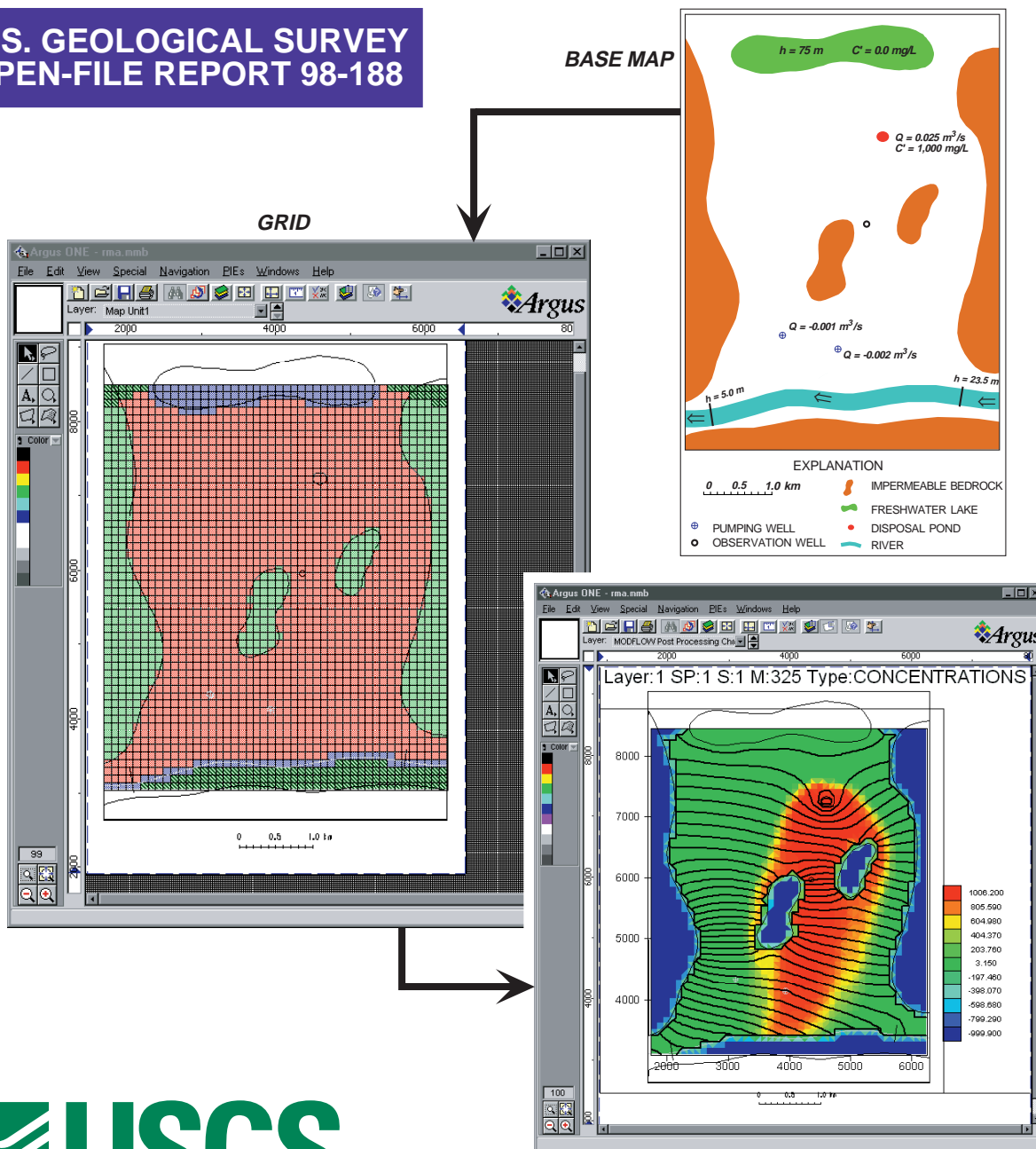


Addition of *MOC3D* Solute-Transport Model Capability to the U.S. Geological Survey *MODFLOW-96* Graphical-User Interface Using Argus Open Numerical Environments

U.S. GEOLOGICAL SURVEY
OPEN-FILE REPORT 98-188



Cover: The illustrations on the cover depict a sequence of modeling stages, starting with a base map that shows the geometry and boundaries of the problem domain (see Figure 16). The Graphical-User Interface for Argus Open Numerical Environments facilitates the definition of parameters and discretization of the model domain into a finite-difference grid (see Figure 25). Argus ONE also exports data sets in a format compatible with *MODFLOW-96* and *MOC3D*, and allows the model to be run from within the Argus ONE environment. Argus ONE visualization capabilities can then be used to visualize the results (in this case, heads as contours and concentrations as colors--see Figure 26).

Addition of *MOC3D* Solute-Transport Model Capability to the U.S. Geological Survey *MODFLOW-96* Graphical-User Interface Using Argus Open Numerical Environments

by G.Z. Hornberger and L.F. Konikow

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U.S. GEOLOGICAL SURVEY
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ABSTRACT

This report describes a Graphical-User Interface (GUI) developed for *MOC3D*, the U.S. Geological Survey (USGS) three-dimensional, method-of-characteristics solute-transport model. *MOC3D* is integrated with *MODFLOW-96*, the USGS modular, three-dimensional, finite-difference ground-water flow model. The GUI for *MOC3D* is developed as an addition to an existing *MODFLOW-96* GUI, which is a Plug-In Extension (PIE) to the commercially available software developed by Argus Interware, Inc. The Argus Interware product, known as Argus Open Numerical Environments (Argus ONE™), is a programmable geographic information system (GIS) that has automated gridding and meshing capabilities to link geospatial information with finite-difference and finite-element discretization, as well as several means of importing geospatial information. The addition of the *MOC3D* interface to the GUI for *MODFLOW-96* includes automatic creation of geospatial information layers required for *MOC3D*, and menus and dialog boxes for input of parameters for *MOC3D* simulation control. The GUI creates formatted ASCII files that can be read by *MOC3D*. *MOC3D* can be executed within the Argus ONE application, and the GUI includes an option to solve only the ground-water flow equation (*MODFLOW-96*). Solute concentrations and ground-water flow velocities calculated by *MOC3D* simulations can be visualized using the GUI's *MOC3D* post-processing capabilities.

INTRODUCTION

This report describes a Graphical-User Interface (GUI) developed for *MOC3D*, the U.S. Geological Survey (USGS) three-dimensional, method-of-characteristics solute-transport model (Konikow and others, 1996). *MOC3D* is integrated with *MODFLOW-96*, the USGS modular, three-dimensional, finite-difference ground-water flow model (Harbaugh and McDonald, 1996a; 1996b). *MOC3D* uses flow components calculated by *MODFLOW-96* to compute velocities across cell faces, and uses these velocities to track particles to simulate advection. The GUI for *MOC3D* is developed as an addition to the *MODFLOW-96* GUI (Shapiro and others, 1997) because *MOC3D* requires the use of *MODFLOW-96*. With this added capability, the *MODFLOW-96* GUI is upgraded to Version 2.0. This documentation describes the functions of the GUI specific to *MOC3D* and is meant to be used in conjunction with documentation for the GUI for *MODFLOW-96* (Shapiro and others, 1997).

