at its top. The uppermost unit includes the layer of nodes at its top.

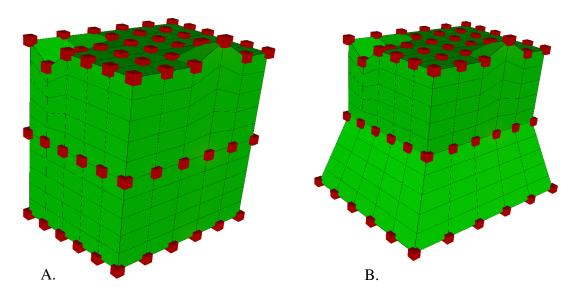


Figure 4. Three-dimensional (3D) meshes in SUTRA containing two units. The nodes marked with red cubes are nodes in Argus ONE two-dimensional meshes indicating the location of the model top and the bottoms of each of the two units. A. Vertically aligned mesh. B. Nonaligned mesh.

The elevation of nodes in the 3D mesh is determined by the **Elevation Top** and **Elevation Bottom Unit[i]** layers. Each such layer is used to assign the elevation of the nodes at the top or bottom of a unit. Nodes in the interior of units are spaced equally between the corresponding nodes on the top and bottom of the unit.

If the user chooses a **vertically aligned** mesh ( $\underline{\text{fig. 4A}}$ ), only a single Argus ONE 2D quad mesh is used and is projected downwards through the 3D mesh. Thus, this 3D mesh type consists of nodes and elements that lie directly beneath the nodes and elements in the Argus ONE mesh. However, the elevations within a layer of nodes can vary, depending on the elevations of the model top and unit bottoms. The 3D mesh is thus vertically extruded from the 2D mesh.

If a **nonaligned** mesh (<u>fig. 4B</u>) is selected, an Argus ONE Quad Mesh must be specified for the bottom of every unit and for the top of the mesh. The 2D meshes on these layers must all have the same number of nodes and elements. In addition, the numbering of the nodes and elements must be the same in each mesh. For example, if one mesh has 10 rows and 20 columns of elements, the others must also. If one mesh has its nodes numbered first along rows and then along columns, the others must also. However, the (X, Y) coordinates of the nodes can vary among meshes. Methods for creating meshes that meet these requirements are discussed in the section of this report entitled "FishNet\_Mesh\_Layout" on page 42.

In **SutraGUI**, the numbering of nodes and elements in the 3D mesh cannot correspond exactly to the numbering of nodes and elements in the 2D mesh created by Argus ONE. Each node and element in the 2D mesh corresponds to several nodes and elements in the vertical dimension. These nodes are numbered sequentially from the top to the bottom of the 3D mesh. For example, if a mesh had 10 elements in the vertical dimension, element 1 in the 2D mesh would correspond to elements 1-10 in the 3D mesh. Element 2 in the 2D mesh would correspond to elements 11-20 in the 3D mesh, and so on. The menu item **PIEs**|**Convert Node and Element Numbers** is a command that can be used to convert node and element numbers in the Argus ONE mesh to those of the 3D mesh and vice-versa when such information is needed.

#### Assignment of Aquifer Properties

Certain variables, such as porosity and permeability must be defined for all nodes or elements in a SUTRA model. The methods for doing so in **SutraGUI** vary somewhat between 2D and 3D models.

#### **Two-Dimensional Models**

The user may define the distribution of porosity, permeability (or hydraulic conductivity), dispersivity, initial pressure (or initial head), initial concentration (or initial temperature), and thickness throughout the 2D model domain. Spatial distributions may be defined in any way provided by Argus ONE, as explained in the Argus ONE User's Guide (Argus Interware, 1997).

#### **Three-Dimensional Models**

The user defines the distribution of porosity, permeability (or hydraulic conductivity), dispersivity, initial pressure (or initial head), and initial concentration (or initial temperature) for each unit. Unless the **Sutra\_Z**() function (described in the next paragraph) is used, the properties do not vary vertically within each unit. (Because pressure changes with elevation, the **Sutra\_Z**() function is often particularly useful in defining specified pressure boundaries and the initial pressure.)

The **Sutra\_Z**() function provided by **SutraGUI** can be used in *Expressions* to set the values of aquifer properties or boundary conditions based on the Z-coordinate (usually the vertical coordinate) of nodes or element centroids. The reader is referred to the Argus ONE User's Guide (Argus Interware, 1997) for an explanation of *Expressions*. The **Sutra\_Z**() function is only meaningful in 3D models.

Note: Because the elevations of the nodes and element centroids are not known except when the input files for SUTRA are generated, values of the **Sutra\_Z()** function are never given interactively by **SutraGUI**. Values of **Sutra\_Z()** exist only during the actual creation of the SUTRA input files, in other words, during export.

The **Sutra\_Z**() function can be used for the source terms in boundary condition layers, for the top and bottom elevations in layers relating to solids and for any of the aquifer properties that are set by node or by element. Table 1 is a complete listing of the layers and parameters for which the **Sutra\_Z**() function is valid. If one of the parameters in table 1 is linked to any other parameter, including ones not in table 1, and the other parameter employs **Sutra\_Z**(), **Sutra\_Z**() will be evaluated correctly during export of the parts of the SUTRA input files related to the parameters in table 1.

## Table 1. Parameters for which the Sutra\_Z() function is valid

1	Note: The reader is referred to the section of this report entitled "Conventions" for an	
e	explanation of "[i]" in layer names.	

Layer	Parameters
Sources of Fluid Solids[i]	total_source, specific_source, concentration_of_source, temperature_of_source, top_elevation, bottom_elevation
Sources of Fluid Points[i]	total_source, concentration_of_source, temperature_of_source
Sources of Fluid Lines[i]	total_source, specific_source, concentration_of_source, temperature_of_source
Sources of Fluid Sheets Vertical[i]	total_source, specific_source, concentration_of_source, temperature_of_source
Sources of Fluid Sheets Slanted[i]	total_source, specific_source, concentration_of_source, temperature_of_source
Sources of Solute Solids[i]	total_source, specific_source, top_elevation, bottom_elevation
Sources of Solute Points[i]	total_source
Sources of Solute Lines[i]	total_source, specific_source
Sources of Solute Sheets Vertical[i]	total_source, specific_source
Sources of Solute Sheets Slanted[i]	total_source, specific_source
Sources of Energy Solids[i]	total_source, specific_source, top_elevation, bottom_elevation
Sources of Energy Points[i]	total_source
Sources of Energy Lines[i]	total_source, specific_source
Sources of Energy Sheets Vertical[i]	total_source, specific_source
Sources of Energy Sheets Slanted[i]	total_source, specific_source
Specified Hydraulic Pressure	specified_pressure, concentration, temperature,
Solids[i]	top_elevation, bottom_elevation
Specified Hydraulic Pressure Points[i]	specified_pressure, concentration, temperature
Specified Hydraulic Pressure Lines[i]	specified_pressure, concentration, temperature
Specified Hydraulic Pressure Sheets Vertical[i]	specified_pressure, concentration, temperature
Specified Hydraulic Pressure Sheets Slanted[i]	specified_pressure, concentration, temperature

Layer	Parameters
Specified Hydraulic Head Solids[i]	specified_hydraulic_head, concentration, top_elevation, bottom_elevation
Specified Hydraulic Head Points[i]	specified_hydraulic_head, concentration
Specified Hydraulic Head Lines[i]	specified_hydraulic_head, concentration
Specified Hydraulic Head Sheets Vertical[i]	specified_hydraulic_head, concentration
Specified Hydraulic Head Sheets Slanted[i]	specified_hydraulic_head, concentration
Specified Concentration Solids[i]	specified_concentration, top_elevation, bottom_elevation
Specified Concentration Points[i]	specified_concentration
Specified Concentration Lines[i]	specified_concentration
Specified Concentration Sheets Vertical[i]	specified_concentration
Specified Concentration Sheets Slanted[i]	specified_concentration
Specified Temperature Solids[i]	specified_temperature, top_elevation, bottom_elevation
Specified Temperature Points[i]	specified_temperature
Specified Temperature Lines[i]	specified_temperature
Specified Temperature Sheets Vertical[i]	specified_temperature
Specified Temperature Sheets Slanted[i]	specified_temperature
Observation Solids[i]	top_elevation, bottom_elevation
Porosity Unit[i]	porosity
Permeability Unit[i]	maximum, middle, minimum, horizontal angle, vertical angle, rotational angle
Hydraulic Conductivity Unit[i]	maximum, middle, minimum, horizontal angle, vertical angle, rotational angle
Dispersivity Unit[i]	longdisp_in_max_permdir, longdisp_in_mid_permdir, longdisp_in_min_permdir, trandisp_in_max_permdir, trandisp_in_mid_permdir, trandisp_in_min_permdir
Initial Hydraulic Head Unit[i]	initial_hydraulic_head
Initial Pressure Unit[i]	initial_pressure
Initial Concentration Unit[i]	initial_concentration
Initial Temperature Unit[i]	initial_temperature

Table 1. Parameters for which the Sutra\_Z() function is valid - Continued

## Assignment of Boundary Conditions and Observations

There are four types of boundary conditions used in SUTRA. These include **Sources of Fluid**, **Sources of Solute** (or **Sources of Energy**), **Specified Pressure** (or **Specified Head**), and

**Specified Concentration** (or **Specified Temperature**). Point, open, and closed contours may be used to specify all the boundary conditions and the locations of observation points in 2D and 3D models. In addition, 3D objects may be used to specify all the boundary conditions and the locations of observation points in 3D models.

For sources of fluid and sources of solute (or sources of energy), either a total source or a specific source may be applied. A total source is the total amount of fluid, solute, or energy to be injected or extracted from all the nodes associated with the contour. A specific source is the amount of fluid, solute, or energy per unit length of contour or per unit area of contour to be injected or extracted from each node associated with the contour. Because point contours have neither length nor area, point contours cannot be used for specific sources.

#### **Total and Specific Sources**

Either a **total\_source** or **specific\_source** for sources of fluid and sources of solute or energy must be defined as contour objects. A contour may have its own value, or its value may come from a background expression.

• If a **total\_source** is defined, the value **total\_source** is divided among all the nodes to which the source applies. The **total\_source** is allocated to each node according to the fraction of the following that falls within the cell of that node: the total length or area of the 2D source contour (open and closed contours), or the total length or area of the 3D source object (line objects or sheet objects).

For solids, the **total\_source** is allocated to each node according to the fraction of the total volume of the cells associated with the 3D solid object represented by the node's cell.

- A **specific\_source** cannot be used with point sources.
- If a **specific\_source** with a line contour is defined, the value is multiplied by the length of the line associated with a node to determine the correct amount to apply to a particular node.
- If a **specific\_source** is defined with a closed contour, the value is multiplied by the area of the contour associated with a node to determine the correct amount to apply to a particular node.
- If a **specific\_source** with a sheet source is defined, the value is multiplied by the area of the contour associated with a node to determine the correct amount to apply to a particular node.
- If a **specific\_source** with a solid source is defined, the value is multiplied by the volume of the cell associated with a node to determine the correct amount to apply to a particular node.

#### Time Dependence

Boundary conditions in SUTRA may be made time-dependent by modifying the subroutine BCTIME in SUTRA and recompiling SUTRA. In such cases, the **time\_dependence** parameter is used to signal that a particular contour specifies a time-dependent boundary condition.

When BCTIME is modified to support time-dependent boundaries, it must be specified how the data for the time-dependent boundaries are to be generated. The data may be generated within

the BCTIME subroutine or BCTIME can read the data from an external file in a format specified by the user. Because there is no standard input format for data files read by the BCTIME subroutine, **SutraGUI** cannot generate such input files. However, users may be able to create an export template for use within Argus ONE that will generate such files for their particular case as described on p. 169-188 of the Argus ONE User's Guide (Argus Interware Inc., 1997).

## Labeling Sources, Boundary Conditions, and Observations

The **comment** parameter holds a string variable that is appended to the SUTRA input file as a comment for all nodes or elements affected by a particular contour. This can be useful for diagnostic purposes or for preparing input files for use in the BCTIME subroutine. For example, this feature may be used to individually name contours that define wells so that time-dependent pumping rates for each named well may be read by the BCTIME subroutine. (The reader is referred to the section of this report entitled "Time Dependence."

## **Two-Dimensional Models**

Two-dimensional (2D) models may use any of the objects defined in Argus ONE to represent boundary conditions and observations. The objects include the following:

- Point contours: these have a single vertex with an X and a Y coordinate.
- Open contours: these have multiple vertices each with an X and a Y coordinate. Open contours do not close back on themselves, so they have a length but no area.
- Closed contours: these have multiple vertices, each with an X and a Y coordinate. Closed contours close back on themselves, so they have both a length and an area.

In 2D models, nodes must lie <u>exactly</u> above point, open (line), and closed contours to be selected as boundary conditions or observations. To specify a boundary condition with a point contour in a 2D model, the location of the point contour must correspond to the location of a node. With open contours, the location of each segment of the contour must lie along the edges or diagonals of elements. Nodes falling within and above a closed contour are selected as boundary conditions or observations.

For sources of fluid, the user must specify a **total\_source** or **specific\_source** and the **concentration\_of\_source** or **temperature\_of\_source** associated with the source. For sources of solute or sources of energy, the user must specify either a **total\_source** or **specific\_source**. For specified pressure or specified hydraulic head, the user must specify the **specified\_pressure** or **specified\_hydraulic\_head** and the **concentration** or **temperature** that correspond to the incoming fluid. For specified concentration or specified temperature, the user must specify the **specified\_concentration** or **specified\_temperature**. If any of these boundary conditions are time-dependent, **time\_dependence** must be set to 'true'.

## **Three-Dimensional Models**

All the boundary conditions and the locations of observation points can be set on layers similar to those used for 2D models. These objects can only be located within the model top and within the bottom surfaces of any model unit in 3D. As in 2D models, these objects must lie directly above nodes or must enclose nodes.

In addition, all boundary conditions can be set using 3D objects, which may be placed anywhere in the 3D domain of the model, within individual units or crossing several units. By itself, Argus ONE does not define 3D objects; it only provides 2D objects. The user can define the shape of the projection of a 3D object on the top of the model and the top and bottom elevations of the object. Any 3D object shape can be constructed in this way using a combination of one or more such objects.

3D objects are defined in SutraGUI using the Argus ONE 2D objects, but additional information must be supplied about the Z-coordinates of the objects. This is done using the parameters defined for each *Information* layer in Argus ONE where 3D objects are defined. There are five types of 3D objects: points, lines, vertical sheets, slanted sheets, and solids. The relations between the 3D objects and the corresponding 2D Argus ONE contours are shown in Table 2.

3D Object	2D Contour-type	Extra information required
Point	Point contour	Z-coordinate
Line	Point or Open contour	Z-coordinates of the first and last vertices of the line (a segmented polyline – need not be linear)
Sheet (vertical)	Open contour	Z-coordinates of the first and last vertices of the line at the top and bottom of the vertical sheet (need not be planar)
Sheet (slanted)	Closed contour	X, Y, and Z-coordinates of three, non-collinear points. These points define a plane; the extent of the contour defines the portion of the plane that is part of the slanted sheet (must be planar).
Solid	Closed contour	A top and bottom elevation. These may be either constants or functions of X and Y. (For simplicity, it is best to avoid making these elevations functions of <b>Sutra_Z().)</b>

Table 2. Summary of methods of specifying three-dimensional (3D) objects using two-dimensional (2D) contours

For points, lines, and sheets, a node will be selected by the 3D object as a boundary condition or observation node in a 3D model if the cell surrounding the node intersects the 3D object. This is in contrast with 2D models, where only nodes directly above the contours themselves are selected. Boundary conditions or observation nodes need not lie exactly above or within contours (objects) in 3D models. For solids, a node will be selected as a boundary condition or observation node if the node is inside the solid. For each type of 3D object, explanations that are more detailed are given in the next sections.

The **follow\_mesh** parameter can modify how certain 3D objects are evaluated when using a nonaligned 3D mesh. The **follow\_mesh** parameter is available for solids, lines, and vertical sheets. It is not available for points or slanted sheets. For more information, the reader is referred to the section of this report entitled "The **Follow\_Mesh** Parameter for Nonaligned Meshes" on page 20.

#### Selecting and Assigning Properties to Nodes Using Points

For points, the 3D object will select a node as a boundary condition node if the point is inside the cell surrounding the node. In <u>figure 5</u>, the red node is selected because the yellow point is inside its cell. The value assigned to the node is the value assigned to the point.

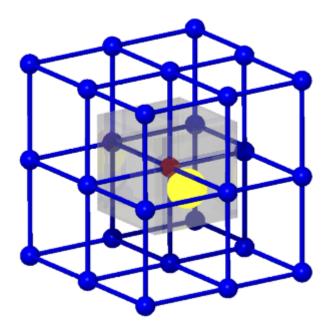


Figure 5. Selecting a node with a point object in three dimensions. The cell of the red node is the shaded region.

For SutraGUI to determine whether a point is inside the cell surrounding the node, the cell is approximated by a polyhedron. The vertices of the polyhedron consist of

- the node itself (if the node is on the edge of the mesh),
- points at the center of the line connecting the node to its neighbors,
- the points at the center of the faces of the elements that include the node, and
- the points at the centers of the elements that include the node.

#### Selecting and Assigning Properties to Nodes Using Lines

For lines, the 3D object selects a node as a boundary condition or observation if the cell surrounding the node intersects the line. In <u>figure 6</u>, the red nodes are selected because the yellow line intersects their cells.

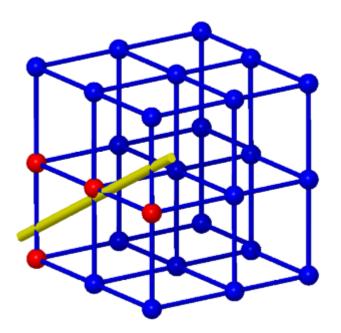


Figure 6. Selecting nodes with a line object in three dimensions.

The values assigned to the selected nodes depend on whether the source is assigned using the **total\_source** or **specific\_source** parameter. If the **total\_source** parameter is used, the value assigned to a node is the value of the **total\_source** parameter times the fraction of the length of the source that is in the cell surrounding the node. If the **specific\_source** parameter is used, the value assigned to a node is the value of the **specific\_source** parameter times the length of the source that was in the cell surrounding the node. (If part of the line lies outside of all cells, that portion is not considered a part of the total length of the line.) For example, suppose that the total length of a source is 500 m and that 100 m of that length lies inside the cell of one node. If the source is a **total\_source** with a value of 2 m<sup>-1</sup>, the value assigned to the node is  $2 \times (100/500) = 0.4$ . If the source is a **specific\_source**, even if part of the line is outside all cells, the total amount assigned to the entire line is distributed by the above method within the mesh.

#### Selecting and Assigning Properties to Nodes Using Sheets

For vertical sheets and slanted sheets, the 3D object selects a node as a boundary condition or observation node if the cell surrounding the node intersects the sheet. In <u>figure 7</u>, the red nodes are selected because the yellow sheet intersects their cells.

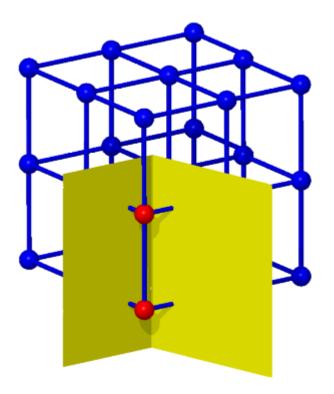


Figure 7. Selecting nodes with a sheet object in three dimensions.

The values assigned to the selected nodes depend on whether the source is a **total\_source** or a **specific\_source**. If the **total\_source** parameter is used, the value assigned to a node is the value of the **total\_source** parameter times the fraction of the area of the source that is in the cell surrounding the node. If the **specific\_source** parameter is used, the value assigned to a node is the value of the **specific\_source** parameter times the area of the source that is in the cell surrounding the node. Only portions of the sheet that lie inside cells count toward the total area of the sheet. For a **total\_source**, even if part of the sheet is outside all cells, the total amount assigned to the entire sheet is distributed by the above method within the mesh.

#### Selecting and Assigning Properties to Nodes Using Solids

For solids, a node is selected as a boundary condition or observation node if the node itself is inside the solid. In <u>figure 8</u>, the red nodes are selected because they are inside the yellow solid.

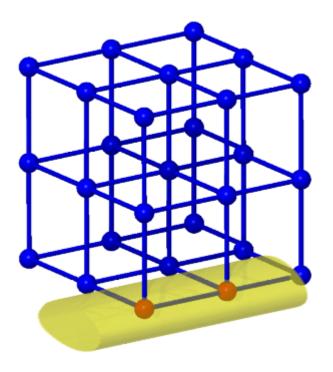


Figure 8. Selecting nodes with a solid in three dimensions.

The values assigned to the selected nodes depend on whether the source is a **total\_source** or a **specific\_source**. If the **total\_source** parameter is used, the value assigned to a node is the value of the **total\_source** parameter times the volume of the cell surrounding the node divided by the volumes of all the cells selected by the solid. If the **specific\_source** parameter is used, the value assigned to a node is the value of the **specific\_source** parameter times the volume of the cell surrounding the node. For a **total\_source**, even if part of the solid object is outside all cells, the total amount assigned to the entire solid is distributed by the above method within the mesh. Note that, in contrast with line and sheet objects, the actual volume of the solid is never calculated and the allocation to nodes, though it preserves the amount of the source, is based on the volume of the cells rather than the volume of the object.

#### The Follow\_Mesh Parameter for Nonaligned Meshes

The **follow\_mesh** parameter can be used to modify how certain 3D objects are interpreted for nonaligned 3D meshes. It is only beneficial to set **follow\_mesh** to 'true' for nonaligned meshes; for vertically aligned meshes, this parameter has no effect.

#### Lines

If **follow\_mesh** is 'true' for lines, the location of the open contour used to define the line is treated as follows. In the uppermost Argus ONE mesh layer, all the nodes whose 2D cells intersect the contour are identified. The contour is treated as if it was aligned with the X and Y coordinates of those nodes. Then it is moved down along a column of nodes to a location where the Z-coordinate matches the Z-coordinate of the original line. In the process, the X and Y coordinates are also adjusted. This new line contour is then evaluated in the usual manner (fig. 9). Thus, when the user specifies a line object on the model top or on any unit bottom, the object is moved up or down to the user-specified elevation along vertical columns of nodes in the mesh.

For nodes at the outer edge of the mesh, this process can lead to lines that lie just outside the mesh and only just touch the mesh along the edges of elements. In such cases, the line would not select any nodes because the line would not be inside the element. Therefore, it is best to avoid setting the **follow\_mesh** parameter to 'true' for lines near the edge of the mesh. In such cases, solids should be used instead.

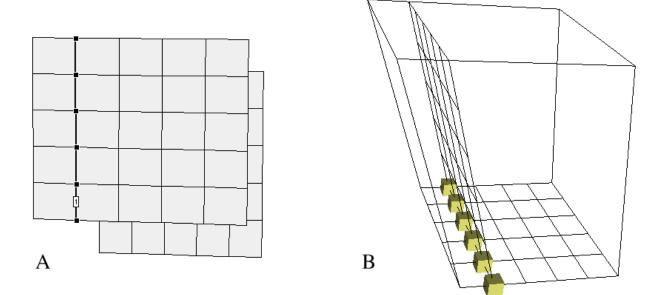


Figure 9. Effect of the follow\_mesh parameter with line objects. A. An open contour in Argus ONE defining a line together with two meshes representing different levels in the three dimensional (3D) mesh. (The "1" on the contour is the parameter value of the contour in Argus ONE.) B. The nodes selected by the line when follow\_mesh is set to 'true' and the elevation of the line is set to the elevation of the lower mesh.

#### **Vertical Sheets**

If **follow\_mesh** is 'true' for vertical sheets, the location of the open contour used to define the line is treated as follows. In the uppermost Argus ONE mesh layer, all the nodes whose 2D cells intersect the contour are identified. A new set of sheets is constructed that comprises the faces of all 3D elements that are in the same column of nodes as the selected nodes on the uppermost 2D mesh. These new sheet contours are then evaluated in the usual manner (<u>fig. 10</u>). As with lines, described just above, this method should not be used at the outer edge of the mesh. Thus, when the user specifies a line object intended to represent a vertical sheet on the model top or on any unit bottom, the entire vertically oriented sheet of nodes that intersects the line is selected between the top and bottom elevations specified by the user.

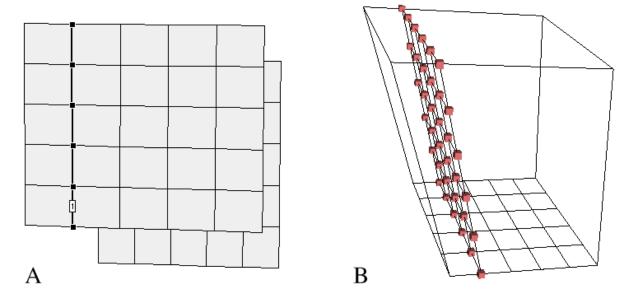


Figure 10. Effect of the follow\_mesh parameter with sheet objects. A. An open contour in Argus ONE defining a line together with two meshes representing different levels in the three dimensional (3D) mesh. (The "1" on the contour is the parameter value of the contour in Argus ONE.) B. The nodes selected by the sheet when follow\_mesh is set to 'true' and the elevations are set to include both meshes.