The GUI for *MODFLOW-96* and *MOC3D* discussed in this report is developed using commercially available software developed by Argus Interware, Inc. The Argus Interware

product, known as Argus Open Numerical Environments (Argus ONE™), is a programmable geographic information system (GIS) that has automated gridding and meshing capabilities to link geospatial information with finite-difference and finite-element discretization, and includes several means of importing geospatial information. Geospatial information and simulation control parameters are exported by the GUI into ASCII text files that can be read by the appropriate numerical model. In addition, Argus ONE allows access to externally developed Plug-In Extensions (PIEs), which are executable codes loaded into the memory of Argus ONE such that they appear as part of Argus ONE, even though they have been developed independently (Argus Interware, 1997).

Although the *MODFLOW-96* GUI is a fully functioning graphical pre- and post-processor, it also allows the user to apply programmable features within Argus ONE to meet the unique demands of each modeling project. Thus, the GUI is intended as a structure from which the user can add capability according to the demands of the modeling project.

This report describes how to use the PIEs as graphical pre- and post-processors for *MOC3D*. This report does not describe the programming that has been used to develop the PIEs. However, the source code and export template for the PIEs (developed using MicrosoftTM Visual C++) are available for those who wish to modify or augment the graphical pre- and post-processing capability developed in this version. Furthermore, it is assumed that the reader has a knowledge of the basic data requirements and underlying principles for using the USGS three-dimensional, method-of-characteristics solute-transport model (*MOC3D*) and the USGS modular, three-dimensional, finite-difference, ground-water flow model (*MODFLOW-96*). Konikow and others (1996) and McDonald and Harbaugh (1988 and 1996a, 1996b) provide thorough discussions of principles underlying *MOC3D* and *MODFLOW-96*. In addition, it is assumed that the reader has a 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 (www.argusint.com).

Acknowledgments. The authors appreciate the thorough evaluation and review comments provided by USGS colleagues P. E. Misut and K. M. Hess, and by Argus Interware. The authors also appreciate the programming support provided by Mr. Shahar Dolev of Argus Interware.

SYSTEM REQUIREMENTS AND INSTALLATION

The pre- and post-processing GUI enhancements developed for *MOC3D* and described in this report use Argus Open Numerical Environments (Argus ONE). Argus ONE operates on multiple computing platforms; the GUI discussed in this report, however, has been developed and tested only for computers operating under Windows 95 and Windows NT. Optimal operation of Argus ONE requires at least

a Pentium 100 Mhz processor with 16 MB of RAM, 7 MB of free disk space, and a video card capable of displaying 256 colors; capability to use 65,000 colors is recommended.

The GUI consists of three PIEs that appear as the files *MFGUI_20.DLL*, *MFPOST20.DLL*, and *MCPOST10.DLL*. The file extension "DLL" is referred to as a dynamically linked library, which is the name of the MicrosoftTM technology that allows external codes to be loaded in the memory of software applications. The file *MFGUI_20.DLL* is the pre-processor for *MODFLOW-96* (Version 2.0), which includes *MOC3D* capabilities. *MFPOST20.DLL* is the post-processor for visualizing head and drawdown results calculated by *MODFLOW-96* or *MOC3D* simulations and *MCPOST10.DLL* is the post-processor for visualizing concentration and velocity fields calculated by *MOC3D* simulations. In addition, the file *MODFLOW.MET* is used for exporting projects and the file *MODFLOW.VAL* contains default values for the project information dialog boxes. These PIEs and files are available without charge from the U.S. Geological Survey and can be distributed freely, but they require an executable version of Argus ONE (version 4.10t or higher) to operate.

The pre- and post-processing PIEs for *MOC3D* and *MODFLOW-96* have been developed using MicrosoftTM Visual C++. The source codes for the PIEs are available at the World-Wide Web site (water.usgs.gov/software/); this information is included under the category "Ground Water." The software can also be retrieved using anonymous File Transfer Protocol (FTP) from water.usgs.gov (path: /pub/software). Detailed installation instructions are included in the *README* file that is included with the software distribution. Additional information about Argus ONE can be found on the World-Wide Web site (www.argusint.com).

The executable versions of *MOC3D* (Version 1.2 or later) and *MODFLOW-96* must also be installed to run these models from the

Argus ONE environment. Remember that the *MODFLOW-96* code and the *MOC3D* code are integrated into one code (*MOC3D*). *MODFLOW-96* (without *MOC3D*) is executed when using the GUI to simulate ground-water flow only, without transport; *MOC3D* is executed when simulating ground-water flow with transport.

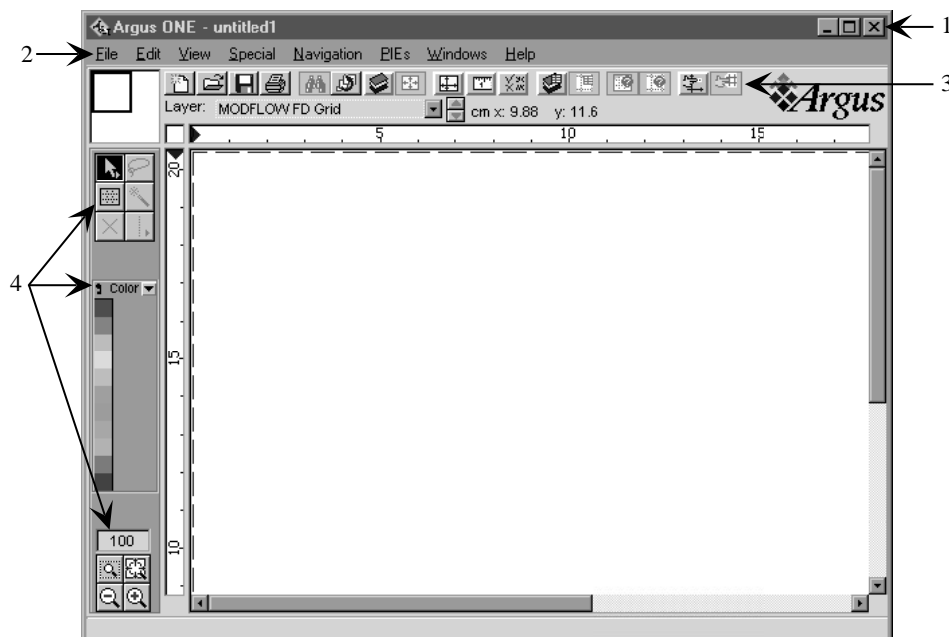
LAUNCHING THE PRE-PROCESSOR

The *MODFLOW-96* GUI automates the use of Argus ONE to create the appropriate geospatial information coverages or layers for *MOC3D*. The GUI also installs menus and dialog boxes specific to *MOC3D* that can be invoked from within the Argus ONE application.

Once Argus ONE is open, the pre-processor is launched by selecting the New

MODFLOW/MOC3D Project menu item from the PIEs menu at the top of the main Argus ONE window (see Figure 1). A pre-existing Argus ONE project made with the *MODFLOW-96* GUI can be opened by choosing Open from the File menu and choosing the name of the project file. To invoke *MOC3D* options for this project, choose Edit Project Info from the PIEs menu.

This opens a window titled *MODFLOW/MOC3D* DataSets, containing pre-processor dialog boxes that are accessed by clicking the tabs at the top of the window. The solute-transport model can be turned "on" by a button in the Stresses/Solvers dialog box in the *MODFLOW/MOC3D* DataSets window; to use this pre-processor for *MODFLOW-96* projects without transport leave the solute-transport button "off" (this is described in the next section). Shapiro and others (1997) describe the basic features of the *MODFLOW-96* GUI.



- 1 Standard Microsoft window controls
- 2 Menu bar
- 3 Icon bar
- 4 Tool palette

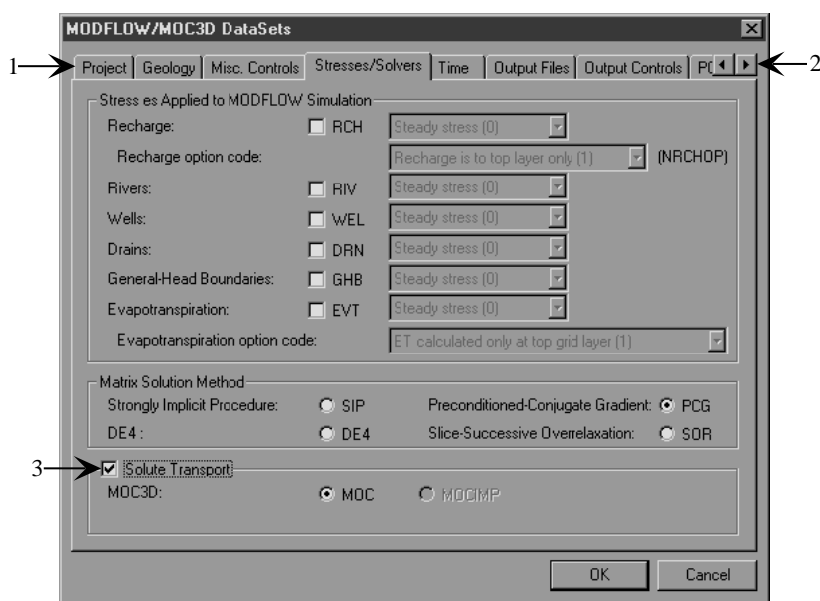
Figure 1. Main Argus ONE window that is displayed after New *MODFLOW/MOC3D* Project is selected from the PIEs pull-down menu.

ENTERING AND EDITING INFORMATION IN THE PRE-PROCESSOR

Geospatial information, such as the spatial distribution of physical parameters, is entered into geospatial information layers (as described in the “Geospatial Information Layers” section of this report.) The pre-processor dialog boxes are used to enter simulation control parameters and other non-spatial information.

In the main Argus ONE window (Figure 1) of a pre-existing *MODFLOW-96* project, access the pre-processor dialog boxes by choosing Edit Project Info from the PIEs menu. The information in the pre-processor dialog boxes is synthesized to build the structure of geospatial information layers needed for a *MODFLOW-96* or *MOC3D* simulation.

MOC3D is activated in the Stresses/Solvers dialog box shown in Figure 2. When the solute-transport checkbox is selected, several *MOC3D* tabs appears at the top right of the dialog box, and *MOC3D* geospatial information layers are created. The MOC solver is the default selection for the *MOC3D* model (other solvers are planned for future releases). The two scrolling arrows that appear at the right side of the strip of labeled tabs provide access to the *MOC3D* dialog boxes. **CAUTION:** Turning *MOC3D* off here (by clicking on the "checked" checkbox) will erase all *MOC3D*-related geospatial information layers and model parameters that may have been entered previously. If you want to deactivate *MOC3D* but preserve entered information relevant to transport, it should be done just prior to exporting and running the model (see section below titled "Creating Data Files and Executing *MOC3D*").



- 1 Tabs to show individual dialog boxes
- 2 Scrolling arrows to view hidden tabs
- 3 Solute-transport checkbox

Figure 2. Stresses/Solvers dialog box in the MODFLOW/MOC3D DataSets window of the pre-processor showing the *MOC3D* package activated. Arrows at the upper right are used to scroll to the *MOC3D* dialog boxes.

MOC3D DIALOG BOXES

MOC3D information related to the simulation of transport is entered in the Transport Subgrid, Particles, and *MOC3D* Output + Dispersivities dialog boxes. Use the scrolling arrows at the top right of the MODFLOW/MOC3D DataSets window to access hidden tabs. The other tabs represent *MODFLOW-96* dialog boxes as described by Shapiro and others (1997). The *MOC3D* tabs will only be visible if the *MOC3D* checkbox has been selected in the Stresses/Solvers dialog box (see Figure 2).

Use the "tab" key or mouse clicks to move between the editable fields. Hitting the "return" or "enter" key is equivalent to clicking the OK button and will return control to the Argus ONE project window. This saves changes made to the project information up to that point. Clicking the Cancel button will ignore any changes made. Wherever possible, the initial selection of any of the data fields in the *MOC3D* dialog boxes will invoke default values (read from the *MODFLOW.VAL* file) that are consistent with the *MOC3D* model.

Help buttons are available for selected parameters. Clicking on a Help button will open an information window that offers a hint, definition, and (or) suggestion relevant to a particular parameter.

Transport Subgrid Dialog Box

The information in the Transport Subgrid dialog box (Figure 3) defines the part of the *MODFLOW-96* grid in which transport calculations will be made, and also includes several other general model parameters required by *MOC3D*.

Number of First and Last Geologic Unit for Transport (ISLAY1 and ISLAY2)

The number of geologic units in the transport subgrid for the simulation is defined with the two parameters, ISLAY1 and ISLAY2 (see *MOC3D* input instructions, Konikow and others, 1996). It is important to note that a distinction is made between geologic units and model layers. A geologic unit may consist of one or more model layers. The pre-processor exports the first (top-most) model layer of the first geologic unit specified for transport, and the last (bottom-most) model layer of the last geologic unit specified for transport. The default response for ISLAY2 ("-1") is a signal to the program to export the *last* Geologic Unit in the *MODFLOW-96* grid. Thus, if Geologic Units are added to the simulation, the last model layer will always be included in the transport subgrid.