#### Solids

If **follow\_mesh** is 'true' for Solids, the location of the closed contour used to define the solid is treated as follows. When each node in the 3D mesh is tested to see whether it lies within the solid, the X and Y locations of the node tested will not be the X and Y coordinates of the node itself but rather the X and Y coordinates of the corresponding node in the uppermost 2D Argus ONE mesh (fig. 11). (The Z-coordinate is the location of the tested node itself.) Thus, when the user specifies a solid object intended to represent a vertical volume on the model top or on any unit bottom, the entire vertically oriented volume of nodes that intersects the line is selected between the top and bottom elevations specified by the user.

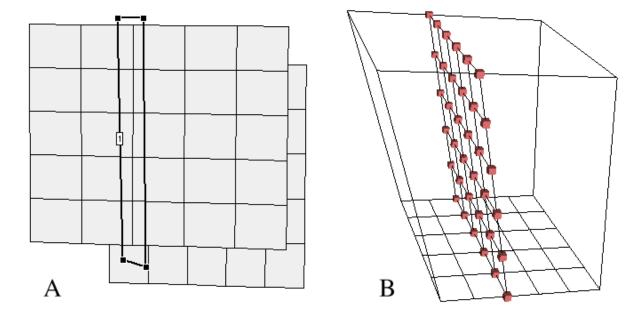


Figure 11. Effect of the follow\_mesh parameter with solid objects. A. A closed contour in Argus ONE defining a solid together with two meshes representing different levels in the three dimensional (3D) mesh. (The "1" on the contour is the parameter value of the contour in Argus ONE.) B. The nodes selected by the solid when follow\_mesh is set to "true" and the bottom elevation is set to below the elevation of the lower mesh and the top elevation is set above the elevation of the upper mesh.

# **Specifying Nonspatial Data**

After starting a new SUTRA project, or when **Edit Project Info**... is selected from the Argus ONE **PIEs** menu, the **SUTRA Project Information** dialog box appears. The **SUTRA Project Information** dialog box allows the user to choose the desired type of SUTRA application (for example, areal solute-transport model, or cross-sectional saturated-unsaturated energy-transport model, etc.) and to enter required information for the SUTRA simulation that is not spatially dependent (for example, time-step size, SUTRA output controls, etc.). It also allows the user to edit this project information at any time from within the Argus ONE environment. (Input of the spatially dependent information is done in geospatial *Information* layers accessible from the standard Argus ONE window after exiting from the **SUTRA Project Information** dialog box.)

The data in the **SUTRA Project Information** dialog box appears on a number of separate panes. A list of the panes appears on the left side of the dialog box. When the user selects one of the items from the list of panes, the corresponding pane appears on the right side of the dialog box.

Most of the information to be entered in the **SUTRA Project Information** dialog box is required in SUTRA input data sets, and with a few exceptions, appears in the same order as normally found in a SUTRA input data set, as described in the SUTRA documentation (Voss and Provost, 2002). The 'initial time' from the SUTRA initial conditions input data set also appears here.

A pane may be accessed by clicking on the pane's title, listed along the left edge of the dialog box. Some data-entry boxes may be grayed out and inaccessible; these parameter values are fixed by the user's choice of problem type (on the **Model Configuration** pane or **Modes**, **Numerical Controls** pane) and need not be altered.

The SUTRA input data-set number and the SUTRA parameter name are given on each pane to allow the user to easily find detailed instructions for each particular data type in the SUTRA documentation (Voss and Provost, 2002). The **SutraGUI** Help system can also be used to find out about the parameters in the **SUTRA Project Information** dialog box. One way to access the Help system for a particular control is to select the control (such as an edit box or check box) and press the F1 button on the keyboard. The reader is referred to the section of this report entitled "Accessing Online Help" on page 5 for more information.

When all entry or modification of data in the **SUTRA Project Information** dialog box is complete, click on the **OK** button to accept changes, or on the **Cancel** button to ignore any changes made; in either case, the user proceeds to the Argus ONE environment. If **Cancel** is selected during the creation of a new SUTRA project, then the creation of that new project is canceled. Because default values are supplied for all parameters, it may not be necessary to access all of the panes in the **SUTRA Project Information** dialog box before closing it. The default values for parameters in the **SUTRA Project Information** dialog box are listed in tables 3 and 4.

Variable	Default	Variable	Default	Variable	Default
SIMULA	SUTRA	NOBCYC	0	NSAVEU	10
	SOLUTE				
	TRANSPORT	NECOL 0	TT 1 1 1	COMPE	0
TITLE1	SUTRA Model	K5COL & K6COL	Unchecked	COMPFL	0
	created using Argus ONE	KOCUL	(=0)		
TITLE2	USGS sample	CNODAL	Unchecked	CW	1
1111112	Interface	CNODAL	(=0)	CW	1
CUNSAT	Unsaturated and	CELMNT	Unchecked	SIGMAW	1E-9 for solute
	saturated flow		(=0)		transport;
					0 for energy
					transport
CSSFLO	Steady-state	CINCID	Unchecked	RHOWØ	1
	ground-water		(=0)		
	flow				
CSSTRA	Steady-state	CVEL	Checked (=1)	URHOWØ	0
CDEAD	solute transport	CDUDC	(1, 1, 1, (1))	DDWDU	0
CREAD	Cold start (first	CBUDG	Checked (=1)	DRWDU	0
	time step of a simulation) (1)				
UP	0	ISTORE	9999	VISCØ	1
GNUP	0.1	Root file	(empty)	COMPMA	0
01101		name	(0		°
GNUU	1.0	Solution type	Noniterative	CS	0
			solution		
ITMAX	1	ITRMAX	1	SIGMAS	0
DELT	1	RPMAX	0	RHOS	2600.0
TMAX	1.0	RUMAX	0	ADSMOD	NONE
ITCYC	9999	CSOLVP	DIRECT	CHI1	0
DTMULT	1.0	ITRMXP	300	CHI2	0
DTMAX	1e99	ITOLP	0	PRODFØ	0
NPCYC	1	TOLP	1E-8	PRODSØ	0
NUCYC	1	NSAVEP	10	PRODF1	0
TSTART	0	CSOLVU	DIRECT	PRODS1	0
NPRINT	9999	ITRMXU	300	GRAVX	0
NCOLPR	9999	ITOLU	0	GRAVY	0
LCOLPR	9999	TOLU	1E-8	GRAVZ	0

Table 3. Default Values for SUTRA Project Information dialog box for General Case<sup>1</sup>

<sup>1</sup> Values in mks units (also known as SI units).

Note: Default values are only initial suggestions, and must be checked and reset, as needed, by the user to appropriate values for the user's project.

~ -		~ -				8	-	~	
Solute tr	-	Solute tra	-	Thermal		Saturated- Saturate		•	
with va		with cor		trans	port	unsaturated flow flow		W	
dens		dens	- 2						
Variable	Default	Variable	Default	Variable	Default	Variable	Default	Variable	Default
SIGMAW	1.0E-9	SIGMAW	1.0E-9	CW	4182.0	IUNSAT	1	IUNSAT	0
RHOW0	1000.0	RHOW0	1	SIGMAW	0.6	ITRMAX	2		
DRWDU	700.0			RHOW0	1000.0			-	
VISC0	0.001			URHOW0	20				
		-		DRWDU	-0.375				
				CS	840.0				
				SIGMAS	3.5				
GRAVY	-9.81			GRAVY	-9.81				
	(for 2D)				(for 2D)				
	0				0				
	(for 3D)				(for 3D)				
GRAVZ	-9.81			GRAVZ	-9.81				
	(for 3D)				(for 3D)				

Table 4. Default Values<sup>1</sup> for SUTRA Project Information dialog for Special Cases<sup>2</sup>

<sup>1</sup> Values in mks units (also known as SI units).

<sup>2</sup> Only values that differ from the defaults in Table 3 are listed.

Note: Default values are only initial suggestions; the user must check and reset these to appropriate values for the user's project.

The following sections provide detailed descriptions of the panes in the **SUTRA Project Information** dialog box.

# About Pane

The **About** pane provides information about the current version of **SutraGUI** and information about SUTRA and Argus ONE documentation. Clicking on a URL in the **About** pane will activate the default web browser and cause it to load the URL that was clicked.

# Model Configuration

The **Model Configuration** pane allows the user to do the following:

- choose the type of simulation problem to be solved with SUTRA,
- set up **SutraGUI** to include the appropriate geospatial *Information* layers, and
- set names of layers and parameters to be appropriate for the chosen problem type.

For example, an areal problem using head will include an *Information* layer called **Hydraulic Conductivity** and refer to "Hydraulic Head" whereas a cross-sectional problem with variabledensity fluid will have a layer called **Permeability** and refer to "Pressure". An unsaturated problem will include an *Information* layer called **Unsaturated Properties** but a saturated-only problem will not have such an *Information* layer.

The SUTRA code solves general equations for flow and transport allowing much flexibility in problem type. This is reflected in the choices available in the **Model Configuration** pane. Internally, the SUTRA code works with its original set of variables, pressure and permeability,

but for the model setup, **SutraGUI** can translate these into the simpler quantities hydraulic head and hydraulic conductivity for ease of use. Should the user prefer to work with the original SUTRA variables, and have access to all possible *Information* layers for SUTRA at once, the "General" option should be selected. Should the user prefer to configure **SutraGUI** for a certain type of problem, the "Specific" option should be selected. This makes available a set of choices to the user in the lower portion of the window, allowing the user to specify the problem type, and the type of meshing. The user may also specify the name and path of the SUTRA executable program on this pane.

## **Orientation of Model**

There are four possible orientations of a model:

- AREAL
- CROSS-SECTIONAL OR DIPPED
- THREE-DIMENSIONAL MODEL (VERTICALLY ALIGNED)
- THREE-DIMENSIONAL MODEL (NONALIGNED)

**AREAL** models are 2D, perfectly horizontal models for constant-density solute transport under saturated conditions (for example, used for typical contaminant plume problems or tracking of natural tracers).

**CROSS-SECTIONAL or DIPPED** models are 2D, vertical cross-sectional models, or nonhorizontal models that potentially allow unsaturated conditions with variable-density solute or energy transport. The gravity vector components in such non-horizontal models can be nonzero, in contrast with AREAL models, in which gravity components are always set to zero. The gravity components for CROSS-SECTIONAL OR DIPPED models would be set to zero if the user is solving for hydraulic head, rather than pressure.

**3D VERTICALLY ALIGNED** models are 3D models in which the X and Y coordinates of all the nodes in each layer of the mesh are at the same X and Y coordinates as the corresponding nodes in all the other layers.

**3D NONALIGNED** models are 3D models in which the X and Y coordinates of all the nodes in each layer of the mesh need not be at the same X and Y coordinates as the corresponding nodes in one or more of the other layers. However, the number of nodes and elements and their pattern of connectivity is the same for all layers, as these are for the VERTICALLY ALIGNED meshes.

## Flow Conditions

The flow conditions in a model may be either **SATURATED** or **SATURATED**. **UNSATURATED**.

- In **SATURATED** models, only saturated conditions are allowed.
- In **SATURATED-UNSATURATED** models, unsaturated conditions can potentially occur in the model. Saturated-unsaturated conditions are used specifically for problems of unsaturated flow and transport.

# **Transport Conditions**

Transport conditions in a **SutraGUI** model may be any of the following:

- **SOLUTE (Variable-density fluid, using Pressure)**. This is for transport problems where solute concentrations affect fluid density. (For example, this can be used for typical saline fluid-intrusion problems or flow near salt domes.)
- **SOLUTE (Constant-density fluid, using Hydraulic Head)** This is for transport problems where solute concentrations do not affect fluid density. (For example, this can be used for typical contaminant plume problems.)
- **ENERGY (Variable-density fluid, using Pressure)** This is for transport problems where temperature changes are to be tracked in the subsurface and where temperature potentially affects fluid density. (For example, it can be used for hydrothermal convection problems, tracking seasonal surface-water recharge, or aquifer energy storage.)

## **Model Thickness**

Model thickness is only used for 2D models.

- If **USER-SPECIFIED** is selected, the user must specify the model thickness in a geospatial *Information* layer. The thickness may be constant or variable. If, conceptually, a thickness is not required, the user should enter a uniform thickness such as 1.
- If **CYLINDRICAL** is selected, model thickness is automatically set such that a radial cross-sectional flow field is obtained. Cylindrical thickness is used for vertical cross sectional simulations only. Thickness at each SUTRA Mesh node is automatically set to 2 X, where X is the radius (the X-coordinate, must be positive or zero) of the node. Most often, the left edge of a cylindrical model would be a vertical line at X = 0, although this is not a requirement.

# Type of Meshing

Two types of mesh are permitted by **SutraGUI:** FISHNET and IRREGULAR.

- With **FISHNET** meshing, the mesh consists of *superblocks* (large contiguous quadrilaterals) each subdivided into a specified number of rows and columns of quadrilateral finite elements. The mesh is created by **SutraGUI** and not by Argus ONE. Detailed instructions for creating such meshes may be found in the section describing the SUTRA Model layer, "**FishNet\_Mesh\_Layout**." FishNet Meshes are presently required for 3D SUTRA models but are optional for 2D models.
- With **IRREGULAR** meshing, the mesh consists of irregularly connected quadrilateral elements created by Argus ONE's quadrilateral meshing engine. Irregular meshes may only be used with 2D models.

# Headings

On the **Headings** pane, two lines of text may be specified that will be used as the title on most SUTRA output files: "lst", "nod", "ele" and "obs".

There is also a text field that may be used to record a description of the project. However, this description is never exported to the SUTRA input files and only appears within **SutraGUI**.

# Structure in Z (3D Only)

The **Structure in Z** pane is only available for 3D models. It is used to control the number of model units in the Z-direction and the discretization within each unit in the Z-direction. Most often in a 3D model, each unit will be a hydrogeologic unit and the Z-direction will be the vertical direction (vertically upwards).

The number of units can be changed either by changing the number displayed in the edit box labeled **Number of Units** or by clicking on the **Delete**, **Insert**, or **Add** buttons. Clicking the **Add** button will add one unit at the bottom of the layer structure. Clicking the **Delete** button will delete the selected unit. Clicking the **Insert** button will insert a unit above the selected unit. Units can also be renamed.

Once the mesh has been created as described in the "SUTRA Mesh" section of this report, the number of nodes and number of elements are displayed on **Structure in Z** pane.

# 3D Surfaces and Objects (3D Only)

The **3D** Surfaces and Objects pane is only available for 3D models. This pane allows the user to select the types of boundary condition, source and observation *Information* layers that appear in the 3D project and are thus available to the user. These *Information* layers have two primary types in 3D: 1- 'In-Surfaces' - layers that will allow boundary conditions, sources or observations to be specified exactly within the model top or within the bottom surfaces of units, and 2- '3D Objects' - layers that will allow boundary conditions, sources or observations to be specified within certain geometric shapes (listed below) that may be placed anywhere in the 3D model domain and the space surrounding it. Thus, the user may choose to specify boundary conditions, sources, or observations in two ways: those that occur exactly on the top or bottom surfaces of units, and those that occur (as 3D objects) anywhere in the 3D model domain.

'3D Objects' - Boundary conditions, sources, and observations that are not exactly located on the top or bottom surfaces of units may be specified as any of five types of 3D objects, **points**, **lines**, **vertical sheets**, **slanted sheets**, and **solids** (for example, points, lines and solids may be used to represent wells). The table on the upper half of the pane allows the user to select the number of Argus ONE layers for each type of object and each type of condition. The table lists the type of 3D object in separate columns and the type of condition to specify in separate rows. The user should specify the number of the Argus ONE layers to be created for each object in the appropriate cell of the table. The layers appear in Argus ONE after **OK** is clicked. The layers may be removed by specifying the value, '0', and the number of layers can be changed at any time. Information in removed layers is lost.

Note: The reason for possibly needing multiple Argus ONE layers for the same 3D object is as follows. Argus ONE allows the user to draw the location of a 3D object only in 2D

map view. Argus ONE does not allow contours describing objects to overlap. If the same condition is required at various Z coordinates, but the objects overlap when seen in map view, each overlapping object must be defined in its own Argus ONE layer to avoid overlap in any layer.

'In-Surfaces' - The lower half of the pane concerns boundary conditions, sources, and observations that are located exactly within the top or bottom surfaces of units (for example, recharge at the top of the model, in the **Sources of Fluid Top** layer). The tree control in the lower half of the pane has a list of units. Within each unit, there is a list of the Argus ONE layers that can appear on the top or bottom of the unit. These layers allow the user to specify boundary conditions, sources, and observations on the tops or bottoms of units. The list of layers may be displayed by clicking the plus sign next to the unit. If the check box next to a layer name is checked, an Argus ONE layer with that name will be included in Argus ONE layer structure after **OK** button is clicked. These layers can be removed from the Argus ONE layer structure by unchecking the check box. Information in removed layers is lost.

Note: Each unit in a 3D SUTRA model has an upper and lower surface. Each of these surfaces need not be a horizontal plane, and may vary in elevation along the surface. The top of each unit is exactly the same surface as the bottom of the unit above it. Because of this, the complete list of Argus ONE layers includes only the bottoms of all units and the top of the uppermost unit (the top of the model domain).

## Modes, Numerical Controls

The Modes, Numerical Controls pane contains two parts: Simulation Mode Options, and Numerical Control Parameters.

# **Simulation Mode Options**

Each of the boxes in **Simulation Mode Options** allows selection of one the following:

- steady-state flow and steady-state transport, or steady-state flow and transient transport, or transient flow and transient transport,
- cold or warm start. (If a warm start has been selected, there will also be an edit box visible in which the user may select the restart file.)

Some options may be disabled depending on the options specified on the **Model Configuration** pane.

# Numerical Control Parameters

The controls in the **Numerical Control Parameters** box allow setting the upstream weight and boundary-condition factors for specified pressure, hydraulic head, concentration or temperature. Ideal selection of the GNUP will cause the simulated pressure to match specified values of pressure at the boundaries to match to six or seven decimal places. Ideal selection of the GNUU will do the same for temperature or concentration. If the simulated and specified values match more closely than that, the flux at the boundary node may not be calculated with sufficient precision. (The reader is referred to Voss and Provost, 2002, for more information.)

Note: The **CheckMatchBC** program distributed with **SutraGUI** may be used to judge whether these criteria have been met after running SUTRA. (The reader is referred to Appendix B.)

The fractional upstream weight (UP) can be used to help control oscillations in the SUTRA transport solution. (The reader is referred to Voss and Provost, 2002, for more information.)

# **Temporal Controls**

The **Temporal Controls** pane is only available if either flow or transport is transient. The controls in the **Temporal Control and Solution Cycling Data** pane determine the duration of the simulation, the size of the time steps, and the cycling of flow and transport solutions.

# Initial Condition Controls

The controls on the **Initial Condition Controls** pane allow users to specify how to use SUTRA restart files as initial conditions for a simulation and to select the starting time of the simulation clock.

**Simulation Starting Time** is the elapsed time at which the initial conditions for simulation are specified. For a cold start, this is usually 0 but it may also be set to a particular starting year (specified in seconds). Argus ONE writes this value to the SUTRA input data set.

The radio buttons under **Read initial conditions from restart file** determine how the restart file will be used. By default, the file is not read. The user may select to read the pressure, concentration (or energy), or both from the restart file. When initial conditions are read from the restart file, the information in the respective Argus ONE initial conditions *Information* layer is ignored when preparing the SUTRA input files.

For 3D models, the user also has the option of interpolating pressure and/or concentration (or energy) results from a simulation on a previously used mesh for use as initial conditions for a new mesh. Finite-element basis functions (equivalent to those used in SUTRA) are used for interpolations to locations that are inside the old mesh. For locations outside the old mesh, the average value at the four nearest nodes in the old mesh is used. Generally, this option would be used to set the initial conditions after refining the mesh. It may require a long execution time by **SutraGUI**.

For 2D models, a similar effect can be accomplished by using an Argus ONE expression to link the initial conditions to data imported into Argus ONE in the process of creating a contour map or other post-processing chart, although Argus ONE interpolation, rather than finite-element interpolation would be used in this case.

# **Output Controls**

The controls under **Output Controls** allow control of the frequency with which output is produced and control what type of output is generated.

If the result of the present simulation is intended for use as an initial condition in a future simulation, the **Save for Restart Option** can be used to control the frequency with which data for the initial conditions will be stored.

# Iterations for Nonlinearity

The radio buttons on the **Iterations for Nonlinearity** pane control iterations for nonlinearities in the system, such as in nonlinear sorption, energy transport, variable-density transport, and unsaturated models.

# Solver Controls

The radio buttons on the **Solver Controls** pane are used to determine the type of matrix-equation solver for the pressure (or head) and solute (or energy) solution. They allow a choice of using a noniterative (direct) or iterative matrix-equation solver. If an iterative solver (CG, GMRES, or ORTHOMIN) is selected, the iteration-control parameters must be entered.

# Fluid Properties

On the **Fluid Properties** pane, values are entered for the properties of the fluid and for the parameters describing the linear dependence of density on concentration or temperature.

# Solid Matrix, Adsorption

Under Solid Matrix Properties, the user enters values for the properties of the solid matrix.

Under Adsorption Parameters the user may choose the equilibrium adsorption isotherm: NONE, LINEAR, LANGMUIR or FREUNDLICH. Depending on the isotherm selected, zero, one, or two additional parameters defining the isotherm must be specified.

# Production, Gravity

Under **Production of Energy or Solute**, the user enters values for the zero-order and first-order production rates.

Under **Gravity Vector**, the user enters values for the X and Y components and additionally for 3D, the Z components of the gravity vector.

# SutraGUI Configuration

In the **SUTRA Path** edit box, the user specifies the full path of the SUTRA program. A **Browse** button next to the edit box can be used to select the full path of the SUTRA program interactively.

Load/Save Default Initial Values for SUTRA Project Information is for advanced users only and deals with the ".val" file. This file contains information about all the controls in the SUTRA Project Information dialog box. If the user clicks on the Save Val File button and uses the default file name and location, a file will be created with the extension ".val." When any new SUTRA models are started within Argus ONE, this file is read and the same options for the SUTRA Project Information are set in the new model. If the user clicks on the Save Val File button and does not use the default file name and location, the ".val" file is not used to set the defaults for all future models. However, the file can then be opened by clicking the Open Val File button and selecting the file. The file is then used to set all the defaults in the current model.

## Problem

The **Problem** pane only appears if **SutraGUI** encounters a problem reading a file. If this pane appears, the best thing to do is to close the model *without saving it* and contact technical support at rbwinst@usgs.gov (as of 2003).

#### Parameter Values – Quick Set

The **Parameter Values – Quick Set** button at the bottom of the **SUTRA Project Information** dialog box opens a separate dialog box that is used to set the values of Argus ONE parameters quickly without entering the Argus ONE *Layers* dialog box. This is convenient, particularly when the same value has to be set for a given parameter in many units in a 3D model (for example, hydraulic conductivity). For new models (before the **SUTRA Project Information** dialog box is exited the first time by clicking **OK**), the value that is entered is the value that will be used. For existing models, it is necessary to click on the **Set Now** button to the left of the appropriate edit box to set the parameter value. The **Set Now** button will appear in **bold text** indicating that it needs to be clicked in order to set the value, and after clicking, the text reverts to the normal font.

Note: It is possible to use Argus ONE expressions, rather than numbers, as values in the boxes. It is advisable to create the expression within the Argus ONE Expression editor for a parameter (found in the Layers dialog) so that the expression has correct syntax, and then copy it into the desired box of the **Parameter Values – Quick Set** pane. Incorrect values entered in the **Parameter Values – Quick Set** pane will appear as expressions in the Layers dialog box and will give incorrect results. The reader is referred to the Argus ONE User's Guide (Argus Interware, 1997) and Winston (2001) for methods of setting parameter Expressions.

# The Argus ONE Window and Argus ONE Layers

Following exit from the **SUTRA Project Information** dialog box, described above, the standard Argus ONE window appears. This window contains many controls for the user environment, and these are all described in the Argus ONE documentation. Only controls that are specifically related to use of the interface for SUTRA simulations are described in this report.

At this point, there will actually be two overlaid windows, the original "Untitled" window, and a new "Untitled1" window that contains the layer structure for a SUTRA model. The user may wish to close or minimize the original "Untitled" window so as not to confuse the two.

For convenience, the new "Untitled1" window may be maximized to full screen by clicking the maximize button containing an upward pointing triangle in the upper-right corner of the window. The appearance of this button may vary depending on the operating system being used.