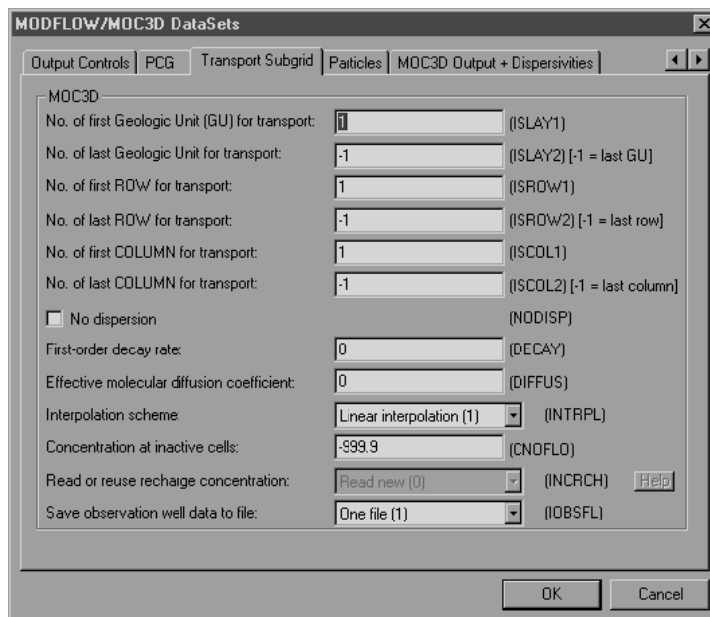


Figure 3. Transport Subgrid dialog box in the MODFLOW/MOC3D DataSets window of the pre-processor.

Non-simulated layers, as defined in the Geology dialog box, are not allowed within the transport subgrid in *MOC3D*. If non-simulated layers exist within the transport subgrid, an error message will be written to the error file (see "Files Created for *MOC3D* Simulations" below) during the export of the data; such layers must be modeled explicitly. Note that the default conditions for the *MODFLOW-96* GUI include an aquitard that is not explicitly modeled. To simulate transport in the aquitard, it must be simulated explicitly. To do this, select the line in the table describing the aquitard, check the "Simulated" box on the first line below the table, and then click Modify (see Figure 4).

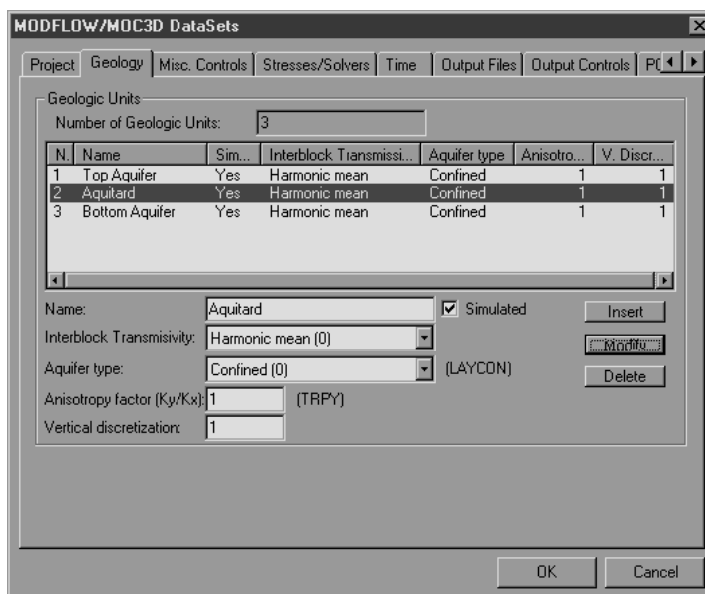


Figure 4. Geology dialog box in the MODFLOW/MOC3D Data Sets window of the pre-processor. The information below the table is linked to the selected geologic unit (Unit 2). The Simulated checkbox has been checked, and Modify was clicked to store the information in the table.

Number of First and Last ROW and COLUMN for Transport

The areal extent of the subgrid is defined in the next four text boxes; they correspond to ISROW1, ISROW2, ISCOL1, and ISCOL2 in the *MOC3D* input instructions. Again, the default value for ISROW2 and ISCOL2 ("-1") will always choose the last ROW or COLUMN, even if the grid density changes, thereby modifying the total number of columns and rows. If the *MOC3D* subgrid does not include the entire model grid, the user may need to re-enter appropriate values for ISROW1, ISROW2, ISCOL1, and ISCOL2 after modifying the grid. *MOC3D* requires the spacing between cells in the row and column directions in the transport subgrid to be uniform, although they do not have to equal one another.

Several *MOC3D* control parameters are also entered in this dialog box. Konikow and others (1996) provide additional information about the definition of these control parameters. Below is an abbreviated description of the parameters.

<i>NODISP</i>	Flag for no dispersion. Activating the checkbox indicates no dispersion.
<i>DECAY</i>	First-order decay rate.
<i>DIFFUS</i>	Effective molecular diffusion coefficient.
<i>INTRPL</i>	Flag for interpolation scheme.
<i>CNOFLO</i>	Concentration associated with inactive cells of subgrid.
<i>INCRCH</i>	Flag to reuse or read new recharge concentrations.
<i>IOBSFL</i>	Flag for writing Observation Well data to one or more files.

Particles Dialog Box

In the Particles dialog box (Figure 5), information describing the use of particles in *MOC3D* is entered. See Konikow and others

(1996) for a detailed description of the input parameters.

<i>NPMAX</i>	Maximum number of particles available for tracking of advective transport in <i>MOC3D</i> (if <i>NPMAX</i> = 0, <i>MOC3D</i> will calculate a default value automatically).
<i>CELDIS</i>	Maximum fraction of cell dimension that a particle may move in one step.
<i>FZERO</i>	Maximum fraction of active cells that can be void of particles before regeneration occurs.
<i>NPTPND</i>	Initial number of particles per cell in transport simulation. Valid options for default geometry of particle placement include 1, 2, 3, or 4 for one-dimensional transport simulation; 1, 4, 9, or 16 for two-dimensional transport simulation; and 1, 8, or 27 for three-dimensional transport simulation (see Konikow and others, 1996, p. 38).

Custom Particle Placement

If the Custom Particle Placement option (see Konikow and others, 1996, p. 73) is checked, relative coordinates for each of the particles are read using the table at the bottom of the Particles dialog box (Figure 5). To edit attributes associated with a particle, use the mouse to select one of the rows in the table. This places the current coordinates of the particle in the editable fields at the bottom of the dialog box. Modify the coordinates of the particle in the editable fields at the bottom of the dialog box. Initial particle coordinates are in a local unit coordinate system relative to the (0, 0, 0) position of a node. Relative positions must lie in the range of -0.5 to 0.5, following the *MODFLOW-96* convention for direction of layers, rows, and columns. Clicking the Modify button accepts the changes made in the editable fields and these changes are displayed in the table at the middle of the dialog box. Clicking Insert will add a particle to the list, and clicking the Delete button will remove a particle from the list.

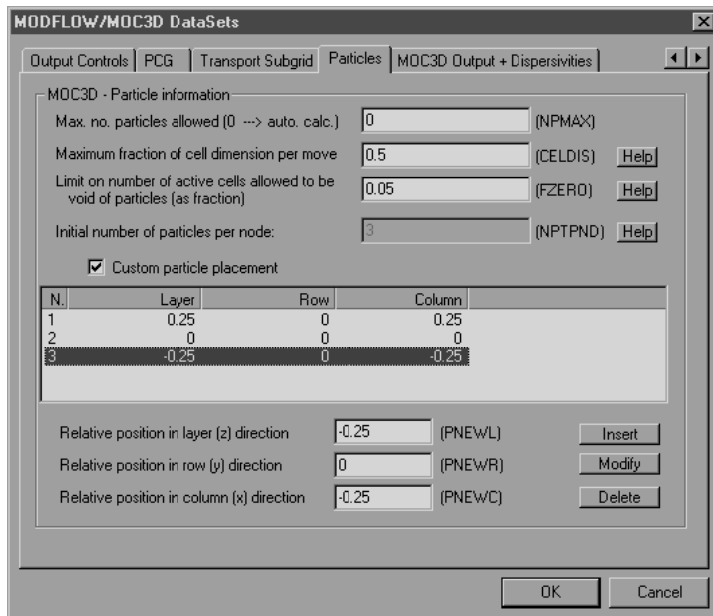


Figure 5. Particles dialog box in the MODFLOW/MOC3D DataSets window of the pre-processor. This example illustrates the use of the custom particle placement option.

MOC3D Output + Dispersivities Dialog Box

The MOC3D Output + Dispersivities dialog box (Figure 6) contains information related to the output controls for *MOC3D* simulations. It also includes a table with input parameters that vary by geologic unit.

Concentrations, velocities, dispersion coefficients, and particle locations from a *MOC3D* simulation can be exported to formatted ASCII text files or binary data files. For each of these output files, a pop-up menu is used to choose either of these file types, or “none” is selected to indicate that an external file will not be generated for a particular data type when executing *MOC3D*. If the post-processing PIE for

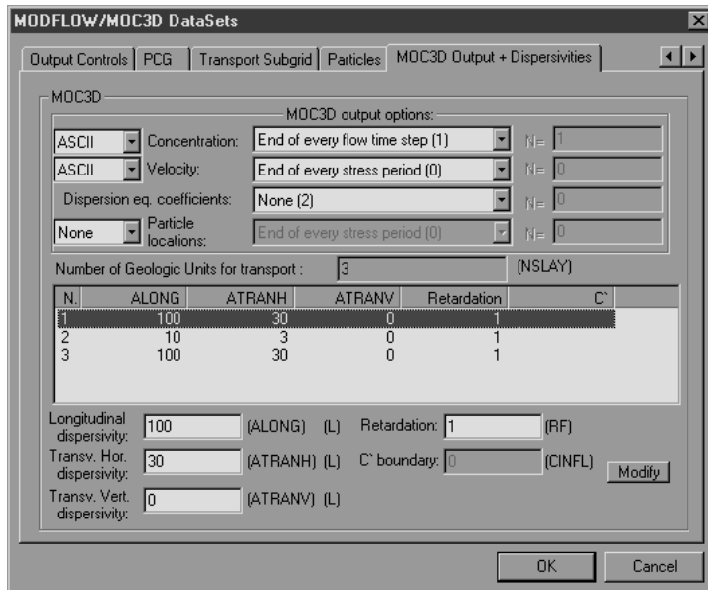


Figure 6. MOC3D Output + Dispersivities dialog box in the MODFLOW/MOC3D DataSets window of the pre-processor.

MOC3D is to be used, then calculated concentrations and velocities from a *MOC3D* simulation must be stored in formatted text (ASCII) files. This is the default setting.

The frequencies of printing the concentrations, velocities, dispersion equation coefficients, and particle locations are also defined using pop-up menus. These options are described in detail in the *MOC3D* documentation (Konikow and others, 1996). When the option called "each Nth move" is used, specify a value of N in the editable field at the right of the dialog box. If this information is not printed out to a separate file, it will be printed in the main *MOC3D* output file. Thus, even if no separate output file is selected, frequency of printing should still be defined.

Several parameters describing hydro-geologic properties are entered in the table in the bottom half of the dialog box. The number of geologic units in the transport subgrid is calculated from the values of ISLAY1 and ISLAY2 entered in the Transport Subgrid dialog box, and is displayed but not editable on this page. The values for longitudinal, transverse horizontal, and transverse vertical dispersivity and for the

retardation factor must be entered for each geologic unit that is included in the transport subgrid. The values of concentration in fluid inflow across the subgrid boundaries (C'), which corresponds to CINFL in the *MOC3D* input instructions, is entered only if the subgrid defined for *MOC3D* is smaller than the *MODFLOW-96* grid. If the subgrid has fewer rows or columns than the flow grid, a value of C' is required for each geologic unit in the subgrid (if not, or if no grid has been created, no value is accepted). Additionally, if the transport subgrid has fewer layers than the *MODFLOW-96* grid, values for C' (but not the other parameters in this table) are required for the layers above and (or) below the active subgrid layers. In this case, the first four

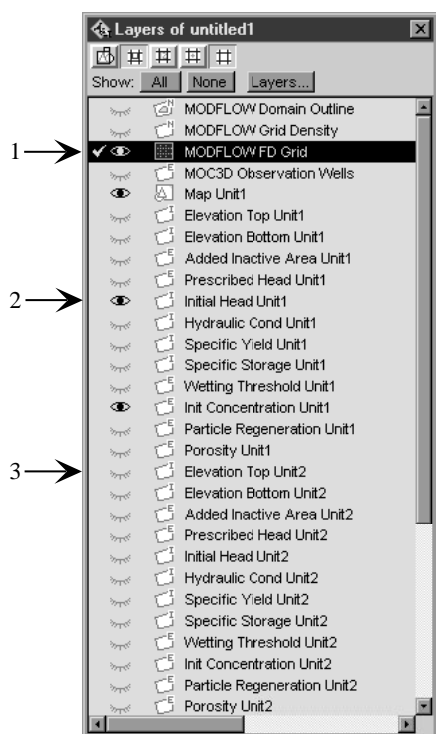
parameters will be blank for the units above or below the subgrid.