Prior to creating or importing information in geospatial *Information* layers, the user should decide on and possibly specify the drawing size of the workspace, and the scale and units of the modeling project. These project parameters can also be changed automatically when importing information that extends beyond the specified ranges.

This information can be entered from the *Drawing Size*... and *Scale and Units*... commands in the *Special* pull-down menu found along the top of the Argus ONE window.

Note: the view of the workspace may be exaggerated or reduced in either direction by selecting Non-uniform: in the Scale and Units dialog box. This is often required for cross-sectional models. Note that this also affects the shape of elements generated in an irregular mesh.

**SutraGUI** assumes that all data are referenced to the same reference elevation or datum. For areal problems, the datum is arbitrary. For cross-sectional problems, the datum is given by the coordinate system selected by the user in the *Scale and Units*... commands in the *Special* pull-down menu along the top of the Argus ONE window. For 3D problems, the X and Y coordinate plane, as viewed on the monitor, may be oriented in any direction in space. However, for most problems, it is recommended that X be directed east, Y north, and Z outward from the screen, representing elevation.

The Argus ONE User's Guide (Argus Interware, 1997) provides information on setting attributes in the dialog boxes that appear when the above commands are used.

## Saving and Retrieving Projects

The nonspatial information for the SUTRA simulations and all information entered into the geospatial *Information* layers in Argus ONE are saved by using the *Save* or *Save As...* command in the *File* menu along the top of the Argus ONE window.

The default extension for the Argus ONE saved project file names is ".mmb."

Starting Argus ONE and opening an existing project file containing SUTRA simulation information (by selecting *Open* in the *File* menu) will retrieve all of the nonspatial project information into the **SUTRA Project Information** dialog box and all of the geospatial information into Argus ONE layers that was entered previously. This returns the user to the same state as when the project was saved.

Saving the project after exiting the **SUTRA Project Information** dialog box and saving regularly during input or edit of geospatial information is a good practice that will protect the user from the need to re-enter data in case of user errors or system problems.

## Layers' Floater Window

The *Layers' Floater* window, which displays a list of available GIS coverages (layers) for the chosen type of SUTRA simulation, may be displayed by clicking on the *Layers*... button along the top of the window. This window is referred to in the Argus documentation as the "*Layers' Floater*" (fig. 12).

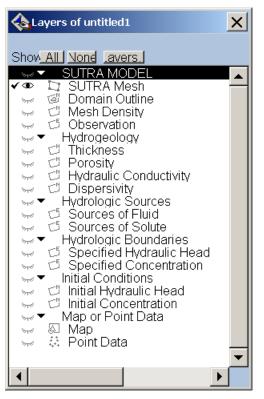


Figure 12. Layers' Floater window

The *Layers' Floater* may be resized to show all of the available layers by dragging and stretching the window from one of the lower corners with the mouse. The window may be moved to cover the unneeded gray area that may appear (depending on the size of Argus work area and on whether screen resolution is high enough) on a side of the Argus ONE window by holding down the mouse button on the top bar and dragging it to this location.

The *Layers' Floater* organizes the available coverages into groups or sublists including: SUTRA Model layers, various Geospatial *Information* layers, and Map or Point Data layers. These are described in detail in the next section "Specifying Spatial Data / Layer Descriptions." The Layer List window also shows the interpretation type (as described in Argus ONE User's Guide (Argus Interware, 1997)).

Opening the list allows the user to see all available layer names within any group. To open or close groups, click on the triangle to the left of the group name. To close an expanded list, click again on the same triangle.

The "eye" icon  $\circledast$  to the left of a layer name in the Layer List window indicates whether a layer is visible. To toggle the visibility of a layer, click on the "eye" icon.

A check mark to the left of a layer name indicates that the layer is the active layer: the layer that receives input from the user. To make a layer active, click in the empty space where the check mark would be. Only one layer can be active at a time.

# Specifying Spatial Data / Layer Descriptions

The arrangement of layers in the SutraGUI list of layers is different in 2D models than it is in 3D models. The following sections describe the arrangement of layers in each.

After introducing each parameter in the following sections, units are given for the parameter in square brackets; for example, for **Permeability.maximum**, the units are given as  $[L^2]$  representing arbitrary length-units squared. Table 5 shows units used and displayed in the GUI with their meanings.

Unit Abbreviations	Unit Meaning
[C]	any consistent concentration units
[degC]	Celsius degrees
[degrees]	angle in degrees
[E]	any consistent energy units
[L]	length units
[M]	mass units
[s]	seconds (time)
[T]	temperature (Celsius)
[1]	unitless, like porosity
[1,0]	true or false
x^2, y^3	x quantity squared, y quantity cubed

Table 5. Unit Abbreviations and Unit Meaning

Parameter names such as **RESULTANT\_FLUID\_SOURCE**, that are uppercase are calculated or linked to other layer parameters. These should not be modified directly. Modifications to such parameters can be done by changing the lowercase parameters of the layers. Advanced users who understand the functions or references in these parameters may modify them to suit specific modeling needs. New users should consider parameters with uppercase names as "read-only" variables. Appendix 1, "Adding and Linking New Layers," explains how to add new layers and link the information from these layers into a SUTRA project.

Depending on the choice of problem type made by the user in the **Model Configuration** pane, some of the layer and parameter names and the units of the parameters will vary. All of the possibilities are included in the descriptions that follow.

# **Two-Dimensional Models**

The arrangement of layers in 2D models (Table 6) is similar to that used in Voss and others (1997). The *Information* layers for **SutraGUI** for 2D models are grouped in the Argus ONE *Layers' Floater* by general type: **SUTRA MODEL**, **Hydrogeology**, **Hydrologic Sources**, **Hydrologic Boundaries**, **Initial Conditions**, and **Map or Point Data**.

Layer Name		
SUTRA MODEL group		
SUTRA Mesh		
FishNet_Mesh_Layout		
Domain Outline		
Mesh Density		
Observation		
Hydrogeology group		
Thickness		
Porosity		
Permeability/Hydraulic Conductivity		
Dispersivity		
Unsaturated Properties		
Hydrologic Sources group		
Sources of Fluid		
Sources of Solute/Sources of Energy		
Hydrologic Boundaries group		
Specified Pressure/Specified Hydraulic Head		
Specified Concentration/Specified Temperature		
Initial Conditions group		
Initial Pressure/Initial Hydraulic Head		
Initial Concentration/Initial Temperature		
Map or Point Data group		
Map		
Point Data		

Table 6. SutraGUI Layer Structure for Two-Dimensional Models

The *Information* layers within the **Hydrogeology** and **Initial Conditions** layer groups are initially assigned the interpretation method *Nearest Contour*. The *Information* layers within the **Hydrologic Sources** and **Hydrologic Boundaries** layer groups are assigned the interpretation method *Exact Contour*. However, the **Unsaturated Properties** layer in the **Hydrogeology** layer group is an exception and it is assigned the *Exact Contour* method.

Note: Some user experimentation with the interpretation methods may be necessary to achieve the best possible spatial distribution for a given parameter.

Each parameter of each layer is assigned a default expression by **SutraGUI**. The expression usually specifies a constant value of a parameter for the entire workspace that is assumed in case no other user input is provided for that parameter. For some parameters, the default expressions are complicated and involve mathematical operations on other data in the model. The values initially specified for parameters by **SutraGUI** are shown in Table 7.

Layer	Parameter	Value <sup>1</sup>
FishNet_Mesh_Layout	elements_in_x	\$N/A
-	elements_in_y	\$N/A
Domain Outline   unused layer1	element_size	0
Mesh Density   unused layer2	element_size	0
Observation	is_observed	0
Thickness	thickness	1
Porosity	porosity	0.1
Permeability or Hydraulic Conductivity	maximum	1.0E-10 or 1.0E-3
	minimum	1.0E-10 or 1.0E-3
	angle_of_max_to_x_axis	0
Dispersivity	longdisp_in_max_permdir	0.5
	longdisp_in_min_permdir	0.5
	trandisp_in_max_permdir	0.5
	trandisp_in_min_permdir	0.5
Unsaturated Properties	region	0
Sources of Fluid	total_source	\$N/A
Sources of Energy or Sources of	specific_source	\$N/A
Solute	concentration_of_source or temperature_of_source	\$N/A
	time_dependence	0
	total_source	\$N/A
Specified Pressure or Specified Hydraulic Head	specific_source	\$N/A
Hydraulic Head	time_dependence	0
	specified_pressure or specified_head	\$N/A
Specified Concentration or	concentration or temperature	\$N/A
Specified Temperature	time_dependence	0
	specified_pressure or specified_head	\$N/A
Initial Pressure or Initial Head	time_dependence	0
	initial_pressure or initial_head	0
Initial Concentration or Initial Temperature	initial_concentration or initial_temperature	0

Table 7. Default Background	Values for	<b>User-Specified Layer Parameters</b>

[\$N/A is a flag for an unassigned variable.]

<sup>1</sup>Note: Default values are only initial suggestions. These must be checked and reset, if needed, by the user to appropriate values for the user's project.

## **SUTRA MODEL**

SUTRA MODEL is a group of layers that define the geometry and discretization of the SUTRA simulation model, and the locations in the model where observations of results will be made. These include the layers **Domain Outline**, **Mesh Density**, **FishNet\_Mesh\_Layout**, and **SUTRA Mesh**, and **Observation**. Not all of these layers are always present. The **FishNet\_Mesh\_Layout** layer is included in the group only when the user-specified **SUTRA Project Information** dialog box specifies a FishNet Mesh, and in this case, some unneeded layers are renamed as **unused layer1** and **unused layer2**.

#### SUTRA Mesh

The **SUTRA Mesh** layer is the layer on which the mesh used in the model is defined. For 2D models, the mesh on a **SUTRA Mesh** layer can be either an irregular mesh or a "FishNet" mesh. The FishNet mesh case is described in the section of this report entitled "FishNet\_Mesh\_Layout" on page 42.

An irregular mesh can be generated automatically using the magic wand tool from the tool palette at the left side of the Argus ONE window as discussed in the Argus ONE User's Guide (Argus Interware, 1997). The User's Guide also explains how to inspect nodal and element geometries and parameters, to move nodes, and to override (change) node or element parameter values that were automatically assigned by Argus ONE. To generate an Irregular Mesh, make the **SUTRA Mesh** layer active, click on the magic wand tool, and then click the magic wand cursor within the area of the domain boundary. Argus ONE then generates a mesh according to the density information contained in the **Domain Outline** layer and, if specified, in the **Mesh Density** layer.

If a mesh already exists in the layer, then the user is prompted to accept deletion of all existing elements before the new mesh is generated. If the view has been rescaled by user selection of *Non-uniform* in the Argus ONE *Scale and Units* dialog box, then elongated elements are produced in an irregular mesh. Horizontally long elements are often appropriate for cross-sectional modeling of aquifer systems.

In some cases, elements with very small or very large angles may be created during the meshing process. Such elements can be found by selecting *Edit*|*Select Acute Elements*. If some exist, the mesh may be manually adjusted or the meshing preferences, which control a scan for odd-shaped elements, may be changed by selecting *Special*|*Preferences* and changing some of the items in the dialog box.

In 2D models, the **SUTRA Mesh** layer contains values for all of the spatially distributed parameters required for running a SUTRA simulation, through references to and functions of the other layers. In 3D models, the **SUTRA Mesh** layer or layers contains values of all the spatially distributed parameters except boundary conditions and observations. Depending on SUTRA's requirements for each parameter, as specified in the documentation for the SUTRA input data sets (Voss and Provost, 2002), a parameter may receive a value for each node or for each element in the mesh. These values are derived from the various *Information* layers described in following sections. The Argus ONE environment refers to the assignment of values in one *Information* layer to another as "linking." The names of the parameters of the **SUTRA Mesh** layer are listed in Table 8. The full Argus ONE name of each parameter is given as

"Layer.Parameter," for example, the first parameter, **NREG**, in the table is **SUTRA Mesh.NREG**.

The uppercase names of **SUTRA Mesh** parameters correspond exactly with variables used by the SUTRA model, and are described in the SUTRA documentation. There is one exception to the above. The SUTRA parameter, **UBC**, representing the concentration or temperature of any fluid that may flow into the model at a node where pressure or hydraulic head is specified, has been changed to **pUBC** in **SutraGUI** to distinguish it from the specified concentration or temperature boundary condition type, which retains its original name (**UBC**).

Two of the **SUTRA Mesh** parameters, **QIN** and **QUIN**, a fluid source and energy or solute source, respectively, have additional logic associated with their values. As noted in the description of the **Sources of Fluid** and **Sources of Energy** or **Sources of Solute** layers, to which these node-wise parameters are linked, these sources may be specified at point, line (open) or closed contours. Depending on which type of contour is specified in the "**Sources**" layer, the resultant source value provided as a parameter in the "**Sources**" layer may require multiplication by the open contour length or closed contour area associated with the node; these multiplications are carried out automatically.

The Z parameter on the SUTRA Mesh layer represents the thickness of the model.

*Note: The properties assigned to any node or element may be viewed (and modified) by double-clicking on the element of interest while the* **SUTRA Mesh** *layer is active.* 

Name	
NREG	
Z	
POR	
LREG	
PMAX	
PMIN	
ANGLE1	
ALMAX	
ALMIN	
ATMAX	
ATMIN	
QIN	
UIN	
time_dependent_fluid_sources	
QUIN	
time_dependent_energy_or_solute_sources	
PBC	
pUBC	
time_dependent_specified_head_or_pressure	
UBC	
time_dependent_specified_concentration_or_temperatu	re
PVEC	
UVEC	
INOB	

 Table 8. SUTRA mesh parameters used in two-dimensional (2D) simulations

## FishNet\_Mesh\_Layout

The **FishNet\_Mesh\_Layout** layer is included only when it is selected in the **SUTRA Project Information** dialog box. **SutraGUI**, rather than Argus ONE, creates FishNet meshes. A FishNet Mesh consists of superblocks (large contiguous quadrilaterals) each subdivided into a specified number of rows and columns of quadrilateral finite elements. This layer, like the **SUTRA Mesh** layer, is a Quad-Mesh layer. However, the elements on it must be drawn manually or imported, rather than being generated automatically by Argus ONE. Each element of the mesh will describe one "superblock" of the **SUTRA Mesh**. The "superblocks" describe the external and internal boundaries of the FishNet Mesh. Each superblock element contains information describing the desired number of quadrilateral finite elements that will fill the superblock in the X and Y directions when the mesh is generated. The use of the **FishNet\_Mesh\_Layout** layer is described in the section of this report entitled "Creating FishNet Meshes" on page 67.

#### Domain Outline

The **Domain Outline** is a special Argus ONE layer type used to define the maximum areal extent of the simulated region when an irregular mesh is used. The outermost contour on the **Domain Outline** will exactly contain the entire finite-element mesh that is generated. Any closed contours inside the outermost one will represent areas where no mesh will be generated (fig. 13). Geospatial information coverage in other layers is required everywhere within the domain outline for the finite-element mesh, and may extend areally beyond the domain outline. If a FishNet mesh is used, SutraGUI does not need a **Domain Outline** layer but one is still needed by Argus ONE. In such cases, the layer is renamed **unused layer1**.

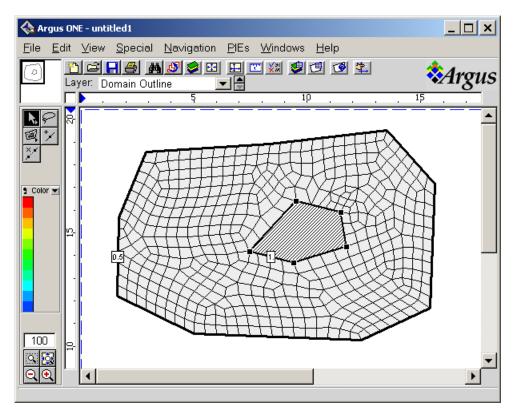


Figure 13. Domain Outline; an example showing vertices on a closed contour and the mesh generated by Argus ONE showing area where no mesh was generated.

The contours in the **Domain Outline** layer contain information controlling the size of finiteelements in an irregular mesh. The **element\_size** defines the desired nominal size of elements in the discretization. This information, in conjunction with the layer **Mesh Density** and the geometry of objects in these layers, determines the distribution and size of mesh elements. Mesh density is strongly affected by the proximity of contours and the size of contour segments, as described in the Argus ONE User's Guide (Argus Interware, 1997). (The **Mesh Density** layer is usually used to refine the discretization in select areas of the model domain and is described below.)

Point and open contours may be specified in the **Domain Outline** layer. Although these do not determine the external boundaries of the mesh, they may be used to define the nominal size of elements along these objects. Nodes and edges of elements will fall exactly along these contours when the mesh is generated.

*Note:* In 2D models, any point or contour objects that must correspond with node location, such as contours in the **Sources of Fluid** layer, must be copied to the **Domain Outline** layer before a useful mesh can be generated. This is not required for 3D models.

The procedure for creating a domain outline follows.

- 1. After the **Domain Outline** layer has been made active, the closed contours in the **Domain Outline** layer can either be generated with the contour drawing tool in the tool palette at the left of the Argus ONE window or they can be imported from text, DXF, or ArcView Shape files.
- 2. To draw a domain-outline contour manually, first click on the closed-contour drawing

tool  $\square$ . To specify the contour's position and shape, click in the white work area of the window in a sequence of positions to form a nearly closed contour. To close the contour, double-click on the last position desired, then move the mouse away from the last point. The contour automatically closes and the *Contour Information* dialog box appears (fig. 14).

Contour Information		
Please enter value for contour:	this	OK Cancel
Contour is:	Closed	
Number of vertices:	45	
Contour area:	121.74	
Contour perimeter:	56.9618	
Contour name:		
Icon: None	A Volue	
Icon: None Parameter element_size	<b>∦</b> x  Value	Units

Figure 14. Contour Information dialog box.

3. This dialog box is used to specify the size of quadrilateral elements. An **element\_size** must be specified that refers to the desired typical size of an element side (in the distance units specified for the project). This number is typed into the data box to the right of the word, "**element\_size**" and just below the label, "Value." In <u>figure 14</u>, an **element\_size** value of 0.5 is specified. Click the OK button to exit the dialog box, and draw additional contours if desired.

Note: Argus ONE User's Guide (Argus Interware, 1997) refers to element\_size as mesh density.

4. To draw an open or point contour, click and hold the mouse button down over the contour drawing tool (<u>fig. 15</u>) and make a selection from the menu that appears. Click in the white work area to draw the selected type of contour. The *Contour Information* dialog box will appear again when the contour is completed for entry of the **element\_size** value.



Figure 15. Contour Tool.

5. Double-clicking on any contour brings back the *Contour Information* dialog box allowing modifications to be made to the values assigned to the object.

More information on drawing contours and on the drawing tools may be found in the Argus ONE User's Guide (Argus Interware, 1997).

Note: Argus ONE requires that the **Domain Outline** and **Mesh Density** layers be present even when the model uses a FishNet Mesh. However, these are ignored in this case. The layers have been renamed "**unused layer1**" and "**unused layer2**" to indicate that they are not to be used. The reader is referred to the **FishNet\_Mesh\_Layout** layer description on page 42 for more information on creating FishNet meshes.

#### Mesh Density

**Mesh Density** is an Argus ONE *Information* layer that is used by the **SUTRA Mesh** layer to define the refinement of the finite-element mesh in an irregular mesh (in addition to the **element\_size** information contained in the **Domain Outline** layer). This layer may contain point contours (that is, points), open contours, and closed contours representing the spatial distribution of **element\_size** desired by the user. Each contour has a value of the **element\_size** associated with it and together, the contours on the **Domain Outline** and **Mesh Density** layers (together with parameters in the Argus ONE *Preferences* dialog box regarding meshing preferences)

define the **element\_size** throughout the mesh. If a FishNet mesh is used, SutraGUI does not need a **Mesh Density** layer but one is still needed by Argus ONE. In such cases, the layer is renamed **unused layer2**.

When regions where increased or decreased discretization within the model domain are desired by the user, the spatial distribution of **element\_size** may be defined in the **Mesh Density** layer. The **element\_size** along the domain boundary will still be based on the value and node-spacing in the **Domain Outline** layer.

When the **Mesh Density** layer is active, as with all *Information* layers, the spatial distribution of **element\_size** may be imported from TEXT, DXF or ArcView Shape files. Alternatively, the point, line, and closed contour tools may be used to specify the approximate size of quadrilateral elements in regions of the modeled domain. After using one of the contour tools to draw a contour, the *Contour Information* dialog box appears where the **element\_size** is entered; the **element\_size** is the desired size of the quadrilateral elements in project units, prescribed at the contour just drawn. Examples of using the **Mesh Density** layer to specify the finite-element discretization may be found in the Argus ONE User's Guide (Argus Interware, 1997). If the **Mesh Density** layer contains no contours (no objects), then the **element\_size** specified for contours in the layer, **Domain Outline**, is used in creating the mesh and the **Mesh Density** layer is ignored.

#### **Observation**

The **Observation** layer is an *Information* layer that contains the spatial distribution of locations at which the user desires "observation-node output" from 2D SUTRA models. As described in the SUTRA documentation, this output provides a detailed time series of pressure, concentration, or temperature, and saturation at user-selected nodes at a user-selected time-step interval. This type of output is used for plotting time-draw down curves or solute breakthrough curves. **GW\_Chart** (Winston, 2000) can be used to prepare such charts (called 'hydrographs' in **GW\_Chart**) from the output.

It is possible to use point, open, or closed contours to specify where observations should be made during the SUTRA simulation. For each contour object, the value of the contour's parameter, **is\_observed**, must be set to "True" (or 1). The frequency of the observations is specified in the **Output Controls** pane of the **SUTRA Project Information** dialog box.

The Observation layer uses the *Exact Contour* method of interpretation so that observations are only defined inside of closed contours, or directly above open and point contours.

Nodes in the **SUTRA Mesh** layer falling within the selected areas or directly above the open or points contours will be marked as observation nodes for input to SUTRA.

For 2D models, note that for the point and open contours, nodes will fall exactly above these locations when the mesh is generated only if these contours are first copied to the **Domain Outline** layer. Information about copying and pasting objects in Argus ONE can be found in the Argus ONE User's Guide (Argus Interware, 1997). Alternatively, the command **PIEs**[Convert...]Mesh Objects to Contours... in the Utility PIE (Winston, 2001) can be used to copy nodes into *Information* layers.

# Hydrogeology

The **Hydrogeology** group of *Information* layers contains information on the spatial distributions of physical and material properties of the entire model.

#### Thickness

The layer **Thickness** contains information on the spatial distribution of the thickness of the 2D medium to be modeled. The layer contains only one parameter, **thickness** [L], which contains the thickness value.

#### Porosity

The **Porosity** layer contains information on the spatial distribution of the porosity of the porosity of the 2D region to be modeled. The layer contains only one parameter, **porosity** [fraction], which contains the porosity value.

# Permeability / Hydraulic Conductivity

The layer called **Permeability** (for cases using pressure) or **Hydraulic Conductivity** (for simulations using hydraulic head) contains information on the spatial distribution of the principal values of permeability/hydraulic conductivity, and the direction of the anisotropy for the medium to be modeled. The layer contains three parameters:

- **maximum** [L<sup>2</sup>] ([L/s] for hydraulic conductivity)
- **minimum**  $[L^2]$  ([L/s] for hydraulic conductivity)
- angle\_of\_max\_to\_x\_axis [degrees]

If the system is isotropic, the maximum and minimum values must be set equal to the desired value, and the angle may be set to any arbitrary number. It may be convenient for isotropic systems to link the value of one of the permeability minimum or maximum parameters to the other. The reader is referred to Appendix A, entitled "Adding and Linking New Layers" on page 106.

#### Dispersivity

The **Dispersivity** layer contains information on the spatial distribution of the longitudinal and transverse dispersivities of the system to be modeled. The layer contains four parameters:

- **longdisp\_in\_max\_permdir** [L] = longitudinal dispersivity for flow in the direction of maximum permeability
- **longdisp\_in\_min\_permdir** [L] = longitudinal dispersivity for flow in the direction of minimum permeability
- **trandisp\_in\_max\_permdir** [L] = transverse dispersivity in the direction of maximum permeability for flow in the direction of minimum permeability
- **trandisp\_in\_min\_permdir** [L] = transverse dispersivity in the direction of minimum permeability for flow in the direction of maximum permeability

The additional components of the dispersivity values in 2D models are extensions to the classical dispersion process provided by SUTRA (Voss, 1984; transverse extension added in 1990 revision). To obtain the classical dispersion model used by most other transport models, set the values of the longitudinal dispersivity parameters equal to each other, and the values of the transverse dispersivity parameters equal to each other.

#### **Unsaturated Properties**

The **Unsaturated Properties** layer is used to specify regions that have different unsaturated flow properties.

Note: Unsaturated-flow simulation with SUTRA requires some <u>user programming</u> in the SUTRA subroutine UNSAT for the user to specify the unsaturated functions for each region as described in Voss and Provost (2002). The FORTRAN source code for SUTRA and a FORTRAN compiler are required to use this feature. Because there is not a standard format for any additional information that must be read into the program for unsaturated properties, **SutraGUI** does not create input files for unsaturated flow properties. However, users may be able to create an export template for use within Argus ONE that will generate such files for their particular case, as described on p. 169-188 of the Argus ONE User's Guide (Argus Interware Inc., 1997).

The **Unsaturated Properties** layer contains information on the spatial distribution of regions having constant unsaturated properties in the unit to be modeled, or for generic studies, in the medium to be modeled. This layer only appears when a saturated-unsaturated problem type has been selected in the **Model Configuration** pane of the **SUTRA Project Information** dialog box. The layer contains only one parameter, region (an integer), which contains the identification number of the region. Usually the *Exact Contour* method should be used to define the location of regions in this layer, in which case only closed contours should be used for specifying regions. The *Exact Contour* method is already specified as the default selection for this layer. After closing a contour, the user must assign its region number in the Contour Information dialog box. Any number of contours may share the same region number. Each region represents one type of material having uniform unsaturated property functions. For example, region 1 may be fine silt, region 2 may be clay, and region 3 may be coarse sand. Each type of material may occur in a number of places within the model domain. The default region number is zero. To create regions that share a boundary (such as geologic layers), turn on the option Special Allow Intersection before drawing contours. If the user wishes to have nodes and element edges occur exactly at region boundaries, then for a FishNet Mesh, these boundaries need to be defined as the edges of superblocks in a FishNet Mesh layout. For an irregular mesh, these must be defined as open contours in the **Domain Outline** layer.

Note: The Argus ONE irregular meshing engine fills only the outermost closed contour on the Domain Outline layer with elements. Any interior closed contours are left empty (<u>fig. 14</u>). The recommended procedure is to define a nearly closed open contour in which the distance between the ends of the contour and the outside closed domain boundary contour is roughly the length of the side of a typical element.

## Hydrologic Sources

The **Hydrologic Sources** group of *Information* layers contains information on fluxes (quantity per time) of fluid, solute, and energy entering or leaving the 2D model domain. In these layers, **SutraGUI** allows specification of fluid sources or sinks and energy/solute sources or sinks at points, along line segments, and for delimited areas. Sources have positive values, whereas sinks are specified with a negative number. Sources of fluid may be either specified as a total amount of fluid per second (that is, **total\_source**), or as the total amount of fluid per second per length or area of the source object (that is, **specific\_source**). Similarly, sources of energy/solute may be either specified as a total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute may be either specified as a total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute may be either specified as a total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute per second per length or per area of the source object (that is, **specific\_source**).

Point sources may be assigned only a **total\_source**. These are created with the point contour drawing tool located along the left side of the Argus ONE window. Point sources typically represent injection or withdrawal wells for fluid sources. For irregular meshes, the points representing point sources must be copied to the **Domain Outline** layer to force a node in the finite element mesh to be located at each point source when the mesh is regenerated. Alternatively, the command **PIEs|Convert...|Mesh Objects to Contours...** in the Utility PIE (Winston, 2001) can be used to copy nodes into information layers as point contours. FishNet meshes must be designed such that the nodes fall exactly at the source locations.

Line or curve sources may be assigned either a **total\_source** or a **specific\_source**. These are created with the open contour drawing tool located along the left side of the Argus ONE window. A fluid line source may represent, for example, recharge occurring along a reach of a river or irrigation canal. Depending on whether the user knows the total recharge along the canal reach, or the recharge per length of canal, the user should specify either **total\_source** or **specific\_source** in the **Sources of Fluid** layer. The contours representing these sources must be copied to the **Domain Outline** layer to force nodes in the finite element mesh to be located along each source contour when the mesh is regenerated. Alternatively, the command **PIEs|Convert...|Mesh Objects to Contours...** can be used to copy nodes and the edges of elements into *Information* layers. FishNet meshes must be organized such that the nodes fall exactly at the source locations.

Area sources may be assigned either a **total\_source** or a **specific\_source**. These are created with the closed contour drawing tool located along the left side of the Argus ONE window. For fluid, an area source may represent, for example, ground-water recharge below a lake (**total\_source** could be specified for the entire lake as one object) or rainfall recharge rate (volume per area) for a particular area (**specific\_source** could be specified in units [L/s] for the object). For energy, an area source may represent, for example, heat production in a magma body (**total\_source** could be specified for the entire body as one object) or radiogenic heat production rate (energy per area) for a particular area (**specific\_source** could be specified in units [E/sL<sup>2</sup>] for the object).

Because contours may not cross one another in Argus ONE, only one type of object may be specified at any location. Furthermore, SUTRA accepts only one source per location; thus two sources, for example, rainfall and a well, cannot be specified separately at the same location, and must be summed externally by the user before entering values into **SutraGUI** for 2D meshes.

To obtain areally distributed values affecting nodes throughout the 2D mesh, rather than exactly along contours in these layers, an expression should be used for the **specific\_source** parameter. The reader is referred to the section of this report entitled "Adding a Precipitation Data Layer and Linking It to Fluid Sources Layer" on page 106.

# Sources of Fluid

The **Sources of Fluid** layer contains information on the spatial distribution of the fluid sources and sinks (such as wells and recharge from rainfall). Additionally the layer contains information on the solute concentration or temperature of the source fluids. The layer contains six parameters. However, two of these (the ones with the uppercase names) are automatically calculated by **SutraGUI** from the others and must not be altered by the user. For any given object in the layer, the user may only specify three of the remaining four parameters, because a choice must be made between **total\_source** and **specific\_source** as described above in the section of this report entitled "Total and Specific Sources" on page 14. When pressure has been selected as the hydraulic variable, fluid sources use units of [M/s]; when hydraulic head has been selected, units of  $[L^3/s]$  are used. The parameters for this layer are:

- total\_source [M/s] ([L<sup>3</sup>/s] when using hydraulic head)
- **specific\_source**  $[(M/s)/(L \text{ or } L^2)] ([(L^3/s)/(L, \text{ or } L^2)]$  when using hydraulic head)
- **concentration\_of\_source** [C] (or **temperature\_of\_source** [°C] for energy transport)
- **time\_dependence** [0 or 1]
- **RESULTANT\_FLUID\_SOURCE**
- QINUIN

# Sources of Solute / Energy

The **Sources of Solute** (or **Sources of Energy**) layer contains information on the spatial distribution of the solute (or energy) sources and sinks (such as dissolving minerals, radiogenic heat production, or thermal conduction through a boundary). The layer contains four parameters. However, one of these (the one with the uppercase name) is automatically calculated by Argus ONE from the others and may not be altered by the user. For any given object in the layer, the user may only specify two of the remaining three parameters, because a choice must be made between **total\_source** and **specific\_source** as described above in the section of this report entitled "Total and Specific Sources" on page 14. The parameters for this layer are:

- **total\_source** [C/s or E/s]
- **specific\_source** [(C/s or E/s)/(L or L<sup>2</sup>)]
- **time\_dependence** [0 or 1]
- RESULTANT\_SOLUTE/ENERGY\_SOURCE

# Hydrologic Boundaries

The Hydrologic Boundaries group of *Information* layers contains information on the known values (or changes in values over time) of pressure, hydraulic head, solute concentration, and temperature in the hydrogeologic unit, at locations where these levels are controlled by forces external to those occurring within the model.

## Specified Pressure / Hydraulic Head

The **Specified Pressure** (or **Specified Hydraulic Head**) layer contains information on the spatial distribution of known or fixed pressures or hydraulic heads. It also contains information on the associated concentration or temperatures of the boundary nodes and whether the boundary conditions are time dependent. The layer contains three parameters:

- specified\_pressure [M/(Ls<sup>2</sup>)] (or specified\_hydraulic\_head [L])
- concentration [C] (or temperature [°C])
- **time\_dependence**[0 or 1]

## Specified Concentration / Temperature

The **Specified Concentration** (or **Specified Temperature**) layer contains information on the spatial distribution of known or fixed values of solute concentration (or temperature). This specification refers not only to the fluid entering the model, but also to the exiting fluid and the fluid within the unit itself. It also contains information on whether the boundary conditions are time dependent. The layer contains two parameters:

- specified\_concentration [C] (or specified\_temperature [°C])
- **time\_dependence** [0 or 1]

## **Initial Conditions**

The Initial Conditions group of *Information* layers contains information on the spatial distribution of pressures or hydraulic heads, and solute concentrations or temperatures at the beginning of the model run, within the region being considered. (Information in the respective layer described below is ignored when SutraGUI creates the SUTRA input files if the user has chosen to read initial conditions from a restart file or to generate initial conditions by interpolation. Both of these options are specified on the **Initial Conditions Control** pane of the **SUTRA Project Information** dialog box.)

## Initial Pressure/Initial Hydraulic Head

The **Initial Pressure** or **Initial Hydraulic Head** layer contains information on the spatial distribution of pressure or hydraulic head at the beginning of the model run within the medium to be modeled. The layer contains only one parameter, **initial\_pressure**  $[M/(Ls^2)]$ , (or **initial\_hydraulic\_head** [L]), which contains the pressure (or hydraulic head) values.

#### Initial Concentration/Initial Temperature

The **Initial Concentration** or **Initial Temperature** layer contains information on the spatial distribution of solute concentration or fluid temperature at the beginning of the model run within the medium to be modeled. The layer contains only one parameter, **initial\_concentration** [C], or **initial\_temperature** [°C], which contains the concentration or temperature values.

## Map or Point Data

This group of layers is provided for the convenience of the user. Bitmap images, maps, or data may be imported into these layers if desired. If not needed, they can be ignored.

#### Мар

The **Map** layer is a special type of Argus ONE layer that can contain an image or contours and points that cannot be modified or linked to other layers. The image in a *Maps* layer can serve as the pattern upon which information in other layers is superposed. *Maps* layers can be used to display point data from Argus ONE Data layers using a variety of post-processing tools provided in Argus ONE. Such display of point data is described in the section, "Displaying Data." The post-processing display of pressure (hydraulic head), saturation, velocity vectors, and concentration (or temperature) for SUTRA simulations is generated in a *Maps* layer created by **SutraGUI**. The user may create additional *Maps* layers. The **Map** layer is provided as a convenience in **SutraGUI**.

One way to use *Maps* layers is to import scanned images into them and then draw contours on *Information* layers by tracing the image after rescaling image size as desired. Objects in *Maps* layers (lines, points and other objects) can be copied from the *Maps* layer and pasted into *Information* layers where attributes associated with the geospatial information can be assigned to these objects.

For example, if the boundary line on a map is associated with a prescribed hydraulic head, the boundary line can be copied from the *Maps* layer to the Specified Hydraulic Head layer. Information about copying and pasting objects in Argus ONE can be found in the Argus ONE User's Guide (Argus Interware, 1997).

## Point Data

*Data* layers are a special type of Argus ONE layer that contain scattered, gridded, or meshed point-wise data that can be linked to the finite-element mesh or displayed in *Maps* layers. Instructions on interpolating and contouring these data are given in the Argus ONE User's Guide (Argus Interware, 1997, Supplement Version 2.5), and a brief description of this is given in the section of this report entitled, "Displaying Data" on page 71. One Data layer, Point Data, is provided as a convenience in **SutraGUI**, and the user may create additional ones as needed. The user cannot simply draw points in a data layer as is done in an *Information* layer. Instead, the data must be imported.

## **Three-Dimensional Models**

This section describes the layers used for 3D SUTRA models (Table 9). Most layers used in 2D are also used for 3D models, although sometimes in an altered form. However, many layers used in 3D models are not used in 2D models.

#### Table 9. SutraGUI Layer Structure for Three-Dimensional (3D) Models

The reader is referred to the section of this report entitled "Conventions" on page 3 for an explanation of "[i]" in layer names.

Layer Name
SUTRA MODEL group
SUTRA Mesh (Top/Bottom Unit[i])
FishNet_Mesh_Layout (Top/Bottom Unit[i])
Unused layer1
Unused layer2
3D OBJECTS group
Hydrologic Sources: 3D Objects group
Sources of Fluid Solids[i]
Sources of Fluid Points[i]
Sources of Fluid Lines[i]
Sources of Fluid Sheets Vertical[i]
Sources of Fluid Sheets Slanted[i]
Sources of Solute Solids[i]/Sources of Energy Solids[i]
Sources of Solute Points[i]/Sources of Energy Points[i]
Sources of Solute Lines[i]/Sources of Energy Lines[i]
Sources of Solute Sheets Vertical[i]/Sources of Energy Sheets Vertical[i]
Sources of Solute Sheets Slanted[i]/Sources of Energy Sheets Slanted [i]
Hydrologic Boundaries: 3D Objects group
Specified Pressure Solids[i]/ Specified Hydraulic Head Solids[i]
Specified Pressure Points[i]/Specified Hydraulic Head Points[i]
Specified Pressure Lines[i]/Specified Hydraulic Head Lines[i]
Specified Pressure Sheets Vertical[i]/Specified Hydraulic Head Sheets Vertical[i]
Specified Pressure Sheets Slanted[i]/Specified Hydraulic Head Sheets Slanted [i]
Specified Concentration Solids[i]/ Specified Temperature Solids[i]
Specified Concentration Points[i]/Specified Temperature Points[i]
Specified Concentration Lines[i]/Specified Temperature Lines[i]
Specified Concentration Sheets Vertical[i]/Specified Temperature Sheets Vertical[i]
Specified Concentration Sheets Slanted[i]/Specified Temperature Sheets Slanted [i]
Observations Layers: 3D Objects group
Observations Solids[i]
Observations Points[i]
Observations Lines[i]
Observations Sheets Vertical[i]
Observations Sheets Slanted[i]

Layer Name
TOP group
Elevation Top
Sources of Fluid Top
Sources of Solute Top
Specified Hydraulic Head Top/Specified Pressure Top
Specified Concentration Top/Specified Temperature Top
Observation Top
UNIT[i] group
Hydrogeology Unit[i] group
Porosity Unit[i]
Permeability Unit[i]/Hydraulic Conductivity Unit[i]
Dispersivity Unit[i]
Unsaturated Properties Unit[i]
Initial Conditions Unit[i] group
Initial Pressure Unit[i]/Initial Hydraulic Head Unit[i]
Initial Concentration Unit[i]/Initial Temperature Unit[i]
BOTTOM UNIT[i] group
Elevation Bottom Unit[i]
Sources of Fluid Bottom Unit[i]
Sources of Solute Bottom Unit[i]/ Sources of Energy Bottom Unit[i]
Specified Hydraulic Head Bottom Unit[i]/ Specified Pressure Bottom Unit[i]/
Specified Concentration Bottom Unit[i]/ Specified Temperature Bottom Unit[i]
Observation Bottom Unit[i]
Map or Point Data group
Map
Point Data

Table 9. SutraGUI Layer Structure for Three-Dimensional (3D) Models - Continued

#### **SUTRA MODEL**

SUTRA MODEL is a group of layers that define the geometry and discretization of the SUTRA simulation model, and the locations in the model where observations of results will be made. These include the layers SUTRA Mesh and FishNet\_Mesh\_Layout. Unused layer1 and Unused layer2 are not used for 3D models but are present because they are required by Argus ONE. The FishNet\_Mesh\_Layout layer is always included in the group because SUTRA currently requires that a FishNet Mesh be used for 3D models. For nonaligned meshes, several Sutra Mesh and FishNet\_Mesh\_Layout layers appear in the SUTRA MODEL group.

## SUTRA Mesh (Top/Bottom Unit[i])

The **SUTRA Mesh (Top/Bottom Unit[i])** layer is (are) the layer(s) on which the mesh used in the model is defined. For 3D aligned meshes, there is only one such layer. For 3D nonaligned meshes, there is one such layer at the top of the model and another at the bottom of each unit with the unit number after its name. All 3D models must use a FishNet Mesh. For 3D models, it must be possible to deform the FishNet Mesh into a grid bounded by a rectangle. (This is not required for 2D models.)

In 3D models, the **SUTRA Mesh** layer (or layers) contains values of all the spatially distributed parameters except boundary conditions and observations. Depending on **SUTRA**'s requirements for each parameter, as specified in the documentation for the **SUTRA** input data sets (Voss and Provost, 2002), a parameter may receive a value for each node or for each element in the mesh. These values are derived from the various *Information* layers described in following sections. The Argus ONE environment refers to the assignment of values in one *Information* layer to another as "linking." The names of the parameters of the **SUTRA Mesh** layer are listed in Table 10. The full Argus ONE name of each parameter is given as "Layer.Parameter," for example, the first parameter, NREG, in the table is **SUTRA Mesh.NREG**.

For 3D nonaligned models, the uppercase names of **SUTRA Mesh** parameters correspond exactly with variables used by the **SUTRA** model, and are described in the **SUTRA** documentation. For 3D vertically aligned models, the uppercase names of **SUTRA Mesh** parameters correspond with variables used by the **SUTRA** model except that they have a number after them that determines to which model unit they belong.

There is one exception to the above. The **SUTRA** parameter, **UBC**, representing the concentration or temperature of any fluid that may flow into the model at a node where pressure or hydraulic head is specified, has been changed to **pUBC** in **SutraGUI** to distinguish it from the specified concentration or temperature boundary condition type, which retains its original name (**UBC**).

Two of the **SUTRA Mesh** parameters, **QIN** and **QUIN**, a fluid source and energy or solute source, respectively, have additional logic associated with their values. As noted in the description of the **Sources of Fluid** and **Sources of Energy** or **Sources of Solute** layers, to which these node-wise parameters are linked, these sources may be specified at point, line (open) or closed contours. Depending on which type of contour is specified in the "**Sources**" layer, the resultant source value provided as a parameter in the "**Sources**" layer may require multiplication by the open contour length or closed contour area or cell volume associated with the node; these multiplications are carried out automatically.

The Z[i] parameters on that layer represent the elevation of the i'th unit boundary. Thus, the Z1 parameter represents the elevation of the top of the uppermost unit and Z2 represents the elevation of the first unit. Z[n+1] represents the elevation of the bottom of unit n.

*Note: The properties assigned to any node or element may be viewed (and modified) by double-clicking on the element of interest while the* **SUTRA Mesh** *layer is active.* 

Name
NREG([i])
Z([i])
POR([i])
LREG([i])
PMAX([i])
PMID([i])
PMIN([i])
ANGLE1(_[i])
ANGLE2(_[i])
ANGLE3(_[i])
ALMAX([i])
ALMID([i])
ALMIN([i])
ATMAX([i])
ATMID([i])
ATMIN([i])
QIN([i])
IS_FLUID_SOURCE([i])
UIN([i])
time_dependent_fluid_sources([i])
QUIN([i])
IS_QUIN_SOURCE([i])
time_dependent_energy_or_solute_sources([i])
PBC([i])
IS_PBC_SOURCE([i])
pUBC([i])
time_dependent_specified_head_or_pressure([i])
UBC([i])
IS_UBC_SOURCE([i])
time_dependent_specified_concentration_or_temperature([i])
PVEC([i])
UVEC([i])
INOB([i])

Table 10. SUTRA Mesh parameters used in three-dimensional (3D) simulations

#### FishNet\_Mesh\_Layout (Top/Bottom Unit[i])

The **FishNet\_Mesh\_Layout** (**Top/Bottom Unit[i]**) layer is always included for 3D models. **SutraGUI**, rather than Argus ONE, creates FishNet meshes. A FishNet Mesh consists of superblocks (large contiguous quadrilaterals) each subdivided into a specified number of rows and columns of quadrilateral finite elements. For 3D models, it must be possible to deform the mesh into a grid bounded by a rectangle. This layer, like the **SUTRA Mesh** layer, is a Quad-Mesh layer. However, the elements on it are usually drawn manually or are imported rather than being generated automatically. Each element of the mesh will describe one "superblock" of the **SUTRA Mesh**. The "superblocks" describe the external and internal boundaries of the FishNet Mesh. Each superblock element contains information describing the desired number of quadrilateral finite elements that will fill the superblock in the X and Y directions when the mesh is generated. The use of the **FishNet\_Mesh\_Layout** layer is described in the section of this report entitled "Creating FishNet Meshes" on page 67.

#### Unused layer1

Unused layer1 is a Domain layer required by Argus ONE that is not used by SutraGUI in 3D.

#### Unused layer2

Unused layer2 is an *Information* layer required by Argus ONE that is not used by SutraGUI in 3D.

## Hydrologic Sources: 3D Objects

SUTRA hydrologic sources may be specified in **SutraGUI** to be located exactly within the top and bottoms of model units, or anywhere in model space as 3D objects. The **Hydrologic Sources: 3D objects** group of *Information* layers is used to set up source boundary conditions specified as 3D objects. The **Hydrologic Sources** group contains information on fluxes (quantity per time) of fluid, solute, and energy entering or leaving the model. These are described separately in the following sections. Points, lines, sheets, and solids can all be used to specify the sources as described in the section of this report entitled "Assignment of Boundary Conditions and Observations" on page 13. The user determines the number and type of layers in this group as described in the section of this report entitled "3D Surfaces and Objects (3D Only)" on page 29. (The reader also is referred to the section of this report entitled "Hydrologic Sources" on page 59 for sources that are to be located exactly on the model top or on bottoms of units.)

# Sources of Fluid Solids[i]/Points[i]/Lines[i]/Sheets Vertical[i]/Sheets Slanted[i]

In addition to the parameters used to specify the geometry of the 3D object that represents a region where a source exists, the user must specify either a **total\_source** or a **specific\_source** for each contour (object). The section of this report entitled "Assignment of Boundary Conditions and Observations" on page 13 explains how these parameters are used to assign values to individual nodes. The concentration or temperature of the source must also be specified. (However, for fluxes out of the model, SUTRA will automatically use the concentration or temperature at the node rather than the specified value.) The user must specify whether a boundary is a time-dependent source. (Time-dependent sources must be programmed into SUTRA in the subroutine BCTIME as described in the SUTRA manual. Because there is no standard method for specifying time-dependent input for SUTRA, **SutraGUI** does not generate input files for the time-dependent data.) If desired, the user can specify a comment for a contour. Such comments will be included in the SUTRA input file created by **SutraGUI**. They can be used to help identify the nodes associated with particular contours, (for example, when

programming subroutine BCTIME to vary sources at certain nodes or groups of nodes representing a hydrologic feature with time).

# Sources of Solutes/Energy Solids[i]/Points[i]/Lines[i]/Sheets Vertical[i]/Sheets Slanted[i]

These layers are used in much the same way as the sources of fluid layers except that the **total\_source** or **specific\_source** refers to sources of solute or energy rather than sources of fluid.

## Hydrologic Boundaries: 3D Objects

SUTRA hydrologic boundaries may be specified in **SutraGUI** to be located exactly within the top and bottoms of model units, or anywhere in model space as 3D objects. The **Hydrologic Boundaries: 3D objects** group of layers is used to set up specified value boundary conditions in 3D models as 3D objects. The boundary conditions may be either specified hydraulic head, specified pressure, specified concentration, or specified temperature. Points, lines, sheets, and solids can all be used to specify the sources as described in the section of this report entitled "Assignment of Boundary Conditions and Observations" on page 13. The user determines the number and type of layers in this group as described in the section of this report entitled "3D Surfaces and Objects (3D Only)" on page 29. (The reader also is referred to the section of this report entitled "Hydrologic Boundaries" on page 61 for boundary conditions that are to be located exactly on the model top or on bottoms of units.)

# Specified Hydraulic Head/Pressure Solids[i]/Points[i]/Lines[i]/Sheets Vertical[i]/Sheets Slanted[i]

In addition to the parameters used to specify the geometry of the 3D object that represents a region where a specified head or pressure exists in the **Specified Hydraulic Head** or **Specified Pressure** layers, the user must set the specified pressure or specified hydraulic head, and concentration or temperature for each contour (object). For specified pressure boundaries, it is often useful to use the **Sutra\_Z(**) function as described in the section of this report entitled "Three-Dimensional Models" on page 11. The user must also specify whether the boundary is time-dependent. The "comment" parameter can be used to identify the nodes in the SUTRA input file that are associated with a particular contour. Such comments will be included in the SUTRA input file created by **SutraGUI**. They can be used to help identify the nodes associated with particular contours, (for example, when programming subroutine BCTIME to vary heads or pressures at certain nodes or groups of nodes representing a hydrologic feature with time).

## Specified Concentration/Temperature Solids[i]/Points[i]/Lines[i]/Sheets Vertical[i]/Sheets Slanted[i]

The **Specified Concentration** or **Specified Temperature** layers are used in much the same way as the specified hydraulic head/pressure layers except that the user sets the specified concentration or temperature rather than the specified pressure or specified hydraulic head.