The values for dispersivity, retardation factor, and C' are defined per geologic unit. These values are assumed to be applied over the entire thickness of the geologic unit. Therefore, if the geologic unit is divided into more than one model layer, the value of these parameters will be applied to each model layer in the vertical dimension.

To edit attributes associated with a given geologic unit, use the table in the middle of the dialog box that lists the units. Clicking one of the rows of the table places the current attributes of the geologic unit in the editable fields at the bottom of the dialog box. Modifications to the attributes can be made in the editable fields at the bottom of the dialog box. Click the Modify button to accept the changes made in the editable fields and these changes are displayed in the table in the middle of the dialog box. The Delete and Insert buttons are absent because the value of the number of geologic units in the transport subgrid is fixed by the values of entered in the Transport Subgrid dialog box.

GEOSPATIAL INFORMATION LAYERS

Argus ONE offers a GIS environment where two-dimensional coverages or layers of information can be superimposed over each other. Note that the term “layer” in the context of Argus ONE does not have the same meaning as either a modeled layer in a *MODFLOW-96* finite-difference grid or a geologic unit. Each layer in Argus ONE can be accessed from the separate floating layers window (see Figure 7). This window can be opened by choosing Show Layers Window under the View menu on the main Argus ONE window (there is also an icon on the icon bar that will open it). The floating layers window allows the user to control which of the layers will be visible (those with an open-eye icon) and which layer is 'active' and therefore available for input or editing (a check-mark will appear to the



- 1 Check mark indicates the active layer
- 2 Open 'eye' indicates the layer is visible
- 3 Closed 'eye' indicates the layer is invisible

Figure 7. The floating layers window.

left of the 'eye'). Clicking on an 'eye' will toggle the layer visibility, and clicking to the left of the eye will make it 'active.' The size of the window can be changed to accommodate projects with a large number of layers.

Information for each layer can be generated using drawing tools that are available in Argus ONE (see Figure 8). The closed-contour tool is used to define a contour of equal value in a layer. If this tool is selected, click once in the workspace for the first vertex in the contour. Drag the mouse to the next vertex and click again. Double-click to finish the contour; this brings up a Contour Information dialog box where parameter information is defined. The line-contour tool is used similarly but will not draw closed contours. Finally, clicking in the work space using the point-contour tool places an object where the pointer is located.

Examples using the contouring tools are described in the step-by-step example problem (see section "Step-By-Step *MOC3D* Sample Problem Using the GUI"). Spatial information

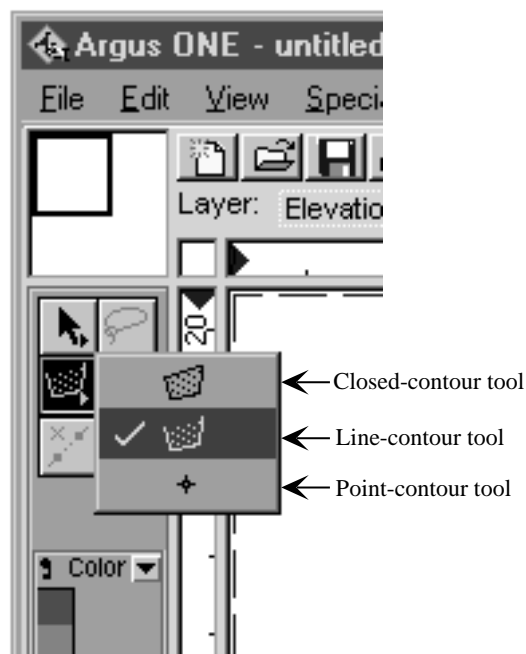
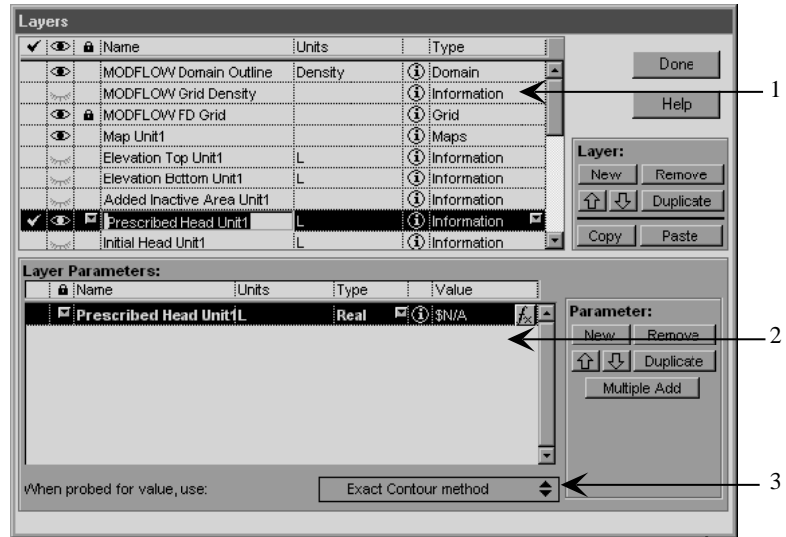


Figure 8. The contouring tools menu in the main Argus ONE window. Check mark indicates the active tool.

can also be imported from a variety of sources including text files, DXF files, and ARC/INFO Shape files. Double-clicking on a contour line will bring up the Contour Information dialog box and the contour values can be edited. Additional information about importing geospatial information into Argus ONE layers can be found in Argus ONE User's Guide and the World-Wide Web site for Argus Interware (www.argusint.com).

Layer information can also be specified in the Layers dialog box (Figure 9). To access the Layers dialog box click on the Layers button in the floating layers window, or click on the Layers Dialog icon on the icon bar, or choose Layers under the View pull-down menu. Select a layer by clicking on it in the top table of the dialog box. That layer's parameters will be listed in the bottom half of the window. The interpretation method for contours in a layer can be changed at the bottom



- 1 Table listing layers in the project.
- 2 Table listing parameters in the selected layer. The f_x button, located to the right of the "Value" column, provides access to the Expression window for that parameter.
- 3 Interpretation method used for the selected layer.

Figure 9. The Layers dialog box, opened by clicking the Layers button in the floating layers window (Figure 7), or by the Layers Dialog icon on the icon bar, or by choosing Layers under the View pull-down menu.