# **Observation Layers: 3D Objects**

SUTRA observations may be specified in **SutraGUI** to be located exactly within the top and bottoms of model units, or anywhere in model space as 3D objects. The **Observation: 3D objects** group of layers is used to set up observation locations in 3D models as 3D objects. Points, lines, sheets, and solids can all be used to specify the observation locations as described in the section of this report entitled "Assignment of Boundary Conditions and Observations" on page 13. The user determines the number and type of layers in this group as described in the section of this report entitled "3D Surfaces and Objects (3D Only)" on page 29. At observation nodes, SUTRA will output a detailed record of pressure, concentration, or temperature and saturation. This type of output is usually used for plotting time-drawdown curves or solute breakthrough curves. **GW\_Chart** (Winston, 2000) can be used to prepare such charts as "hydrographs'. (The reader is referred to the section of this report entitled "Observation Top" on page 62 for observations that are to be located exactly on the model top or on bottoms of units.)

The user only needs to specify the geometry of the 3D objects used to select the boundary nodes. No additional information is required.

## TOP

The **TOP** group of layers is only present in 3D models. It includes layers that are related to the top of the model. It contains the **Elevation Top** layer and, depending on the user's selections, may contain **Sources of Fluid**, **Sources of Solute / Energy**, **Specified Pressure / Hydraulic Head**, **Specified Concentration / Temperature**, and **Observation** layers. See the section of this report entitled "3D Surfaces and Objects (3D Only)" on page 29 for more information on specifying which layers should be present.

## Elevation Top

The **Elevation Top** layer is used to specify the elevation of the top layer of nodes in the model. It has one parameter, **elevation top** [L], which is the elevation.

#### Hydrologic Sources

Two types of layers that represent hydrologic sources: **Sources of Fluid Top** and **Sources of Solute Top** / **Sources of Energy Top**. These *Information* layers contain information on fluxes (quantity per time) of fluid, solute, and energy entering or leaving a unit. The section of the report entitled "Hydrologic Sources: 3D Objects" on page 57 describes how to specify sources within units.)

In these layers, **SutraGUI** allows specification of fluid sources or sinks and energy/solute sources or sinks at points, along line segments, and for delimited areas. Sources have positive values, whereas sinks are specified with a negative number. Sources of fluid may be either specified as a total amount of fluid per second (that is, **total\_source**), or as the total amount of fluid per second (that is, **specific\_source**). Similarly, sources of energy/solute may be either specified as a total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute per second (that is, **total\_source**), or as the total amount of energy/solute per second per length or per area of the source object (that is, **specific\_source**). For 3D models where elevations of the top may vary, the areas used are the projection of these surfaces in the X-Y plane.

Point sources may be assigned only a **total\_source**. Point sources typically represent injection or withdrawal wells for fluid sources. The command **PIEs|Convert...|Mesh Objects to Contours...** in the Utility PIE (Winston, 2001) can be used to copy nodes into information layers as point contours. The mesh must be organized such that the nodes fall exactly at the source locations.

Line or curve sources may be assigned either a **total\_source** or a **specific\_source**. A fluid line source may represent, for example, recharge occurring along a reach of a river or irrigation canal. Depending on whether the user knows the total recharge along the canal reach, or the recharge per length of canal, the user should specify either **total\_source** or **specific\_source** in the **Sources of Fluid** layer. The command **PIEs**[**Convert...**]**Mesh Objects to Contours...** can be used to copy nodes and the edges of elements into *Information* layers. The mesh must be organized such that the nodes fall exactly at the source locations.

Area sources may be assigned either a **total\_source** or a **specific\_source**. These are created with the closed contour drawing tool located along the left side of the Argus ONE window. For fluid, an area source may represent, for example, ground-water recharge below a lake (**total\_source** could be specified for the entire lake as one object) or rainfall recharge rate (volume per area) for a particular area (**specific\_source** could be specified in units [L/s] for the object). For energy, an area source may represent, for example, heat production in a magma body (**total\_source** could be specified for the entire body as one object) or radiogenic heat production rate (energy per area) for a particular area (**specific\_source** could be specified in units [E/sL<sup>2</sup>] for the object).

Because contours may not cross one another in Argus ONE, only one type of object may be specified at any location. Furthermore, SUTRA accepts only one source per location; thus two sources, for example, rainfall and a well, cannot be specified separately at the same location, and must be summed externally by the user before entering values into **SutraGUI** for sources specified on the top of a 3D model mesh. (For 3D models, multiple sources can be specified at one location using 3D source objects. **SutraGUI** will combine these into a single source before exporting the data to SUTRA.)

To obtain areally distributed values affecting nodes throughout the mesh, rather than exactly along contours in the top, an expression should be used for the **specific\_source** parameter. The reader is referred to the section of this report entitled "Adding a Precipitation Data Layer and Linking It to Fluid Sources Layer."

#### Sources of Fluid Top

The **Sources of Fluid Top** layer contains information on the spatial distribution of the fluid sources and sinks (such as wells and recharge from rainfall). These sources occur on the top of the uppermost unit. The reader is referred to the section of this report entitled "Sources of Fluid Solids[i]/Points[i]/Lines[i]/Sheets Vertical[i]/Sheets Slanted[i]" on page 57 for a description of how to specify sources of fluid within units. Additionally the layer contains information on the solute concentration or temperature of the source fluids. The layer contains six parameters. However, two of these (the ones with the uppercase names) are automatically calculated by **SutraGUI** from the others and must not be altered by the user. For any given object in the layer, the user may only specify three of the remaining four parameters, because a choice must be made between **total\_source** and **specific\_source** as described above in the section of this report entitled "Total and Specific Sources" on page 14. When pressure has been selected as the

hydraulic variable, fluid sources use units of [M/s]; when hydraulic head has been selected, units of  $[L^3/s]$  are used. The parameters for this layer are:

- total\_source [M/s] ([L<sup>3</sup>/s] when using hydraulic head)
- **specific\_source** [(M/s)/(L, L<sup>2</sup>, or L<sup>3</sup>)] ([(L<sup>3</sup>/s)/(L, L<sup>2</sup>, or L<sup>3</sup>)] when using hydraulic head)
- **concentration\_of\_source** [C] (or **temperature\_of\_source** [°C] for energy transport)
- **time\_dependence** [0 or 1]
- **RESULTANT\_FLUID\_SOURCE**
- QINUIN

#### Sources of Solute / Energy Top

The **Sources of Solute Top** (or **Sources of Energy Top**) layer contains information on the spatial distribution of the solute (or energy) sources and sinks (such as dissolving minerals, radiogenic heat production, or thermal conduction through a boundary). These sources occur at the top of the uppermost unit. The reader is referred to the section of this report entitled "Sources of Solutes/Energy Solids[i]/Points[i]/Lines[i]/Sheets Vertical[i]/Sheets Slanted[i]" on page 58 for a description of how to specify sources of solute or energy within units. The layer contains five parameters. However, one of these (the one with the uppercase name) is automatically calculated by Argus ONE from the others and may not be altered by the user. For any given object in the layer, the user may only specify three of the remaining four parameters, because a choice must be made between total\_source and specific\_source as described above in the section of this report entitled "Total and Specific Sources" on page 14. The parameters for this layer are:

- total\_source [C/s or E/s]
- **specific\_source** [(C/s or E/s)/(L or L 2 )]
- **time\_dependence** [0 or 1]
- RESULTANT\_SOLUTE/ENERGY\_SOURCE

#### Hydrologic Boundaries

There are two types of layers representing hydrologic boundaries: **Specified Pressure / Hydraulic Head Top**, and **Specified Concentration / Temperature Top**. These layers contain information on the known values (or changes in values over time) of pressure, hydraulic head, solute concentration, and temperature in the hydrogeologic unit, at locations where these levels are controlled by forces external to those occurring within the unit or generic model. These layers appear under the **TOP** layer and represent boundary conditions at the top surface of the model.

#### Specified Pressure Top / Hydraulic Head Top

The **Specified Pressure Top** (or **Specified Hydraulic Head Top**) layer contains information on the spatial distribution of known or fixed pressures or hydraulic heads. These conditions occur on the top surface of the model. The reader is referred to the section of this report entitled "Specified Hydraulic Head/Pressure Solids[i]/Points[i]/Lines[i]/Sheets Vertical[i]/Sheets Slanted[i]" on page 58 for a description of how to specify these boundary conditions within units. It also contains information on the associated concentration or temperatures of the boundary nodes and time dependent boundary conditions. The layer contains three parameters:

- specified\_pressure [M/(Ls<sup>2</sup>)] (or specified\_hydraulic\_head [L])
- concentration [C] (or temperature [°C])
- **time\_dependence**[0 or 1]

#### **Specified Concentration Top / Temperature Top**

The **Specified Concentration Top** (or **Specified Temperature Top**) layer contains information on the spatial distribution of known or fixed values of solute concentration (or temperature). These conditions occur on the top surface of the model. The reader is referred to the section of this report entitled "Specified Concentration/Temperature Solids[i]/Points[i]/Lines[i]/Sheets Vertical[i]/Sheets Slanted[i]" on page 58 for a description of how to set up specified concentration or specified temperature boundaries within units. It also contains information on time dependent boundary conditions. The layer contains two parameters:

- **specified\_concentration** [C] (or **specified\_temperature** [°C])
- **time\_dependence** [0 or 1]

## **Observation Top**

The **Observation Top** layer is an *Information* layer that contains the spatial distribution of locations at which the user desires "observation-node output" from locations exactly within the top of a 3D SUTRA model. As described in the SUTRA documentation, this output provides a detailed time series of pressure, concentration, or temperature, and saturation at user-selected nodes at a user-selected time-step interval. This type of output is used for plotting time-drawdown curves or solute breakthrough curves. **GW\_Chart** (Winston, 2000) can be used to prepare such charts (as 'hydrographs') from the output. The reader is referred to the section of this report entitled "Observation Layers: 3D Objects" on page 59 for a description of how to set up observation locations within units.

It is possible to use point, open, or closed contours to specify where observations should be made on the model top during the SUTRA simulation. For each contour object, the value of the contour's parameter, **is\_observed**, must be set to "True" (or 1). The frequency of the observations is specified in the **Output Controls** pane of the **SUTRA Project Information** dialog box.

The **Observation Top** layer uses the *Exact Contour* method of interpretation so that observations are only defined inside of closed contours, or directly above open and point contours.

Nodes in the top **SUTRA Mesh** layer falling within the selected areas or directly above the open or points contours will be marked as observation nodes for input to SUTRA. The command **PIEs**[Convert...]Mesh Objects to Contours... in the Utility PIE (Winston, 2001) can be used to copy nodes into *Information* layers.

# UNIT[i]

The UNIT[i] group of layers is only present in 3D models. It includes layers that are related to a specific unit. Following the UNIT[i] layer are the Hydrogeology Unit[i] and Initial Conditions Unit[i] layers, which pertain to unit[i].

# Hydrogeology Unit[i]

The **Hydrogeology Unit**[i] group of *Information* layers contains information on the physical and material properties of unit[i].

# Porosity Unit[i)

The **Porosity Unit[i]** layer contains information on the spatial distribution of the porosity of the 3D unit to be modeled. The layer contains only one parameter, **porosity** [fraction], which contains the porosity value.

# Permeability Unit[i] / Hydraulic Conductivity Unit[i]

The layer called **Permeability Unit[i]** (for cases using pressure) or **Hydraulic Conductivity Unit[i]** (for simulations using hydraulic head), contains information on the spatial distribution of the principal values of permeability/hydraulic conductivity, and the direction of the anisotropy for the unit to be modeled, or for generic studies, for the medium to be modeled. In 3D models, the layer contains six parameters:

- **maximum**  $[L^2]$  ([L/s] for hydraulic conductivity)
- **middle** [L<sup>2</sup>] ([L/s] for hydraulic conductivity)
- **minimum** [L<sup>2</sup>] ([L/s] for hydraulic conductivity)
- horizontal angle [degrees]
- vertical angle [degrees]
- rotational angle [degrees]

If the system is isotropic, the maximum, middle, and minimum values must be set equal to the desired value, and the angle(s) may be set to any arbitrary number. It may be convenient for isotropic systems to link the value of one of the permeability minimum or maximum parameters to the other. The reader is referred to Appendix A, entitled "Adding and Linking New Layers" on page 106.

## Dispersivity Unit[i]

The **Dispersivity Unit[i]** layer contains information on the spatial distribution of the longitudinal and transverse dispersivities of the unit to be modeled, or for generic studies, of the medium to be modeled.

In 3D models, the layer contains six parameters:

- **longdisp\_in\_max\_permdir** [L] = longitudinal dispersivity for flow in the direction of maximum permeability
- **longdisp\_in\_mid\_permdir** [L] = longitudinal dispersivity for flow in the direction of intermediate permeability
- **longdisp\_in\_min\_permdir** [L] = longitudinal dispersivity for flow in the direction of minimum permeability
- **trandisp\_in\_max\_permdir** [L] = transverse dispersivity in the direction of maximum permeability for any flow in the mid-min plane
- **trandisp\_in\_mid\_permdir** [L] = transverse dispersivity in the direction of intermediate permeability for any flow in the max-min plane
- **trandisp\_in\_min\_permdir** [L] ] = transverse dispersivity in the direction of minimum permeability for any flow in the max-mid plane

The additional components of the dispersivity values in 3D models are extensions to the classical dispersion process provided by SUTRA (Voss, 1984; transverse extension added in 1990 revision, 3D extension added by Voss and Provost, 2002). To obtain the classical dispersion model used by most other transport models, set the values of all the longitudinal dispersivity parameters equal to each other, and the values of all the transverse dispersivity parameters equal to each other.

#### Unsaturated Properties Unit[i]

The **Unsaturated Properties Unit**[i] layer is used to specify regions that have different unsaturated flow properties.

Note: Unsaturated-flow simulation with SUTRA requires some <u>user programming</u> in the SUTRA subroutine UNSAT for the user to specify the unsaturated functions for each region as described in Voss and Provost (2002). The FORTRAN source code for SUTRA and a FORTRAN compiler are required to use this feature. Because there is not a standard format for any additional information that must be read into the program for unsaturated properties, **SutraGUI** does not create input files for unsaturated flow properties. However, users may be able to create an export template for use within Argus ONE that will generate such files for their particular case, as described on p. 169-188 of the Argus ONE User's Guide (Argus Interware Inc., 1997).

The **Unsaturated Properties Unit[i]** layer contains information on the spatial distribution of regions having constant unsaturated properties in the unit to be modeled, or for generic studies, in the medium to be modeled. This layer only appears when a saturated-unsaturated problem type has been selected in the **SUTRA Project Information** dialog box. The layer contains only

one parameter, **region** (an integer), which contains the identification number of the region. Usually the *Exact Contour* method should be used to define the location of regions in this layer, in which case only closed contours should be used for specifying regions. The *Exact Contour* method is already specified as the default selection for this layer. After closing a contour, the user must assign its region number in the *Contour Information* dialog box. Any number of contours may share the same region number. Each region represents one type of material having uniform unsaturated property functions. For example, region 1 may be fine silt, region 2 may be clay, and region 3 may be coarse sand. Each type of material may occur in a number of places within the model domain. The default region number is zero. To create regions that share a boundary (such as geologic layers), turn on the option *Special Allow Intersection* before drawing contours. If the user wishes to have nodes and element edges occur exactly at region boundaries, then for a FishNet Mesh, these boundaries need to be defined as the edges of superblocks in a FishNet Mesh layout.

# Initial Conditions Unit[i]

This group of *Information* layers contains information on the spatial distribution of pressures or hydraulic heads, and solute concentrations or temperatures at the beginning of the model run, within unit[i].

## Initial Pressure Unit[i]/Initial Hydraulic Head Unit[i]

The **Initial Pressure Unit[i]** or **Initial Hydraulic Head Unit[i]** layer contains information on the spatial distribution of pressure or hydraulic head at the beginning of the model run. The layer contains only one parameter, **initial\_pressure**  $[M/(Ls^2)]$ , (or **initial\_hydraulic\_head** [L]), which contains the pressure (or hydraulic head) values. (For 3D models using pressure, it is often useful to make the initial pressure a function of **Sutra\_Z**().)

## Initial Concentration Unit[i]/Initial Temperature Unit[i]

The **Initial Concentration Unit[i]** or **Initial Temperature Unit[i]** layer contains information on the spatial distribution of solute concentration or fluid temperature at the beginning of the model run. The layer contains only one parameter, **initial\_concentration** [C], or **initial\_temperature** [°C], which contains the concentration or temperature values.

# **BOTTOM UNIT[i]**

The **BOTTOM UNIT[i]** group of layers is only present in 3D models. It includes layers that are related to the bottom of unit[i]. It contains the **Elevation Bottom Unit[i]** layer and may also contain **Sources of Fluid Bottom Unit[i]**, **Sources of Solute Bottom Unit[i] / Energy Unit[i]**, **Specified Pressure Bottom Unit[i] / Hydraulic Head Bottom Unit[i]**, **Specified Concentration Bottom Unit[i] / Temperature Bottom Unit[i]**, and **Observation Bottom Unit[i]** layers. These layers are equivalent to those layers described previously in the section of this report labeled "TOP" on page 59, but here concerning locations exactly within the bottoms of units, rather than on the top surface of the model.

The **Elevation Bottom Unit[i]** layer is used to specify the elevation of the layer of nodes at the bottom of a unit in the model. It has one parameter, **elevation bottom unit[i]** [L], which is the elevation.

## Map or Point Data

This group of layers is provided for the convenience of the user. Bitmap images, maps, or data may be imported into these layers if desired. If not needed, these layers can be ignored.

### Мар

The **Map** layer is a special type of Argus ONE layer that can contain an image or contours and points that cannot be modified or linked to other layers. The image in a *Maps* layer can serve as the pattern upon which information in other layers is superposed. *Maps* layers can be used to display point data from Argus ONE Data layers using a variety of post-processing tools provided in Argus ONE. Such display of point data is described in the section, "Displaying Data" on page 71. The user may create additional *Maps* layers. The **Map** layer is provided as a convenience in **SutraGUI**.

One way to use *Maps* layers is to import scanned images into them and then draw contours on *Information* layers by tracing the image. Objects in *Maps* layers (lines, points and other objects) can be copied from the *Maps* layer and pasted into *Information* layers where attributes associated with the geospatial information can be assigned to these objects.

For example, if the boundary line on a map is associated with a prescribed hydraulic head, the boundary line can be copied from the *Maps* layer to the **Specified Hydraulic Head** layer. Information about copying and pasting objects in Argus ONE can be found in the Argus ONE User's Guide (Argus Interware, 1997).

#### Point Data

*Data* layers are a special type of Argus ONE layer that contain scattered, gridded, or meshed point-wise data that can be linked to the finite-element mesh or displayed in *Maps* layers. Instructions on interpolating and contouring these data are given in the Argus ONE User's Guide (Argus Interware, 1997, Supplement Version 2.5), and a brief description of this is given in the section or this report entitled, "Displaying Data" on page 71. One Data layer, Point Data, is provided as a convenience in **SutraGUI**, and the user may create additional ones as needed. The user cannot simply draw points in a data layer as is done in an *Information* layer. Instead, the data must be imported.

# **Creating FishNet Meshes**

A FishNet Mesh (for example, <u>fig. 3</u> on page 9) consists of superblocks (large contiguous quadrilaterals) that are each subdivided into a specified number of quadrilateral finite elements, four of which are connected to each internal node. The mesh may be considered similar to a deformed finite-difference grid. FishNet meshes are created as follows.

## Prepare to Draw the Layout of the FishNet Mesh

- 1. On the **Model Configuration** pane of the **SUTRA Project Information** dialog box, choose to use a FishNet Mesh. (FishNet meshes are mandatory for 3D models.)
- 2. Make the **FishNet\_Mesh\_Layout** layer active.

## Draw the First Superblock

- 3. Select the element-drawing tool 🖾 at the left of the window.
- 4. Draw an element in the white work area of the window by clicking at the desired location of each corner, proceeding either clockwise or counter-clockwise around the element (fig. 16).

Argus ONE - untitled1										
File	Edit	View	<u>S</u> pecial	<u>N</u> avigation	<u>P</u> IEs	<u>W</u> indows	; <u>H</u> elp			
	Lay			5		10		<sup>™</sup> <b>Arg</b> ı	ıs	
	15  				<u>, , , , , , , , , , , , , , , , , , , </u>		<u> </u>		•	

Figure 16. Example of a completed superblock.

5. Select the Arrow button **b** at the left side of the window and double-click on the element.

6. The *Element Information* dialog box appears. Enter the desired number of elements in the X and Y directions (for example, 10 and 15) next to the names **elements\_in\_x** and **elements\_in\_y** below the word "Value". These values determine how many rows and columns of quadrilateral finite elements this superblock will be divided into when the mesh is generated. To exit the dialog box, click OK to accept the values or Cancel to leave the values unaltered.

Note: To determine the X and Y directions for the element, identify the two nodes with the largest X-coordinates. Of those two, the one with the largest Y coordinate is treated as being in the upper right corner of the element. If the nodes have the same Y-coordinate, the one with the larger X coordinate is treated as being in the upper right corner of the element. If the nodes with the second and third highest X-coordinates have the same X-coordinate, then the one with the higher Y-coordinate is selected as one of the two with the highest X-coordinate.

Note: Superblocks may contain redundant information concerning number of rows and columns of elements. For example, each superblock in a pair of superblocks side-by-side in the X direction will have a value for **elements\_in\_y**. Because the FishNet Mesh design requires there to be the same number of rows of elements across both blocks, the user should provide each superblock with the same value for **elements\_in\_y**. **SutraGUI** is designed so that if these numbers do not agree, then the higher value is applied throughout that row or column of superblocks.

#### Draw Additional Superblocks

- 7. Usually, the user will want to join at least one side of each new superblock to a previously drawn one. To draw the next superblock, select the element tool again and move the cursor over one of the nodes of the previous superblock along the side to which the new one will be joined. The cursor will change to a large hollow plus sign when it is over one of the nodes of the other element. Click with the mouse at this point to begin drawing a new element that includes the node under the mouse.
- 8. If another node of a previous superblock is to be shared with the new superblock, then move the cursor over the next previously existing node and click again when the cursor becomes a hollow plus sign.
- To complete the element, click at the other locations where corners of the element are desired. Assign each element appropriate values of elements\_in\_x and elements\_in\_y.
- 10. Begin a new superblock according to step 8, if desired. If no more superblocks are needed, then continue with step 11.

#### Create the Mesh from the Layout of the FishNet Mesh

- 11. Make the **SUTRA Mesh** layer active.
- 12. Select **PIEs**|Create SUTRA FishNet Mesh. SutraGUI then generates a mesh according to the specifications given in the FishNet\_Mesh\_Layout layer and places the mesh into the SUTRA Mesh layer.

Note: The **SUTRA Mesh** layer must be empty (that is, contain no old mesh) for this choice to be available. Old meshes must be deleted first by clicking **Edit** Select All, and then pressing the delete key.

A completed **FishNet\_Mesh\_Layout** layer is shown in <u>figure 17</u>. In it, **elements\_in\_x** and **elements\_in\_y** have both been set to 5. The resulting mesh that appears in the **SUTRA Mesh** layer is shown in <u>figure 18</u>. Almost any arrangement of superblocks is possible.

Note: although the mesh in <u>figure 18</u> is suitable for a 2D model, it is not suitable for a 3D model. This is because it cannot be deformed into a simple rectangle consisting of rows and columns of elements, where each row has the same number of elements as all other rows and each column has the same number of elements as all other columns (like a rectangular finite-difference grid containing rectangular cells).

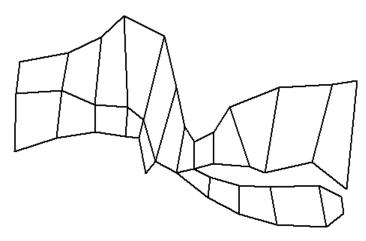


Figure 17. Example of FishNet Mesh showing structure of superblocks.

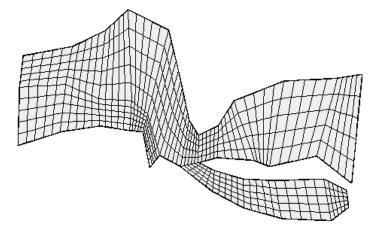


Figure 18. Completed FishNet Mesh, for layout shown in figure 17.

For 3D nonaligned meshes, one 2D mesh must be created for the bottom of each unit plus an extra mesh for the top of the model; however, each mesh must have the same number and relative arrangement of nodes and elements.

It is possible to copy a mesh from one layer to another using the following procedure from the Utility PIE (Winston, 2001):

- Select **PIEs Import**...
- Click on the Copy Quad Mesh... radio button and then click on the OK button.
- Select the layers from which and to which the mesh should be copied and then click on the **OK** button.

Only the geometry of the mesh is copied; parameter values are not copied and must be reentered.

# **Displaying Data**

This section describes how the user can check the values assigned to elements and nodes.

# Element Data

It is important for the user to check whether the elementwise mesh parameters have been assigned by element as desired. The user can double-click on an individual element to check or modify its values. The spatial distribution of any elementwise parameter of the **SUTRA Mesh** layer can be easily displayed as a color map, as follows.

When the **SUTRA Mesh** layer is active, holding the mouse button down over the triangle next to the word "*Color*" above the color band along the left edge of the Argus ONE window provides a list of possible elementwise mesh parameters by which elements can be colored. Figure 26 on page 87 shows the list and a mesh colored by parameter **PMAX**, where the closed contours are regions of constant permeability specified for the **permeability.maximum** layer parameter.

Note: It is sometimes useful to make the **SUTRA Mesh** layer transparent, which can be done by turning off the option View Opaque Elements.

Note: It is sometimes useful for the user to display the spatial distribution of a new Information layer or parameter added by the user. This may be accomplished by also creating a new **SUTRA Mesh** layer parameter and linking its value (selected as "**Type:** element parameter") to the user's new information layer or parameter.

# Node Data

It is important for the user to check whether the nodewise mesh parameters have been assigned by node as desired. The spatial distribution of any nodewise parameter of the SUTRA Mesh layer can be easily displayed as a contour map, as follows.

- 1. Activate the **Map** layer, or create a new map type layer and activate it.
- 2. Hold the mouse button down over the post-processing tool at the lower right of the tools found at the upper left edge of the Argus ONE window, and select the contour drawing tool from the pull-down list .
- 3. Click and drag the cursor anywhere in the workspace to form a small rectangle and release the mouse. This opens the *Contour Diagram* dialog box.
- 4. In the "Layer:" box, select SUTRA Mesh (if it is not already selected).
- 5. In the "Value:" box, select the nodewise parameter of the SUTRA Mesh layer that should be contoured.
- 6. Click the Position tab along the top of the window and then click on "Overlay Source Data" to force the plot to exactly overlay the model domain.
- 7. Click OK, and the plot is drawn. This creates a contour plot of the nodewise parameter of interest overlaying the mesh. Double-clicking this plot with the arrow tool brings back the *Contour Diagram* dialog box, allowing modifications to be made

to plot style. The reader is referred to "Post-Processing Tools and Objects (p 23 s2.5) of the Argus ONE User's Guide (Argus Interware, Inc., 1997)" for more information.

Note: If the mesh or the Information layer (to which the nodewise parameter plotted is linked) is changed, this process must be repeated to display the new node-wise parameter distribution.

Another way to display the nodewise data is to make a Data layer, such as **Point Data**, the active layer and select *Edit Read Data From Layer*... Then select the parameters in the **SUTRA Mesh** layer that should be displayed and click on the *OK* button. The data points can then be colored in the same way as the elements as described above in the section entitled "Element Data." Again, note that the data points will not be automatically updated if the node values change.

# Exporting SUTRA input files and Running SUTRA

Once a SUTRA model has been prepared, the next steps are to export the SUTRA input files and run SUTRA. To export the input files for SUTRA, make **SUTRA Mesh** (or **Sutra Mesh Top** or **SUTRA Mesh Bottom Unit[i]**) the active layer. Then select **PIEs**[**Run Sutra...** from the menu. The **Run SUTRA** dialog box will appear (fig. 19).

Run SUTRA									
Main Options Memory options									
Root file name for simulation	<b>√</b> <u>0</u> K								
Model input Create SUTRA input files	X <u>C</u> ancel								
Create SUTRA input files and run SUTRA	<u>E</u> dit Params >>								
<ul> <li>Alert level</li> <li>Show <u>all warnings</u></li> <li>Warn <u>only about problems that will cause invalid model input</u></li> <li>Show <u>n</u>o warnings</li> </ul>									
External calibration program running Argus ONE     SUTRA Path     C:\SutraSuite\SUTRA_2D3D_1\bin\sutra_2D3D_1.exe     Browse     Browse									
<ul> <li>Save temporary files for reuse by SutraGUI.</li> <li>(This reduces the execution time of SutraGUI when not all data sets are exported.)</li> </ul>									
Slow data sets to export NBI: Data Set 3 (bandwidth) Data Set 8D (Observation nodes) Data Set 14B (Node locations, porosity, unsaturated flow regions) Data Set 15B (Element unsaturated flow regions, permeability, permeability angle) Data Set 17 (Fluid sources and sinks) Data Set 17 (Fluid sources and sinks) Data Set 18 (Energy or solute mass sources and sinks) Data Set 19 (Specified pressures) Data Set 19 (Specified concentrations or temperatures) Data Set 20 (Specified concentrations or temperatures) Data Set 22 (Element incidence) Data Set ICS 2 (Initial pressure) Data Set ICS 3 (Initial temperatures or concentrations) All None									

Figure 19. The Run SUTRA dialog box.

The **Run SUTRA** dialog box provides several options that the user can select. First, there is the "root file name for simulation." This is the part of the file name before the extension that will be used to create all of the file names for the input and output files for SUTRA. For example if the root file name is "A\_Name," the main SUTRA input file would be "A\_Name.inp" and the name of the node output file would be "A\_Name.nod."

Next is a pair of radio buttons. Depending on which one is selected, **SutraGUI** will either only create the SUTRA input files or will create the SUTRA input files and then run SUTRA.

Next there are three radio buttons that can be used to control how much error checking will be done during the export of the SUTRA input files. The first choice (Show all warnings) is selected by default. The user also can choose either to show only warnings that would cause an invalid SUTRA input file to be created or to show no warnings.

Next, there is a check box that, if checked, indicates that an external calibration program such as UCODE (Poeter and Hill, 1998) or PEST (Doherty, 1994) is running Argus ONE. If the calibrate checkbox is checked, several changes will be made to the batch file that **SutraGUI** creates to run SUTRA. First, a "wait" option will be included after SUTRA. This will cause the operating system to wait until after SUTRA has finished running before processing the next line of the batch file. Second, a new line will be added to the batch file after the one that starts SUTRA. This will call the program "WaitForMe" described in Winston (1999). The external program that is running Argus ONE should also call WaitForMe just after sending the commands to Argus ONE to start creating the SUTRA input file. When WaitForMe is run a second time, the first and second copies of WaitForMe will close, which will signal the calibration program that it can now read the results from SUTRA. The third change made to the batch file if the "Calibrate" checkbox is checked is that the "pause" command will not be included at the end of the batch file.

Below the calibrate check box, there is the **SUTRA Path** edit box in which the user specifies the full path of the SUTRA program. A "Browse" button next to the edit box can be used to select the full path of the SUTRA program interactively.

Below the **SUTRA Path** edit box, there is a checkbox labeled **Save temporary files for reuse by SutraGUI**. If this checkbox is checked, certain temporary files created by **SutraGUI** will be saved for reuse the next time the SUTRA input files are created. The temporary files that are saved contain the input data for certain data sets in SUTRA. If those data sets have not changed since the last time the SUTRA input files were generated, the user can save time by not exporting those data sets again. However, the data sets must still be present in the SUTRA input file. To solve this problem, **SutraGUI** creates a separate temporary file (saved in the working directory for the project) for each data set and then combines them in the final SUTRA input file. If the checkbox to save the temporary files is checked, the temporary files are not deleted after the final input file is generated and can be reused the next time the SUTRA input files are generated. If the **Save temporary files** checkbox is not checked, and only some data sets should be exported, **SutraGUI** will disassemble the prior versions of the input files (that must be located in the working directory for the project) to create a temporary file for each data set. Those files that are not replaced during the export process will then be incorporated into the new input file.

After the **Save temporary files** checkbox, there is a group of checkboxes with the names of data sets in the SUTRA input file. In order to save some execution time for **SutraGUI** export, if some of the data sets can remain the same as they were when they were last exported, the user can uncheck the corresponding checkbox and the data sets will not be exported again. Only those data sets that can require a substantial amount of time to export have corresponding checkboxes. The other data sets are always exported. The **None** and **All** buttons beneath the checkboxes will cause none or all of the checkboxes to become checked, respectively.

Finally, on the separate **Memory options** tab, there is a set of options that affect memory usage during export of the SUTRA input files in 3D models. During the export process, **SutraGUI** must determine the polyhedron around each node that represents the cell of that node. This can be a computationally intensive and time-consuming process. However, in large models, the

amount of memory required to store the polyhedrons can be prohibitive. The **SutraGUI** has several options for dealing with this situation. In almost all cases, the best choice is the default choice, which is to recalculate the polyhedrons each time they are needed. For some small models, a better choice may be to calculate the polyhedrons once and them keep them in memory. However, for larger models, the computer may start to use virtual memory, which tends to be slow. When the computer is using virtual memory, some items that would normally be in physical memory are stored on the hard drive and then read back into physical memory when needed. Another option provided by the **SutraGUI** is to save the polyhedrons to a file on the disk. This allows the polyhedrons to be read from the disk file during a future run. However, it is usually faster to compute the polyhedrons than to read them from disk so this option will not be advantageous in most circumstances.

# **Evaluating Model Results**

**SutraGUI** can display model results only from 2D SUTRA models, but can do this in a variety of ways within Argus ONE. Results from 2D and 3D SUTRA models can be displayed in both Model Viewer (Hsieh and Winston, 2002), which provides 3D color visualizations, or SutraPlot (Souza, 1999), which mainly provides 2D views slicing through the 3D results.

To display 2D SUTRA results in **SutraGUI**, select **PIEs**|**SUTRA 2D Post Proc...** Then select the node or element file to display the results from it. A dialog box will appear in which the user can select the data sets to plot. Any data set that is set to **YES** will be plotted. By default, no data sets are plotted. If a particular data set is absent from the output file, it is shown in the dialog box as an uppercase **NO**. If the data set is present but has not been selected, it is shown in the dialog box as a lowercase **no**. Clicking on a column heading will change all the data sets labeled **no** in that column to **YES**. After data sets have been selected, the user clicks the **OK** button to create Argus ONE Data layers containing data points with the data and an Argus ONE Map containing contour maps of the data. The data in the Data layers may be used to create other sorts of post-processing charts as described in the Argus ONE User's Guide (Argus Interware, Inc., 1997).

# Example Applications of SutraGUI

This section provides the user the opportunity to begin using **SutraGUI** quickly for a few applications without reading any other parts of this report. In-depth details and discussions of the various steps, windows, and dialog boxes encountered below may be found in other parts of this report. The following step-by-step examples should be followed in sequence.

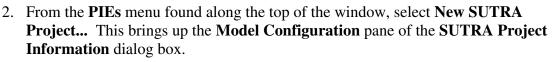
## Areal Ground-Water-Flow Model

This example shows how to create an areal steady-state ground-water-flow model (ignoring solute transport), run SUTRA, display simulation results, and save the project for use in subsequent step-by-step examples.

Assume that there are four lakes, one at each corner of a closed alluvial valley. The lakes control the hydraulic head at each corner, and no flow crosses the bedrock sides of the valley. A hydraulic head value will be specified where each lake exists. Assume that three of the lakes are at the same elevation, which is somewhat higher than the fourth lake.

# Entry of Hydrogeologic Data

1. Double-click on the Argus ONE icon. This opens Argus ONE.



3. The **Model Configuration** pane is where the type of problem to be simulated is chosen. To select the default type of **AREAL**, click on **OK**. This sets up a problem of areal flow with constant-density solute transport using an irregular finite-element mesh.

The other panes allow the user to specify values for the SUTRA simulation that are not spatially variable; that is, those that may have only a single value, such as "time step." These may be inspected on the various panes by clicking on the list of panes on the left. Rather than making changes here now, accept the default values by clicking **OK**. This brings up a new Argus ONE window, called "untitled1."

Default values are given in Table 3 and Table 4. The default values set up simulation of steady-state ground-water flow (and solute transport of a non-reactive solute) in a sandy-type aquifer.

4. The Argus ONE window is where the model will be designed, run, and evaluated. It contains many layers in a stack; each layer will hold either model or mesh information. Additionally, another window, the *Layers' Floater* can be shown by clicking on the *Layers* button 2. It allows users to see which layers are available. This window may be resized to display the full layer names.

The *Layers' Floater* shows which layers are available for the particular problem type (AREAL) chosen in step 3. It allows the user to control which of the layers will be visible (those with the open eye ) and which layer is active and thus available for

input from the screen. Clicking on an "eye" toggles the layer visibility. (The icon changes to a closed eye >.) Clicking to the left of an "eye" makes the layer active and puts a check mark next to it.

- 5. One way to begin a modeling project is to enter hydrogeologic information for the area into the appropriate geospatial *Information* layers provided in **SutraGUI**. The layers listed in the *Layers' Floater* (for example, **Porosity**, and **Hydraulic Conductivity**) have already been assigned default values by the interface (these values are shown in Table 7.) Rather than modify any of these values, in this step-by-step example, the defaults will be accepted. A situation will be considered in which only boundary conditions need be assigned to make a model.
- 6. To enter the lakes into the model, activate the **Specified Hydraulic Head** layer by clicking to the left of its "eye" in the *Layers' Floater* window. A check mark should appear where the dialog box was clicked indicating that the layer is now the active layer.
- 7. Draw a lake by first activating the contour-drawing tool . Then move the cursor into the white workspace and click at three locations, creating the first vertices of a closed contour. Try to create a lake similar to one of the four shown in <u>figure 20</u>. Then, double-click on the location desired for the last vertex. The *Contour Information* dialog box appears.

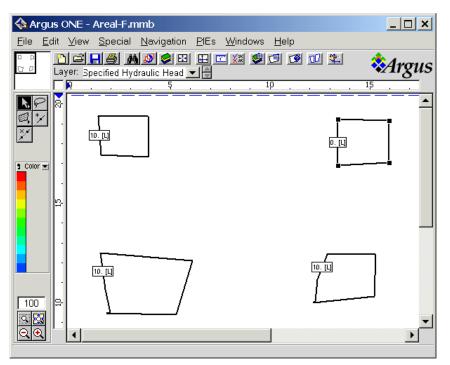


Figure 20. Lakes in Areal Ground-Water-Flow Step-by-Step Example.

8. The specified head value and concentration of water potentially entering the aquifer from the lake must be specified in the dialog box. This is done by clicking next to **specified\_hydraulic\_head** (below *Value*) and entering the head, then clicking next to concentration and entering a concentration, and finally clicking *OK*. For the first

lake, specify 10.0 for the head, and enter 0.0 for the concentration. For this step-bystep example, all the lakes contain no solute. The other parameters in the *Contour Information* dialog box can be ignored for the time being.

9. Draw the other three lakes by clicking to create small closed regions similar to the ones shown in <u>figure 20</u>. For each lake, double-click on the last vertex to close the shoreline. This brings up the *Contour Information* dialog box for each lake. For two of the remaining lakes, enter 10.0 for the head, and for the last lake, enter 0.0 for the head. For all lakes, enter 0.0 for the concentration.

This completes entry of hydrogeologic data for simulating ground-water flow in this system.

#### **Mesh Generation**

- 10. Now draw the model boundary. Make the **Domain Outline** layer active by clicking to the left of its "eye" in the *Layers' Floater*. This makes the **Domain Outline** layer active, although the **Specified Hydraulic Head** layer remains visible. The purpose of the **Domain Outline** layer is to contain model boundary locations. The model boundary will follow the valley walls and the corners will be placed at the center of the lakes.
- 11. Draw a model boundary by first activating the *Domain-Outline-drawing tool* . Then move the cursor into the white workspace and click in the center of one of the lakes. Proceeding around the workspace, click at the center of each lake. Try to create a domain outline that looks like the one shown in <u>figure 21</u>. Then, double-click at the center of the last lake to close the model domain contour.

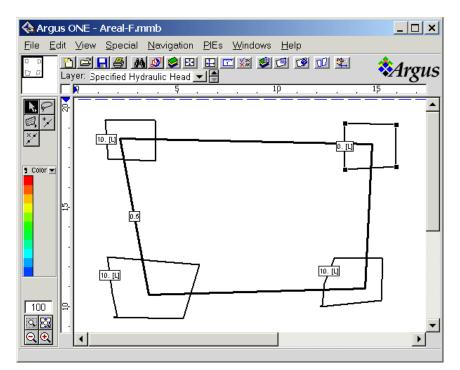


Figure 21. Model boundary in areal ground-water-flow step-by-step example.

- 12. The *Contour Information* dialog box appears. In it, specify the desired typical size of finite elements to be created by the mesh generator is specified. Type 0.5 in the space below the label, *Value*. This sets the desired width of an element to 0.5 in the units shown in the rulers around the periphery of the workspace. The result should look similar to the model boundary shown in <u>figure 21</u>. Click *OK* to exit the dialog box.
- 13. Next, the finite-element mesh will be created. Activate the **SUTRA Mesh** layer by clicking to the left of its "eye" in the *Layers' Floater*.
- 14. Click on the 'magic wand' and then click the magic-wand cursor inside the model boundary just drawn. An irregular finite-element mesh containing elements with a size of about 0.5 is generated and displayed. Figure 22 shows the type of mesh that may be expected.
- 15. The bandwidth of a newly generated irregular mesh always needs to be reduced. Select the *Special Renumber*... This brings up the *Renumber* dialog box. Click on *Optimize Bandwidth* and then *OK*. The mesh numbering is then optimized for the matrix solver currently used by SUTRA.

The entry of data and preparation of the mesh for simulating ground-water flow in this system is now completed.

## **Running SUTRA**

16. Save the project so far by selecting *File*|*Save As...* menu item. Select the desired directory and type in the desired name (for example, "Areal-F" for areal flow model) and then click on Save. A project file called Areal-F.mmb is created in the directory chosen by the user, and the window name becomes the same, as shown in <u>figure 22</u>.

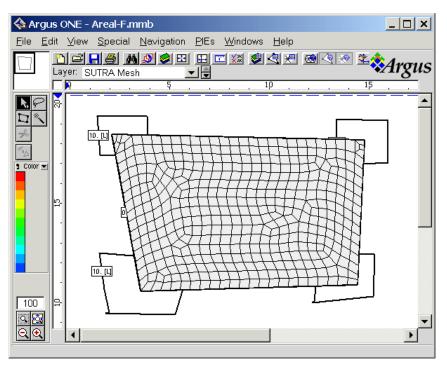


Figure 22. SUTRA mesh in areal ground-water-flow step-by-step example.

- 17. The model information now needs to be exported from Argus ONE creating input files that SUTRA requires, and the simulation can then be run. (Note: the SUTRA Mesh layer must be active to export.) Select PIEs Run SUTRA. The Run SUTRA dialog box appears.
- 18. This dialog box allows the user to choose only creation of SUTRA input files, or creation of files and running of SUTRA (the default). Click **OK** to proceed. An **Enter export file name** dialog box appears.
- 19. Select the directory into which the SUTRA input files will be placed by Argus ONE. Then select the name of the files by typing in the space next to File Name (for example, "Areal-F.inp"). The files created will all begin with the name entered here and the suffixes will be appended (for example, Areal-F.inp, Areal-F.ics).

Note: the Save as type box can be ignored.

20. Click on the **Save** button and the export takes place while the barber pole is visible, and then the SUTRA simulation is run while the DOS window is visible. If requested, hit any key to exit the DOS window. Now, the completed SUTRA simulation has created (at least four) output files (Areal-F.lst, Areal-F.rst, Areal-F.nod, and Areal-F.ele) in the directory that was selected.

## **Displaying Results**

- 21. To display the results, select **PIEs**|**SUTRA 2D Post Proc...** An Open File dialog box appears in which the user can select the "nod" or "ele" files produced by the model.
- 22. Find the directory selected above for the SUTRA files and double-click the appropriate nod or ele file (Areal-F.nod or Areal-F.ele). This brings up the **Select SUTRA results to display** dialog box.

23. This dialog box contains a list of all results available from the SUTRA simulation for visualization. Because the simulation was for steady-state conditions, only one time step appears. Click on the **no** below Pressure to change it to **YES** (this selects a contour map of head). Also, select a velocity vector map by changing the **no** below Velocity to **YES**. Then click on **OK** and the plots of velocity vectors and head contours (similar to that in <u>figure 23</u>) are created.

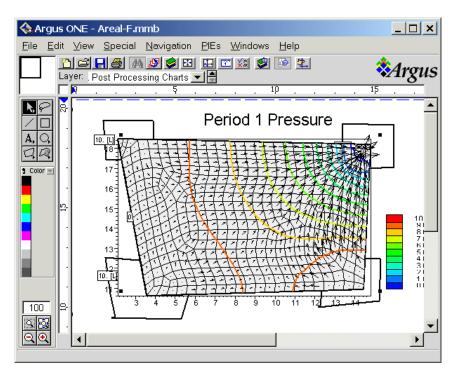


Figure 23. Head and vector plot in areal ground-water-flow step-by-step example.

- 24. Because the **SUTRA Mesh** layer was active, the mesh hides the plots. To make them visible, activate the **SUTRA Post Processing Charts** layer (click left of the "eye" for that layer in the *Layers' Floater*).
- 25. The plot appears, but the window is too cluttered because the mesh is also visible. Make the mesh invisible by clicking on the 'eye' next to **SUTRA Mesh** in the *Layers' Floater*.
- 26. Save the current state of the project by selecting *File Save*.
- 27. The Argus ONE application may now be closed by selecting File|Quit. When the project is reopened, it will be in the same state as when it was closed.

Ground water flows into the aquifer from three of the lakes and exits at the fourth lake. Hydraulic head in the aquifer decreases near the outflow lake.

## Areal Solute Transport Model

This step-by-step example continues the basic areal steady-state ground-water-flow model and considers steady-state solute transport that occurs in the steady-state flow field. Then SUTRA is run, simulation results are displayed, the display is modified, and the project is saved for use in subsequent examples.

- 1. Double-click on the Argus ONE icon to open Argus ONE.
- 2. Select *File*|*Open...*, to bring back the project that was saved in the previous step-bystep example. In the *Choose file to open:* dialog box that appears, move to the appropriate directory and double-click on the ".mmb" project file that was saved in the above example (for example, Areal-F.mmb). This returns the user environment to the same state as when the project was previously saved (<u>fig. 23</u>).

Assume that the lake in the corner diagonally opposite the lake with the lowest water level contains a solute with a concentration of 100 units. The other lakes have no solute, as was previously entered. This information will be treated as the concentration of fluid that enters the aquifer from the lake, and is associated with the specified head boundary condition at the lake.

- 3. To input this information, activate the **Specified Hydraulic Head** layer. This brings to the top the layer in which the lakes were entered.
- 4. Next, select the lake diagonally across from the low-head lake by double-clicking on it. This brings up the *Contour Information* dialog box. Double-click next to concentration (below *Value*) and type in 100 to enter the concentration of fluid from the lake that may flow into the aquifer. Note that the **specified\_hydraulic\_head** is still set to 10. Click *OK* to exit the dialog box. This is the only modification required before exporting the data from Argus ONE and rerunning the simulation.
- 5. To export and run, activate the SUTRA Mesh layer again. Select PIEs|Run SUTRA.
- 6. Click **OK** in the **Run SUTRA** dialog box, select the directory into which the SUTRA input files will be placed, and select the name of the new files that will run a solute transport simulation (for example, "Areal-T"). Ignore the **Save as type** box. Click on **Save** to export and run.
- 7. If needed, press any key to exit the DOS window in which the SUTRA code was run.
- 8. This time, results for concentration and velocity will be plotted. First, the old plots of heads and velocities will be removed. Activate the **SUTRA 2D Post Processing Charts** layer and select *Edit Select All*. (If *Select All* is disabled, everything is already selected.) Then press the delete key to remove both plots.
- 9. To display the new results, select **PIEs**|**SUTRA 2D Post Proc...** The **Open File**: dialog box appears.
- 10. Find the directory selected above for the SUTRA files and double-click the appropriate "inp" file (for example, Areal-T.inp). This brings up the **Select SUTRA** results to display dialog box.

- 11. Click on the no below Concentration to change it to YES (this selects a contour map of concentration). Also, select a velocity vector map again by changing the no below Velocity to YES. Then click on OK. SutraGUI will prompt the user to either overwrite the previously imported data or create new layers. Choose to overwrite the existing data. The user must make that choice for each of the three layers whose data are being overwritten. Once that is done, the plots are created.
- 12. The plot is too cluttered because the mesh is visible. Make the mesh invisible by clicking on its "eye." A plot of velocity vectors and concentration contours (similar to that shown in <u>figure 24</u> but with fewer contours) will be shown.

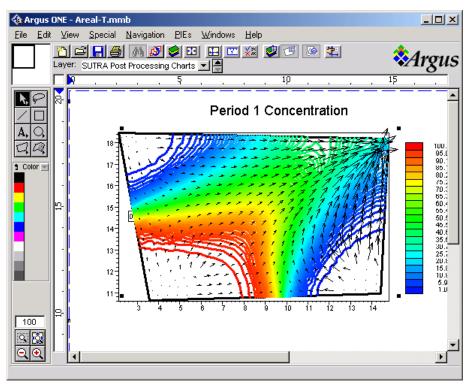


Figure 24. Concentrations and velocities in areal solute transport step-by-step example.