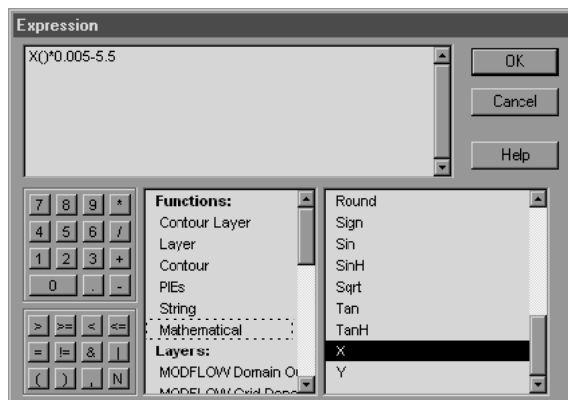


Figure 10. The Expression window, invoked by clicking the f_x button in the Layers dialog box (Figure 9). The box at the top of the window shows the value or function for the current parameter. Functions and layer parameters in the lower middle table can be used to define the parameter.

of the Layers dialog box (see Argus ONE User's Guide, p. 116, for a description of interpretation methods). Each layer parameter is given a default value when it is created. This value is constant for the entire layer. To change the default value click on the f_x button to the right of the Value column of the parameter. This brings up the Expression dialog box (Figure 10) in which a constant value for the layer may be entered, or a spatially varying field may be defined using mathematical functions or functions relating to other information or data layers. The Argus ONE User's Guide provides more detailed information about the use of the Layers dialog box and the Expression dialog box.

MOC3D geospatial information layers are created for every geologic unit in the model, regardless of its inclusion in the *MOC3D* subgrid. Only the information layers relating to geologic units in the *MOC3D* subgrid will be exported. In

addition, input fields for source-fluid concentration data are added to geospatial information layers within each geologic unit for each of the fluid stresses that are specified. The exceptions are for the recharge stress (for which a separate geospatial information layer named Recharge Concentrations is created), and evapotranspiration and drain stresses (which have no concentrations associated with them). If new geologic units are added or removed, the *MOC3D* geospatial information layers are renumbered automatically to reflect the new order associated with the geologic units.

The values for recharge concentration, initial concentration, particle regeneration, and porosity are assumed to be applied over the entire thickness of the geologic unit for which they are defined. Therefore, if the geologic unit is divided into more than one model layer, the value of these parameters at a given areal location will be applied to each model layer in the vertical dimension.

The geospatial information layers created for *MOC3D* by the pre-processor are described below. Reference to geospatial information layers for geologic units is denoted by [i], where the "i" denotes the sequence number of the geologic unit, starting with the uppermost geologic unit.

Recharge Concentration

The recharge concentration must be specified if the *MODFLOW-96* Recharge package is used. The information in the Recharge Concentration layer can be specified to be a constant and uniform value, or closed-contour information describing a spatially varying recharge concentration can be imported or generated. The default recharge concentration is zero. The recharge concentration can vary between stress periods, in which case a concentration parameter for each stress period must be entered. The option to read or reuse recharge concentrations (the INCRCH flag in *MOC3D*) is defined in the Transport Subgrid dialog box.

MOC3D Observation Wells

Observation wells (node locations in the simulation grid for which values of head and concentration calculated after each transport time increment will be written to a separate file) are assumed to represent piezometers that are only open to the aquifer at a single point in three-dimensional space. They can be specified in the *MOC3D* Observation Wells layer using the point-contour tool. The well object is defined by its elevation in the simulation. Up to five observation points may be specified at any horizontal point by entering different elevations. The elevation values are used to calculate in which *MODFLOW-96* layer the observations will be made for each well. The IOBSFL flag in the Transport Subgrid dialog box controls the options to print observation well data to a separate file or to include all observation well data in one file (see "Files Created by Executing *MOC3D*" below).

Initial Concentration Unit[i]

The initial concentration can be specified to be a constant and uniform value; alternatively, closed-contour information describing spatially varying initial concentration can be imported or generated. The default initial concentration is zero for all geologic units.

Particle Regeneration Unit[i]

The Particle Regeneration Unit (a flag to treat fluid sources and/or sinks as either "strong" or "weak"; see Konikow and others, 1996, p. 76) can be entered using the point-, line-, or closed-contour tools. A value of "1" designates a "strong" fluid source or sink, where moving particles will be added or removed as appropriate. The default value of this unit is zero ("weak" or no fluid source).

Porosity Unit[i]

The porosity of the geologic unit can be specified to be a constant and uniform value; alternatively, closed-contour information describing spatially varying initial concentration can be imported or generated. The default initial porosity is 0.2 for all geologic units.

Prescribed Head, Well, River, and General Head Boundary Information Layers

Objects defining areas of prescribed head and all fluid source objects require concentration information for *MOC3D* simulations. Concentration associated with prescribed head objects will be attributed to every finite-difference cell within that object. For each stress period, a concentration associated with the fluid source is required for each well, river segment, and general head boundary object. Data fields for concentration information appear in the dialog box opened when the user double clicks on an existing fluid source object, or creates a new one, when the solute transport option is being used. If solute transport is turned off or is not being used, this information is absent.

VISUALIZING GEOSPATIAL INFORMATION LINKED TO THE FINITE-DIFFERENCE GRID

The procedure for grid generation described in the original *MODFLOW* GUI documentation (Shapiro and others, 1997) should also be used for *MOC3D* simulations. Note that the transport subgrid must have constant cell widths and heights. Visualization of geospatial information linked to the finite-difference grid is conducted in the layer *MODFLOW* FD Grid. Making this the active layer and clicking the down arrow to the right of the color legend in the

tool palette opens a menu with a list of the parameters linked to the finite-difference grid (see Figure 11). Selecting one of parameters on the list will color the grid according to the geospatial information for the selected parameter. In addition, the spatial information attributed to a finite-difference cell can be examined by double clicking a single finite-difference cell in the layer *MODFLOW* FD Grid; a window appears showing a list of the parameter values linked to that cell (Figure 12).

The geospatial information linked to the finite-difference grid by the pre-processor for *MOC3D* is described below.

Init Concentration Unit[i]

Selecting Init Concentration Unit[i] displays, by color, the grid cell values of initial concentration from the layer Init Concentration Unit[i].