The steady-state solute plume from the lake containing solute fills the central portion of the aquifer, but due to dispersion, is somewhat diluted before it discharges to the low-head lake. The distribution of no-solute waters from the side lakes also is apparent, and these waters increase in solute concentration due to dispersion from the plume before discharging.

13. Each plot may be edited. For example, the contours may be made denser as follows. Double-click on the contour plot to bring up the *Contour Diagram* dialog box. Note that there are two plots visible and each has separate controls. The dialog box for the wrong one may appear if the wrong plot on the screen was double-clicked. The plot frames are visible on the screen and the user should click on a spot bounded by only *one* frame, the one desired. This may require some experimentation. If the wrong dialog box appears (that is, the *Vector Diagram* dialog box), click on *Cancel* in the dialog box and try again. Clicking on the color scale for the concentration diagram will probably select the concentration diagram.

- 14. To make contours thicker, select *3 Points* near the bottom of the dialog box. To plot more contours, change the numbers in the box. For example, set Minimum to 1.0, set Maximum to 100.0, and set Delta to 1.0. Click on *OK* and the plot is drawn. The plume is displayed in nearly solid color. (The smoothness of the color scale shown depends on the type of graphics available on the computer, and on the number of colors and resolution selected in the operating system.)
- 15. Save the current state of the project by selecting *File*|*Save As...* and choose a new project name (for example, Areal-T.mmb) to distinguish this from the previous model of only ground-water flow.
- 16. The Argus ONE application may now be closed or continue with step 2 of the following step-by-step example.

# Areal Solute Transport Model with Barrier

This step-by-step example continues the areal steady-state transport model and considers the change that occurs in steady-state solute transport observed above if there is a low-conductivity barrier within the aquifer. The barrier is added, its discretization is evaluated visually, the information is exported, the simulation is run, and the results are displayed. Finally, the barrier's properties are changed and the simulation is run again.

- 1. Start Argus ONE, and open the ".mmb" project file that was saved in the above example (for example, Areal-T.mmb). Note that this may also be done by double-clicking the ".mmb" project file name in any 'file manager' window.
- 2. Activate the *Hydraulic Conductivity* layer. A low-conductivity region will be created that extends partway across the aquifer.
- 3. Hide the **SUTRA Post Processing Charts** layer to simplify the workspace.

4. With the closed-contour drawing tool, create a closed contour that extends across one side and partway across the model domain (<u>fig. 25</u>), partly blocking the outflow lake. After closing the contour, enter the value 0.0001 for the **maximum** and **minimum** values of hydraulic conductivity, and click *OK* in the *Contour Information* dialog box. (Any contour object or region in the **Hydraulic Conductivity** layer has three parameters that contain the spatial distributions of maximum and minimum conductivity components and the angle of the maximum direction to the X-direction in the workspace. Thus, conductivity may be set to be anisotropic.) This decreases the conductivity of the region by ten times relative to the background value (0.001) used for conductivity.

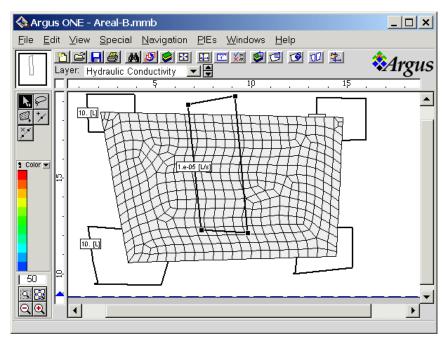


Figure 25. Low-conductivity barrier in areal solute transport step-by-step example.

- 5. Because the conductivity distribution includes a specific 'object' of low value, the interpretation method that Argus ONE uses by default for assigning values throughout the workspace must be changed. (The default method is intended for interpreting contour maps of conductivity.) To change the method, click on the *Layers* button in the *Layers' Floater*. This brings up the *Layers* dialog box.
- 6. In the *Layers* dialog box, many attributes of available layers may be changed and new layers may be added or existing ones deleted. Select the **Hydraulic Conductivity** layer in the top half of the dialog box by clicking on the line in which it is found. If it is already highlighted then it is not necessary to click on it. (Note that the default values of the layer's parameters are shown in the bottom half of the dialog box.)
- 7. At the bottom of the dialog box, *Nearest Contour method* appears as the interpretation method for this layer. Hold the mouse button down over this box and select *Exact Contour method* instead. Then click *Done*.
- 8. To visually determine whether the barrier shape is discretized sufficiently by the current mesh, make the **SUTRA Mesh** layer active.

- 9. Hold down the mouse button over the triangle next to the word *Color* along the tool palette on the left edge of the window. A list of parameters of the **SUTRA Mesh** layer appears that vary by element (rather than by node). Select **PMAX** (the maximum component of hydraulic conductivity. The reader is referred to Table 8, "SUTRA mesh parameters used in two-dimensional (2D) simulations" and section 7.1 of the SUTRA documentation (Voss and Provost, 2002) for more information about PMAX.
- 10. The elements are colored according to maximum conductivity value (The reader is referred to <u>figure 26</u> for an example). The barrier may now be examined to determine whether it was sufficiently discretized. For example, the user may wish to avoid having high-conductivity 'holes' through the barrier because elements are too large. If adjustments are needed, it is suggested that, for simplicity, the barrier be widened rather than refining the mesh at this point. Try adjusting the shape of the barrier by activating the *Hydraulic Conductivity* layer, clicking on one of its vertices, and dragging it to a new position. Note that the zonation shown in the mesh layer adjusts automatically to the new barrier shape.

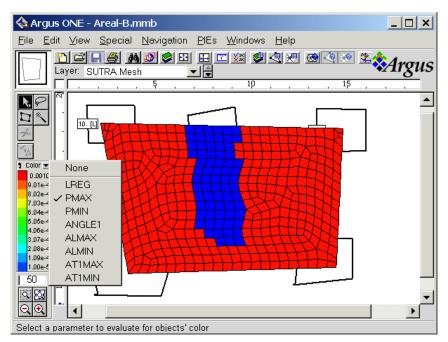


Figure 26. Mesh representation of low-conductivity barrier, areal solute transport step-by-step example.

- 11. When the barrier is satisfactory, the project may be exported (use a new name for SUTRA files, for example, Areal-B) and run. Activate the *SUTRA Mesh* layer, export, and run as before.
- 12. Display the new steady-state concentration contours and velocity field to evaluate the effect of the barrier.

- 13. Evaluate the effect of further reducing the conductivity of the barrier by ten times by activating the *Hydraulic Conductivity* layer, double-clicking on the contour, and adjusting the **maximum** and **minimum** values in the *Contour Information* dialog box. Then re-export, re-run and display the results.
- 14. Save the revised project as a new project file (for example, Areal-B.mmb).

## Areal Model with Transient Solute Transport

Rather than evaluating only the steady state of the solute plume, as in the previous step-by-step examples, its evolution over time is simulated and displayed in two ways in the following example.

- 1. Select *File*|*Open...* to restore one of the projects modeling transport or if Argus ONE was not closed after the last example, continue to the next step.
- 2. To make the most recent steady-state transport simulation into a transient simulation, the **SUTRA Project Information** must be modified. Bring up this dialog box by using **PIEs**|**Edit Project Info...**
- 3. In the **SUTRA Project Information** dialog box, parameters that are not spatially dependent in the SUTRA code may be modified. They are all assigned default values initially. Select the pane named **Modes, Numerical Controls**.
- 4. Hold the mouse button down over the entry that says Steady-state ground-water flow: Steady-state solute transport, and select Steady-state ground-water flow: Transient solute transport instead. Also, set the Hydraulic Head Boundary Condition factor, GNUP to 1.0E-3 to provide a good match of specified and calculated heads.
- 5. Select the **Temporal Controls** pane to adjust the time steps for the simulation. Set the number of time steps to run to 50 (**ITMAX** = 50) and the time-step size in seconds to 100 (**DELT** = 100). In order that the simulation not stop because of the maximum allowed simulation time, set **TMAX** = 1.E99.
- 6. Select the **Output Controls** pane to adjust the frequency of output to every 5 time steps by setting **NCOLPR=5**.
- 7. Click **OK** to exit the dialog box. Save the project (for example, to Areal-tr.mmb).
- 8. Set the active layer to **SUTRA Mesh**, export the project (for example, to filename prefix Areal-tr), and run the simulation.
- 9. Inspect transient transport results by using **PIEs**|**SUTRA 2D Post Proc...** and select the nod file (for example, Areal-tr. nod) just created. Results for time steps 5, 10, 20, and 40 seconds will be viewed.
- 10. The Select SUTRA results to display dialog box appears.

Because the simulation used steady-state flow, velocity may only be plotted for the first time step (a **no** is available to toggle to **YES** only for **Time Step** 1 under **Velocity**). Although it appears that **Pressure** is also available to plot for all time steps, the pressures are all the same because the flow is at steady state. **Concentration** for any time step may be viewed.

To view results for **Time Step 5**, toggle the **no** to **YES** for **Velocity** and **Concentration** in the appropriate line of the dialog box, and click on **OK**.

- 11. When prompted, choose to overwrite the old plot and data. Then activate the SUTRA Post Processing Charts layer, and make the SUTRA Mesh layer invisible. This produces a viewable plot of concentrations after time step 5, and steady-state velocities.
- 12. Because the velocities and concentrations come from different time steps, they are not automatically overlain. To change this, first move one of the charts to the edge of the visible area by clicking on it and dragging it to the desired position. Then doubleclick on the other chart and go to the *Position* tab. On it, make sure that the *Overlay Source Data* button is checked. Then go to the other chart and do the same to it.
- 13. Because results for a few time steps will be viewed sequentially, it is advisable to use the same concentration contour levels each time. To pick these levels and adjust the contour plot, double-click on the chart to bring up the *Contour Diagram* dialog box.
- 14. Set the *Minimum* value to 1.0, the *Maximum* to 100.0, and the *Delta* to 1.0. When the user clicks *OK*, the plot is redrawn. Note the position of the leading edge and bulk of the plume for comparison with a later simulation time.
- 15. Now view results for Time Step 10, by again by selecting PIEs|SUTRA 2D Post Proc... Re-select the nod file created for this simulation. In the Select SUTRA results to display dialog box, toggle the no to YES for Concentration in the line for Time Step 10, and click on OK. Choose to overwrite the data in the layers for the data and plots.
- 16. The new plot appears. Reset the contour levels, as was done for time step 5, and note that the leading edge and bulk of the plume have progressed downstream.
- 17. The plot may be printed to a printer or file at this point, by selecting **File**|**Print...**, and modifying the **Print** dialog box that appears.
- 18. Repeat steps 15 through 17 to view results for time step 20, and then once again for time step 40. Save the project.
- 19. Finally, the progression of the plume may instead be viewed for all time steps at once. First, make all layers invisible except the **SUTRA Post Processing Charts** layer, by clicking on the *Show: None* button at the top of the *Layers' Floater*.
- 20. Select **PIEs**|**SUTRA 2D Post Proc...** and then reselect the nod file (for example, Areal-tr.nod).
- 21. In the Select SUTRA results to display dialog box, click on the word Concentration along the top of the window; this makes each no in the column into a YES and selects plots of all the available concentration results. Then click OK.
- 22. Click **OK** again to allow the layer to be cleared when so prompted, and the new plots appear. If these appear small, then they may be zoomed into view by clicking on the

zoom tool at the lower left corner of the window . Then click and drag a box around the group of small plots to increase their size. This type of plot can provide a good preview of the concentration results for all of the time steps selected for output in the SUTRA simulation. Save the project.

## Areal Model with Transient Solute Transport and Observations

In some cases, a graph of head or concentration plotted against time at some particular location is required. This example shows how to create such a plot using **GW\_Chart** (Winston, 2000).

- 1. Using **File**|**Open...**, restore the projects modeling transient solute transport. Alternatively, if Argus ONE was not closed after the last example, continue to the next step.
- 2. Make the **Observation** layer the active layer.
- 3. Create a point contour somewhere in the middle of the solute plume and assign the is\_observed parameter a value of 1 or True.
- 4. Copy the contour to the clipboard and paste it on the **Domain Outline** layer.
- 5. Double-click on the contour pasted on the **Domain Outline** layer and assign it a value of 0.
- 6. Make the **SUTRA Mesh** layer the active layer, click on the *Magic Wand* tool, and then click inside the domain outline.
- 7. In the dialog box, choose *Delete All*. A new mesh will be created including a node exactly at the position of the contour pasted into the **Domain Outline** layer.
- 8. Select **PIEs** Edit Project Info... and go to the **Output Controls** pane. Change NOBCYC to 1 and click the OK button.
- 9. Select *Special Renumber* and choose to optimize the bandwidth.
- 10. Run SUTRA and save the project.
- 11. Start **GW\_Chart** (Winston, 2000).
- 12. Select Chart Type|Hydrographs.
- 13. In the group of radio buttons labeled **Data**, choose **SUTRA**.
- 14. Click on the Read button and select the observation file (with the extension .obs) for the model.
- 15. In the group of radio buttons labeled **SUTRA Data**, choose the one labeled Concentration.
- 16. In the upper left is a table with a list of the observation node numbers. In the column labeled Plot, change the No to Yes and then click somewhere outside the cell. A plot of concentration vs. time should appear.

# Henry Seawater-Intrusion Problem with Variable-Density Flow

This step-by-step example reproduces a classic simulation example for testing variable-density transport codes that is presented as an example simulation in the SUTRA documentation (Voss, 1984, section 6.5, page 196). It involves creating a rectangular cross-sectional model domain containing a FishNet Mesh, and applying boundary conditions exactly along the two vertical edges of the domain. Along one edge, a total fluid inflow is specified and SutraGUI is allowed to distribute the value of fluid sources along the edge. Along the other edge, the user creates a specified pressure condition in a single object that linearly increases with depth representing hydrostatic seawater. The user should read the above-mentioned section of the SUTRA documentation for background on this problem before beginning.

- 1. Start Argus ONE. In the **SUTRA Project Information** dialog box, select a crosssectional orientation with saturated flow, solute transport with variable-density fluid, using pressure, user-specified model thickness, and a FishNet Mesh.
- 2. In the **SUTRA Project Information** dialog box, a number of changes to the initial default values are required to match the Henry problem.
  - On the **Headings** pane, set **TITLE1** to "Henry Problem from SUTRA Documentation." Clear **TITLE2**.
  - On the Modes, Numerical Controls pane, select Transient ground-water flow: Transient solute transport
  - On the **Temporal Controls** pane, set **ITMAX**=100, **DELT** = 60, and **TMAX** = 1.E9
  - On the **Output Controls** pane, set **NPRINT=50**
  - On the Fluid Properties pane, set SIGMAW=18.8571E-6, and VISCØ = 1.E-3,
  - On the **Production**, **Gravity** pane, set **GRAVY** = -9.8

Then click **OK**.

- 3. In the Argus ONE window, select **Special Drawing Size...** and set the size as follows:
  - Horizontal Extent: = 4
  - Vertical Extent: = 3
  - Horizontal Origin: = -1
  - Vertical Origin: = -1
- 4. The workspace shrinks because of the reduced drawing size. Resize it using the zoom tool and resize the window if necessary.

The next steps create the 2 by 1 model domain by first approximating the shape and then editing to make it exact.

- 5. Activate the **FishNet\_Mesh\_Layout** layer.
- 6. Click on the *Element drawing tool*
- 7. While holding down the shift key on the keyboard, place four vertices at about (0,0), (0,1), (2,1) and (2,0). The shift key causes lines to be drawn horizontally and vertically.
- 8. Choose the Arrow button **b** and double-click on the element. This brings up the *Element Information* dialog box. Set elements\_in\_x=20 and elements\_in\_y=10. Click OK.

Click outside the element to deselect it. Then double-click on the lower left node. In the *Node Information* dialog box, set *Position X* to 0 and *Position Y* to 0. Double-click on each node in turn and adjust their positions so that their coordinates are (0, 0), (2, 0), (2, 1), and (0, 1) and then save the file.

The next steps create a line source exactly along the left vertical edge of the domain representing inflow of fresh water to the cross section. The total inflow across this boundary (0.066) and the solute concentration of inflowing freshwater (0.0) are specified.

- 10. Select **PIEs**|**Convert...** In the dialog box that appears, select (**Mesh Objects to Contours...**). Click the **OK** button.
- 11. In the next dialog box, choose the **FishNet\_Mesh\_Layout** layer and click the **OK** button.
- 12. In the next dialog box, choose the Sources of Fluid layer and click the OK button.
- 13. In the next dialog box, click on the left side of the rectangle that represents the element in the **FishNet\_Mesh\_Layout** layer and click the **OK** button.
- 14. When prompted to turn "Allow Intersection" on, click the No button.
- 15. Activate the **Sources of Fluid** layer and double-click on the open contour just imported in to it to bring up its *Contour Information* dialog box.
- 16. The user may specify either a total source value for the open contour object, or a source per length of the object. Only one of these may have a value, and the other **must** be set to \$N/A, meaning 'undefined'. Set:
  - $total\_source = 0.066$
  - specific\_source = N/A
  - concentration\_of\_source = 0.0

and click OK. Save the project.

The following steps create a background value for the **Specified Pressure** layer that represents the pressure of seawater under hydrostatic conditions. This background value provides a pressure everywhere in the workspace. Sea level is set at elevation y=1 and pressure increases below this point. The density of seawater is given by the linear fluid density expression used by SUTRA, (1000. + 700. \* 0.0357), gravity is 9.8, and depth is given by (1. - y).

- 17. Open the *Layers* dialog box either by clicking the appropriate tool button along the top of the window or the *Layers*... button in the *Layers' Floater*.
- 18. In the upper window, click on the Specified Pressure layer to select it.
- 19. In the lower window, hold the mouse button down over the *Value* column of **specified\_pressure** and click the *fx* button.
- 20. In the *Expression Editor* that appears, type the following equation:

(1000. + 700. \* 0.0357) \* 9.8 \* (1. - Y())

Then click OK.

*Note: Y*(*) is an Argus ONE function and may be automatically inserted by clicking on Mathematical (under Functions) in the lower left list, and then clicking on Y in the lower right list.* 

- 21. Click on **concentration** in the *Layer Parameters* (lower half of the dialog box). Then click in the *Value* column and click the *fx* button.
- 22. In the *Expression Editor*, set the value to 0.0357, and click *OK*. Click *Done* in the *Layers* dialog box. Save the project.
- 23. Activate the **Specified Pressure** layer and move the cursor up and down in the workspace to observe the varying background pressure value just specified. (The value is shown in the lower left margin of the window.) Note that zero occurs along the top edge of the model domain and pressure increases with depth.

The next steps create a specified pressure boundary condition exactly along the right vertical edge of the superblock by copying the edge from the **FishNet\_Mesh\_Layout** layer and modifying the object's values.

- 24. Select **PIEs Convert...** In the dialog box that appears, select (**Mesh Objects to Contours...**). Click the **OK** button.
- 25. In the next dialog box, choose the **FishNet\_Mesh\_Layout** layer and click the **OK** button.
- 26. In the next dialog box, choose the **Specified Pressure** layer and click the **OK** button.
- 27. In the next dialog box, click on the right side of the rectangle that represents the element in the **FishNet\_Mesh\_Layout** layer and click the **OK** button.
- 28. When prompted to turn "Allow Intersection" on, click the No button.
- 29. Double-click on the newly imported object to bring up its *Contour Information* dialog box. The values shown in the dialog box should be based on the expressions specified for **specified\_pressure** and **concentration**. Click **OK**. Save the project.

When this domain is meshed, nodes falling exactly along this object will be automatically assigned specified pressure values varying with depth and seawater concentration to create the desired boundary condition. In the next steps, the initial default parameter values for various layers will be set to the values required for the Henry problem.

- 30. Bring up the Layers dialog box.
- 31. Highlight the **Porosity layer** in the upper window. In the lower window, reset the initial default value of 0.1 to 0.35 by bringing up the *Expression editor* for the **porosity** parameter.

- 32. Highlight the **Permeability layer** in the upper window. In the lower window, select **maximum** and set its default value to 1.020408E-9.
- 33. Select the **minimum** parameter and set its value to that of **maximum**. To do this, in the *Expression Editor*, select **Permeability** from the lower left list, then double-click **maximum** in the lower right list. The parameter **maximum** then appears in the upper expression window. Click *OK* to exit it.
- 34. Highlight the **Dispersivity layer** in the upper window and set all four dispersivity parameters to zero (0.0).
- 35. Click Done to exit the Layers dialog box. Save the project.

This completes entry of information for the Henry problem. Next, the mesh is created and numbering optimized.

- 36. Activate the SUTRA Mesh layer.
- 37. Select **PIEs**|**Create SUTRA FishNet Mesh**. This creates the FishNet Mesh. (Compare this with the mesh shown on page 197 of the SUTRA documentation.) The bandwidth does not need to be optimized with a FishNet Mesh.
- 38. Inspect the values assigned to nodes and elements in the mesh by double-clicking the node or element of interest. Note the distribution of inflow (**QIN**) along the left-hand boundary nodes, where the upper and lower nodes are assigned half the inflow of the others along the boundary to correctly create a uniform inflow. Note also the distribution of specified pressure (**PBC**) along the right-hand boundary nodes is equivalent to the pressure of a hydrostatic column of seawater.

Finally, the simulation is run, and results plotted.

- 39. Export and run SUTRA.
- 40. Select **PIEs**|**SUTRA 2D Post Proc...** and plot concentration and velocity for time step 100. To plot each 10% of seawater concentration, set *Minimum*: to 0.00357, *Maximum*: to 0.0357, and *Delta*: to 0.00357 in the *Contour Diagram* dialog box. The contours can be made somewhat smoother by changing the contouring algorithm from "Linear" to "Algorithm 626 (use layer triangulation)." Then, to compare with the results found in the SUTRA documentation (Voss and Provost, 2002, fig. 6.11 on page 156), plot each 25% by setting both *Minimum*: and *Delta*: to 0.008925. Save the project.

The user may wish to continue by experimenting with various aspects of this problem. For example, the mesh size may be halved in each direction, a low conductivity barrier or high conductivity channel may be added, or parameters such as dispersivity and diffusion coefficient may be changed and the simulation rerun and results displayed.

### Example Three-Dimensional Model

This step-by-step example shows how to create an example 3D steady-state ground-water-flow and transport model, run SUTRA, and display simulation results.

- Start Argus ONE and start a new SUTRA project. In the SUTRA Project Information dialog box, change the number of dimensions to 3 and select a vertically aligned 3D model. Select SOLUTE (constant-density fluid, using Hydraulic Head).
- On the Structure in Z pane, change the Z discretization (not Number of Units) to 10. Then click the OK button.
- 3. Make the **FishNet\_Mesh\_Layout** layer the active layer and draw one element on it. Click on the arrow button , double-click on the element and assign **elements\_in\_x** and **elements\_in\_y** each a value of 10.
- 4. Make the **SUTRA Mesh** layer the active layer and select **PIEs Create SUTRA FishNet Mesh**. This creates a mesh with 10 rows and 10 columns.
- 5. Make the **Elevation Top** layer the active layer. Click on the *Layers* button or select *View*|*Layers*... Click on the *fx* button for the **elevation top** parameter and change the expression for the parameter to *10*. Click the *OK* button to close the *Expression Editor* and then click the *Done* button.
- 6. This step will set up a low hydraulic conductivity zone reaching from the top of the model to near the bottom. Make the Hydraulic Conductivity Unit1 layer the active layer. Click on the *Layers* button or select *View*|*Layers*... Change the evaluation method for the layer from *Nearest* to *Exact*. Click on the *fx* button for the maximum parameter and change the expression for the parameter to *If((ContourArea()>0)&(Sutra\_Z()>3), 1e-7, 1e-3)*. (When using a digital version of this documentation, the user can select the expression in this document, copy it to the clipboard and paste in the *Expression Editor*. Use Ctrl-V to paste.) Click the *OK* button to close the *Expression Editor*. Click on the *fx* button for the middle parameter and change the expression for the parameter to *maximum* by clicking on Hydraulic Conductivity Unit1 in the lower left window and then by double-clicking on *maximum* in the lower right window, and finally click on *OK*. Set the Expression for the minimum parameter to *maximum* in the same way and then click the *Done* button.

This expression has several parts. First, there is the *If* function: *If*(*Condition*, *True\_Value*, *False\_Value*). The *If* function can be found below *Mathematical* in the expression editor. For this example, if (*ContourArea*()>0)&(*Sutra\_Z*()>3) evaluates to True, the hydraulic conductivity will be set to 1e-7 (the *True\_Value*). Otherwise, it will be set to 1e-3 (the *False\_Value*). The *Condition*, in this case, has two parts: (*ContourArea*()>0) and (*Sutra\_Z*()>3). Both must evaluate to *True* for the entire condition to evaluate to True. When using the *Exact* interpretation method, *ContourArea*() is greater than 0 only inside closed contours. (Using the *Nearest* method, it would be 'true' everywhere in a layer on which there was at least one closed contour, so the *Exact* method must be used.) In the *Expression Editor*, the *ContourArea*() function can be found under *Contour*. **Sutra\_Z**() is the elevation of a node or element in the 3D mesh. In the Expression Editor, the **Sutra\_Z**() function

can be found under **PIEs**. Thus, this condition will only be 'true' inside closed contours on the **Hydraulic Conductivity Unit1** layer for elements whose centers have an elevation higher than 3. The top elevation of the model was set to 10 and the bottom elevation is, by default, 0. The vertical discretization was set to 10 elements. Thus, if a closed contour is drawn on the **Hydraulic Conductivity Unit1** layer and it uses the default values for the **maximum**, **middle**, and **minimum** parameters, a low hydraulic conductivity zone that reaches down to an elevation of 3 will be defined.

7. Draw a closed contour on **Hydraulic Conductivity Unit1** layer similar to that shown in <u>figure 27</u>. It should encompass several columns of cells from the northern to the southern ends of the model but should not reach all the way to the east and west edges of the model. Use the default values for all parameters in the model, so simply click *OK* to exit the *Contour Information* dialog box that appears when the contour is closed.

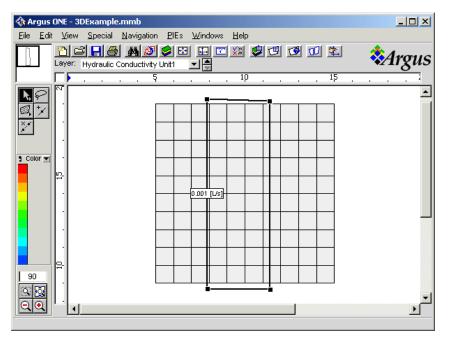


Figure 27. Low hydraulic conductivity zone in three-dimensional example.

8. Next, the dispersivities for the model are set to 0.3. The same methods as before can be used to set the *Expressions* but, in this case, a simpler method is used to set them all at once.

Select **PIEs Edit...** In the dialog box, select **Set Multiple Parameters** and click the **OK** button. A dialog box will appear with a list of all the group layers. Next to each layer is an empty check box. If the group layer has one or more layers controlled by it, it will also have a box with a + or - sign in it. Click the box with the + sign next to **Hydrogeology Unit1** to expand the list of layers in that group. The + sign will change to a - sign and the group of layers will expand to show all the layers underneath **Hydrogeology Unit1**. Next to each of the layers, there is an empty check box. Any of the layers that have parameters that can be set will also have another box

with either a + sign or a – sign. Click on the + sign next to **Dispersivity Unit1** to show the parameters for that layer. Click in the empty check box for one of the parameters. Note that the check boxes for **Dispersivity Unit1** and **Hydrogeology Unit1** change from empty to gray. This indicates that some, but not all, of the check boxes beneath those units are checked. Click on the check box for **Dispersivity Unit1 Unit1**. Note that all of the check boxes for the parameters under **Dispersivity Unit1** become checked.

When the **OK** button is clicked, the expression for all the parameters whose check boxes are checked are changed to the value shown in the **Value** edit box. Change the value in the **Value** edit box to 0.3 and click the **OK** button.

9. Next, the boundary conditions are set. On the right side of the model near the top, there will be a specified head boundary with a head of 10. On the left side, there will be three specified head boundaries with heads of 11. One of those boundaries will have a solute concentration of 100. The rest will all have concentrations of 0.

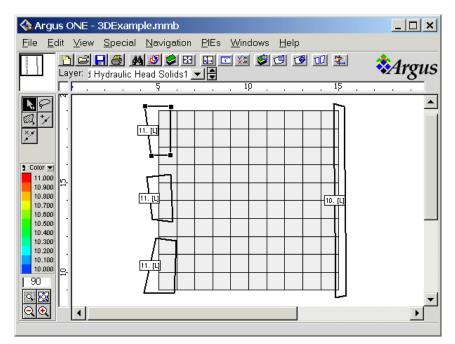


Figure 28. Specified hydraulic heads in three-dimensional example.

Make the **Specified Hydraulic Head Solids1** layer the active layer. On it, draw four closed contours similar to the ones in <u>figure 28</u>. For all the contours, assign **top\_elevation** a value of 11 and **bottom\_elevation** a value of 9.5. For the three contours on the left, assign **specified\_hydraulic\_head** values of 11. For the contour on the right, assign **specified\_hydraulic\_head** a value of 10. For the middle contour on the left, assign **concentration** a value of 100. For the rest, assign **concentration** a value of 0.

Note: If several contours are selected, the Contour Information dialog box will have a "Set All" button. If this button is clicked all the parameters that have a check mark next to their name will be set to the values displayed in the Contour Information dialog box for all the selected contours. An individual parameter can have the check mark next to its name removed by clicking the check mark. The "None" and "All" buttons can also be used to remove or restore check marks.

- 10. To set the initial conditions, make Initial Hydraulic Head Unit1 the active layer. Click on the Layers button or select View|Layers... Click on the fx button for the initial\_hydraulic\_head parameter and change the expression for the parameter to 10.5. Click the OK button to close the expression editor and then click the Done button.
- 11. To run the model, make **SUTRA Mesh** the active layer and select **PIEs**|**Run SUTRA**. Select a root name for the files to be created. Click the **OK** button to export the SUTRA input files and begin running SUTRA. After the SUTRA input files have been created, a DOS window opens and SUTRA runs in it.
- 12. After SUTRA has finished running, start Model Viewer (Hsieh and Winston, 2002).
- 13. In **Model Viewer**, select **File**|**New** to start a new **Model Viewer** project. Change the type of model to **SUTRA** and click on the **OK** button.
- 14. In the next dialog box, click on the **nod** radio button and then click on the **Browse** button next to it. Select the "nod" file for the project created by SUTRA. Then click on the **Browse** button next to **Please specify the "ele" file** and select the "ele" file for the project created by SUTRA. Finally click on the **Browse** button next to **Please specify the "inp" file** and select the "inp" file for the project used by SUTRA. Finally, click on the **OK** button.
- 15. **Model Viewer** will prompt the user to convert the ASCII files to binary ones. **Model Viewer** can read binary files faster than ASCII files; once the conversion is made, using binary files is faster. (The ASCII files are not destroyed when the data in them are converted to binary format. Instead, a new file is created with the required information.) If the user chooses to create a binary file, the extension ".bin" should be used as part of the file name. Using that extension will make it easier to later find the file for use in **Model Viewer**. After making a choice (**No** is suggested for a file as small as this model), click on the **OK** button.
- 16. In the next dialog box, change the data type to **Concentration** and click on the **OK** button.

17. After a short wait, Model Viewer shows an empty box from the top. From the Model Viewer menu, select Show Isosurfaces. Model Viewer then displays isosurfaces of equal concentration (fig. 29). An isosurface is the 3D equivalent of a contour line. It is a surface through locations where some quantity has equal values. In this case, it is a set of surfaces through locations where the concentrations are the same.

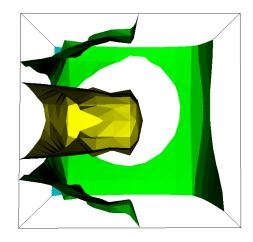


Figure 29. Isosurfaces generated by Model Viewer.

- 18. Hold down the left mouse button and move the mouse. Notice how the image rotates in response to the mouse movements.
- 19. Release the left mouse button, hold down the right mouse button, and move the mouse up and down. Notice how the magnification of the image changes in response to the mouse movements.
- 20. Release the right mouse button, and hold down the left mouse button and the Shift button on the keyboard. Move the mouse. Notice how the position of the image changes in response to the mouse movements.
- 21. Release the Shift button, and hold down the left mouse button and the Ctrl button on the keyboard. Move the mouse. Notice how the image moves laterally in response to the mouse movements.

22. Select Show|None and then Show|Model Features. In the dialog box that appears, click on spec. pressure and then click on the Show --> button. Then click on the up arrow next to Size a few times. Click on the Done button. This has hidden the isosurfaces and shown the locations of nodes that are specified pressure boundaries (fig. 30). (Isosurfaces and boundary nodes can be viewed simultaneously. Hiding the isosurfaces, however, makes the image less cluttered.)

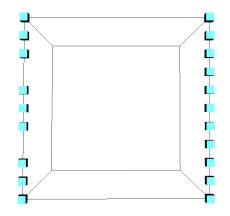


Figure 30. Specified pressure boundaries as seen in Model Viewer.

23. The user may make changes in the model and see how they affect the results displayed in **Model Viewer**. However, if **Model Viewer** has the input or output files for the SUTRA model open, it will not be possible to run SUTRA because the files will be locked by **Model Viewer**. Therefore, **Model Viewer** should be closed before trying to run SUTRA.

#### Nonaligned 3D Model

This example is similar to the previous example except that the mesh is not aligned vertically. It shows how to create such a mesh and assign aquifer properties of boundary conditions to it. Use of the **follow\_mesh** parameter is illustrated in assigning boundary conditions.

- Start Argus ONE and start a new SUTRA project. In the SUTRA Project Information dialog box, change the number of dimensions to 3 and select a nonaligned 3D model. Select SOLUTE (constant-density fluid, using Hydraulic Head).
- 2. On the **Structure in Z** pane, change the **Z** discretization to 10. Then click the **OK** button.
- 3. Make the **FishNet\_Mesh\_Layout Top** layer the active layer and draw one element on it. Click on the arrow button , double-click on the element and assign both **elements\_in\_x** and **elements\_in\_y** a value of 20.
- Make the FishNet\_Mesh\_Layout Bottom Unit1 layer the active layer and draw one element on it. Make its width smaller than the element in FishNet\_Mesh\_Layout Top. Click on the arrow button, double-click on the element and assign both elements\_in\_x and elements\_in\_y a value of 20.

- 5. Make the **SUTRA Mesh Top** layer the active layer and select **PIEs**|**Create SUTRA FishNet Mesh**. This creates a mesh with 20 rows and 20 columns. Repeat this step with the **SUTRA Mesh Bottom Unit1** layer.
- 6. Make the **Elevation Top** layer the active layer. Click on the *Layers* button or select *View*|*Layers*... Click on the *fx* button for the **elevation top** parameter and change the expression for the parameter to *10*. Click the *OK* button to close the *Expression Editor* and then click the *Done* button.
- 7. This step will set up a low hydraulic conductivity zone from the top of the model to near the model's bottom. Make the Hydraulic Conductivity Unit1 layer the active layer. Click on the *Layers* button or select *View*|*Layers*... Change the evaluation method for the layer from *Nearest* to *Exact*. Click on the *fx* button for the maximum parameter and change the expression for the parameter to If((ContourArea()>0)&(Sutra\_Z()>3), 1e-7, 1e-3). Click the OK button to close the *Expression Editor*. Click on the *fx* button for the minimum parameter and change the expression for the same with the minimum parameter and then click the *Done* button.
- 8. Draw a closed contour on **Hydraulic Conductivity Unit1** layer similar to that shown in <u>figure 31</u>. It should encompass several columns of cells from the northern to the southern ends of the model but should not reach all the way to the east and west edges of the model. Use the default values for all parameters in the model, so simply click *OK* to exit the *Contour Information* dialog box that appears when the contour is closed.

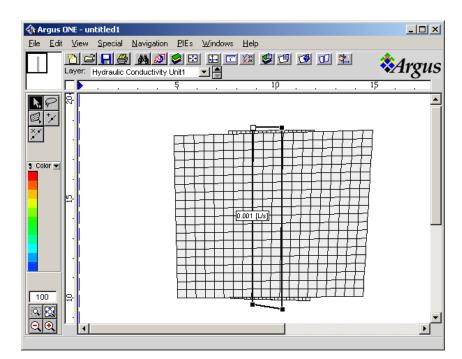


Figure 31. Specified hydraulic heads in nonaligned, three-dimensional example.

9. Next, the dispersivities for the model are set to 0.3. The same methods as before can be used to set the *Expressions* but, in for demonstration purposes, another method is used to set them.

Select **PIEs**|Edit Project Info.... At the bottom of the SUTRA Project Information dialog box, click on the **Parameter Values – Quick Set** button. A dialog box will appear with a list of some model parameters. At the bottom, type in the value 0.3 into each box for **dispersivity**; there are six boxes to fill in. The **Set Now** buttons to the left become **bold** indicating that the value has changed. To actually set the values just entered, click each **Set Now** button or click **Set All** at the bottom of the dialog box. When each button is clicked, the expression for each parameter whose value is referred to is changed to the value just entered in the edit box. Click **Done** to exit the dialog box and then **OK** or **Cancel** to exit the **SUTRA Project Information** dialog box.

10. Next, the boundary conditions are set. On the right side of the model extending from the top to the bottom of the model, there will be a specified head boundary with a head of 10. On the left side, there will be three specified head boundaries with heads of 11. One of those boundaries will have a solute concentration of 100. The rest will all have concentrations of 0. The **follow\_mesh** parameter will be used to make sure the boundary on the right only applies to all the nodes on the edge of the model.

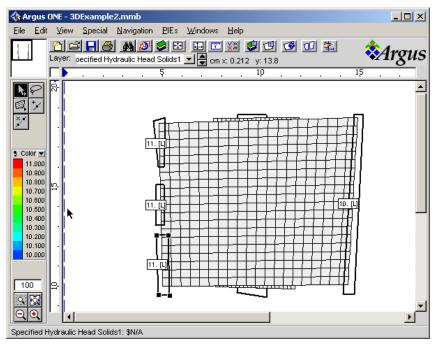


Figure 32. Specified hydraulic heads in nonaligned, three-dimensional (3D) example.

Make the **Specified Hydraulic Head Solids1** layer the active layer. On it, draw contours similar to the ones in <u>figure 32</u>. For all the contours, assign **top\_elevation** a value of 11 and **bottom\_elevation** a value of 9.5. For the three contours on the left, assign **specified\_hydraulic\_head** values of 11 and **bottom\_elevation** a value of 9.5. For the contour on the right, assign **specified\_hydraulic\_head** a value of 10,

**bottom\_elevation** a value of -1, and **follow\_mesh** to 1 or True. For the middle contour on the left, assign **concentration** a value of 100. For the rest, assign **concentration** a value of 0.

- 11. To set the initial conditions, make Initial Hydraulic Head Unit1 the active layer. Click on the Layers button or select View Layers... Click on the fx button for the initial\_hydraulic\_head parameter and change the Expression for the parameter to 10.5. Click the OK button to close the Expression Editor and then click the Done button.
- 12. To run the model, make **SUTRA Mesh Top** or **SUTRA Mesh Bottom Unit1** the active layer and select **PIEs Run SUTRA**. Select a root name for the files to be created. Click the OK button to export the SUTRA input files and begin running SUTRA. After the SUTRA input files have been created, a DOS window opens and SUTRA runs in it.
- 13. Use Model Viewer to view the results of the model as in the previous example. Model Viewer was used to create <u>figure 33</u>, which shows isosurfaces of concentration along with the locations of specified pressure boundaries.

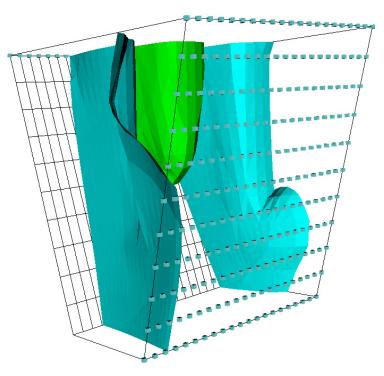


Figure 33. Isosurfaces and boundary conditions displayed by Model Viewer.

# **Summary and Conclusions**

**SutraGUI** is a graphical user-interface for SUTRA. It supports two-dimensional (2D) and threedimensional (3D) simulations. **SutraGUI** is based on a commercial package, Argus ONE<sup>TM</sup> (Argus Interware, Inc., 1997), which provides 2D Geographic Information System and meshing support. For 2D models, the new version of **SutraGUI** described in this report is much the same as the previous version (Voss and others, 1997). For 3D models, the model domain is divided into a stack of tabular units and these units are used to assign aquifer properties, boundary conditions, and initial conditions to different, vertically separate parts of the model. In addition, 3D objects are used to assign boundary conditions. Three-dimensional objects are defined by associating elevations with 2D objects built into Argus ONE. Another feature of this version of **SutraGUI** is a comprehensive Help system.

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# Appendix A. Adding and Linking New Layers

Two examples are presented below that demonstrate a few aspects of adding and linking new layers. The first example involves creation of an areal fluid source from a precipitation map and the second involves defining the thickness of the aquifer from top and bottom elevations.

# Adding a Precipitation Data Layer and Linking it to a Fluid Sources Layer

- 1. Start a 2D SUTRA model.
- 2. Bring up the *Layers' Floater* by clicking on the *Layers*... button along the top of the Argus ONE window.
- 3. Click on the **Layers** button at the top of the *Layers' Floater* window. This brings up the *Layers* dialog box.
- 4. To create the new layer (that will contain the areal distribution of rainfall), use the down arrow to position the highlighted layer to **Sources of Fluid**, and click on button *New* below the label "Layer" (not below the label "Parameter, which would add a parameter to layer Sources of Fluid).
- 5. Set the layer name by typing "Rainfall" to replace the default layer name, "New Layer."
- 6. Change the *Type* to *Data* (from the default of *Information*) by clicking on the word "Information," which will bring up a menu of choices.
- 7. For the **Rainfall** layer to be useful, data will need to be imported into it. The reader is referred to the Argus User's Guide (Argus Interware, 1997) for information on importing data. Close the *Layers* dialog box, import data into **Rainfall**, and then reopen the *Layers* dialog box. A number of parameters may be associated with the imported data; assume that the first parameter contains the rainfall amounts in units [m/year].
- 8. To link the imported information, click on the **Sources of Fluid** layer to highlight it.
- 9. In the parameter listing area, highlight the line containing **specific\_source**, then find the button labeled " $f_x$ ", below the label "Value". Click this button to show the *Expression Editor*.
- 10. In the *Expression Editor*, scroll the left scroll bar until an entry for the **Rainfall** layer can be seen.
- 11. Click on **Rainfall**. The parameter names imported into the layer will then appear in the box to the right.
- 12. The first parameter, "Imported Parameter 1" contains the rainfall values for this example. Double-click on the entry in the right-hand box, and the parameter name will appear in the expression box at the top of the *Expression Editor*.
- 13. To convert the value to [m/s] append the expression "/(365.25\*86400)" to divide the rainfall by the number of seconds in a year. To indicate that only 25% of the rainfall becomes ground-water recharge, click to the left of the parameter name and type "0.25\*." The final expression should be

"0.25\*Imported Parameter 1/(365.25\*86400)."

- 14. Click OK button.
- 15. If the user plans to add point or contour objects to the **Sources of Fluid** layer in addition to the recharge from rainfall, the interpretation method listed at the bottom of the *Layers* dialog box must be set to *Exact Contour method*. (This is the default interpretation method for the layer.) Any other interpretation method will cause the objects to override the distributed rainfall source everywhere in the layer.
- 16. In the *Layers* dialog box click *Done*. The default value of the parameter **Sources of Fluid.specific\_source** is now set to the recharge calculated from the rainfall distribution.

#### Calculating a Thickness from Two New Layers or Two New Parameters

In the following dual example, it is shown how, for a 2D model, thickness may be calculated in two ways. In the first, the two new layers that are added are the elevations for the top and bottom of the aquifer. These layers are then linked to the thickness layer, which calculates the aquifer thickness. In the second example, two new parameters are instead added to the **Thickness** layer in a 2D model. The first example follows:

- 1. Start a 2D SUTRA model.
- 2. Bring up the *Layers' Floater* by clicking on the **Layers...** button along the top of the Argus ONE window.
- 3. Click on the Layers button at the top of the Layers' Floater.
- 4. In the *Layers* dialog box, use the down arrow to position the highlighted layer to be **Thickness**, and click on button *New* below the label *Layer* (not below the label *Parameter*, which would add a parameter to layer **Thickness**).
- 5. Set the new layer name by typing "Top" to replace the default layer name, "New Layer." This layer will be used to set the elevation of the top of the aquifer. The default interpretation type is **Nearest Contour**.
- 6. Add a second new layer and name it "Bottom."
- 7. Click on the *Thickness* layer line to highlight it.
- 8. In the parameter listing area, click the button labeled fx to show the *Expression Editor*.
- 9. In the *Expression Editor*, scroll the left scroll bar until an entry for layer **Top** can be seen.
- 10. Click on entry "Top." That entry will then appear in the box to the right.
- 11. A list of parameters of this layer appears in the right-hand box. In this case, there is only one parameter, "Top." Double-click on the entry in the right-hand box, and the layer (and implicitly for single parameter layers, the parameter "Top" in layer **Top**) name will appear in the expression box at the top of the *Expression* dialog box.

Expression			
Top -		•	OK Cancel Help
7 8 9 * 4 5 6 / 1 2 3 + 0 ≥ ≥ < ≤ = = & 1 () . N	Layers: SUTRA Mesh Domain Outline Mesh Density Observation Thickness Top Bottom Porosity	Top	

Figure 34. Constructing an Equation in the Expression Dialog, example

- 12. Insert a minus sign after "Top" (The reader is referred to figure 34).
- 13. Repeat step 10 to add layer **Bottom** to the expression. The expression "Top-Bottom" should now be in the upper box.
- 14. Click OK.
- 15. If the user plans to add point or contour objects to the *Thickness* layer in addition to the thickness calculated from top and bottom elevations, the interpretation method listed a the bottom of the *Layers* dialog box must be set to *Exact Contour method*. Any other interpretation method will cause the objects to override the calculated thickness everywhere in the layer.
- 16. In the Layers dialog box click Done.

From now on, elevations of objects in layer **Bottom** will be subtracted from elevations in layer **Top** to calculate values for layer **Thickness**.

*Note: Objects with specified thickness value drawn directly into layer* **Thickness** *would override the calculation.* 

The Argus ONE User's Guide (Argus Interware, 1997) provides details of adding *Information* layers and linking *Information* layers to each other using mathematical expressions.

In the second example, thickness may be calculated from "Top" and "Bottom" information contained in a single layer. In this case, it would be necessary to add two parameters to the **Thickness** layer as follows.

- 1. Bring up the *Layers' Floater* by clicking on the *Layers*... button along the top of the Argus ONE window.
- 2. Click on the button *Layers* at the top of the *Layers' Floater*.
- 3. In the *Layers* dialog box, use the down arrow to position the highlighted layer to be **Thickness**, and click on button *New* below the label *Parameter* twice (not below the label *Layer*, which would add a new layer). Each click creates a new parameter.
- 4. Set the first parameter name by typing "Top" to replace the default parameter name after clicking on "New Parameter." This parameter will be used to set the elevation of the top of the aquifer.
- 5. Set the second parameter name by typing "Bottom" to replace the second default parameter name after clicking on "New Parameter 1." This parameter will be used to set the elevation of the bottom of the aquifer.
- 6. In the parameter listing area, click on the line containing parameter *thickness* in the list found on the lower part of the dialog box. Then click on the *fx* button.
- 7. In the *Expression Editor*, scroll the left scroll bar until an entry for layer "Thickness" is visible and click on it. Click on entry "Top." That entry will then appear in the box to the right.
- 8. A list of parameters of this layer appears in the right-hand box. In this case, there are three parameters. Double-click on the "Top" entry in the right-hand box, and the parameter "Top" will appear in the expression box at the top of the *Expression Editor*.
- 9. Insert a minus sign after "Top."
- 10. Repeat step 8 to add parameter "Bottom" to the expression. The expression "Top Bottom" should now be in the upper box.
- 11. Click OK.
- 12. In the Layers dialog box, click Done.

From now on, elevations of objects in parameter "Bottom" will be subtracted from elevations in parameter "Top" to calculate values for parameter "Thickness." This method somewhat restricts the flexibility of the distributions possible for "Top" and "Bottom" as they are defined as parameters of the same graphic objects. For the previous example, where new layers were defined, the contours of "Top" and "Bottom" could, in effect, cross one another.

# Appendix B. The CheckMatchBC program

The **CheckMatchBC** program is used to compare the values of specified pressure and concentration boundaries as specified in the SUTRA input file as compared to the actual values calculated for such boundaries by SUTRA. Ideal selection of the GNUP and GNUU in Dataset 5 cause the simulated and specified values to match from six to eight decimal places. If the simulated and specified values match more closely than that, the flux at the boundary node may not be calculated with sufficient precision.

To run the program, double-click on it in Windows Explorer, click on the **Select Files** button and select the input (\*.inp) and node (\*.nod) file for a SUTRA model. The program will display the maximum and minimum relative differences for pressure and concentration along with the node numbers at which these occur, the specified value, the calculated value, and the number of digits that match. The relative difference is calculated as follows:

Rel. Dif. = Abs[(specified value - calculated value)/(specified value + calculated value)],

where

Rel. Dif. = relative difference Abs = absolute value

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