Porosity Unit[i]

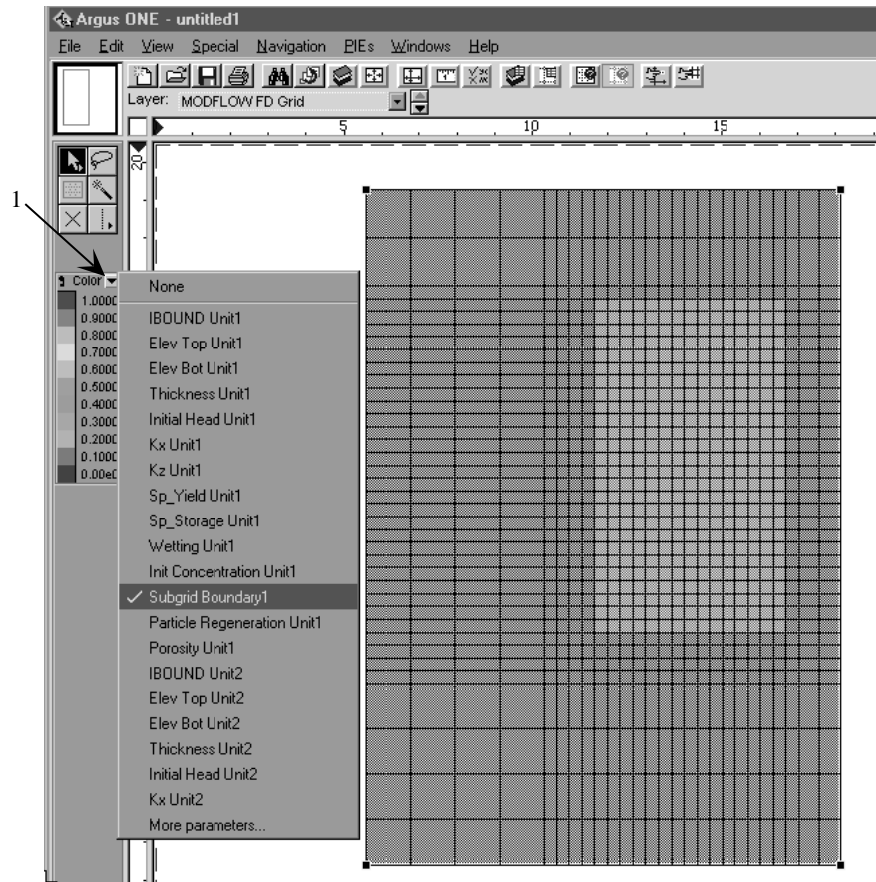
Selecting Porosity Unit[i] displays, by color, the grid cell values of porosity from the layer Porosity Unit[i].

Particle Regeneration Unit[i]

Selecting Particle Regeneration Unit[i] displays, by color, the grid cell values from Particle Regeneration Unit[i].

Subgrid Boundary[i]

Selecting Subgrid Boundary displays, by color, the area in which the solute-transport problem will be solved. This corresponds to the input data fields ISROW1, ISROW2, ISCOL1, ISCOL2 in the Transport Subgrid dialog box in the project information dialog boxes.



¹ Down arrow used to open the parameter list.

Figure 11. Example visualization of geospatial information linked to the MODFLOW FD Grid layer. Using the cursor to click-hold the down arrow to the right of the color legend in the tool palette opens a menu with the list of the parameters linked to the finite-difference grid. Selecting a parameter (subgrid boundary in this example) will color the grid according to the parameter's value.

CREATING DATA FILES AND EXECUTING *MOC3D*

To save an Argus ONE project, use the Save command under the File menu. This will allow the user to return to the information layers and project information dialog boxes in future sessions. To save a *MODFLOW*-only project, the user can first save the project with *MOC3D* active (retaining all *MOC3D* information), then turn the *MOC3D* option off, and finally save the project again using a different project name.

Saving a *MOC3D* Argus ONE project does not create files necessary to run *MOC3D*, however. These files must be created from the geospatial information layers and project information by exporting the data using an export template. The file *MODFLOW.MET* is the export template used by *MFGUI_20.DLL* to export and format the ASCII files needed to execute *MOC3D*.

The ASCII files used to execute *MOC3D* are created from the MODFLOW FD Grid layer in Argus ONE. While the MODFLOW FD Grid

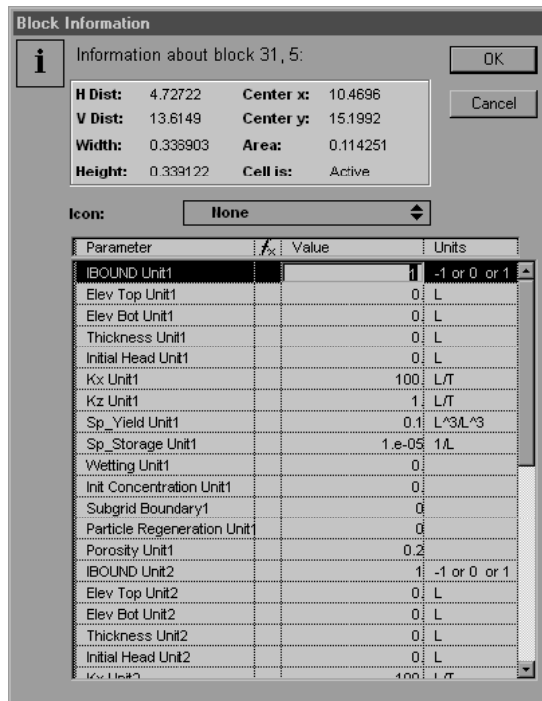


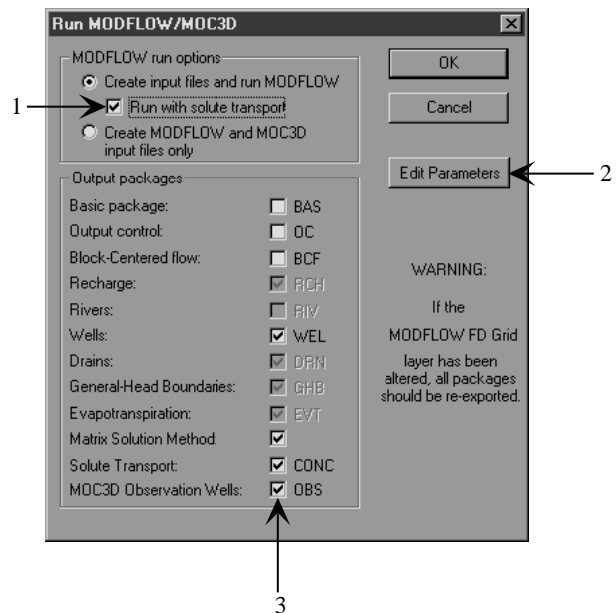
Figure 12. Block Information window for a cell in the MODFLOW FD Grid, invoked by double-clicking on the cell itself.

layer is active, select the Run MODFLOW/MOC3D command in the PIEs pull-down menu. A dialog box appears with several options (Figure 13).

The user is able to run the simulation with or without solving the transport problem by toggling the checkbox labeled "Run with solute transport" below the "Create input files and run MODFLOW" radio button. This feature is included because it is much more efficient to solve the flow equation alone; in the early stages of designing a transport simulation, it is often worthwhile to evaluate the reasonableness of the calculated flow field before proceeding with the transport simulation. If the simulation is run without transport by toggling the "Run with solute transport" checkbox, all information intended for use with *MOC3D* will be ignored, but will still be saved in the Argus ONE project and exported to files. Running a simulation without transport uses the *MODFLOW-96* executable. If it is desired to run *MODFLOW-96* alone as a preliminary or

intermediate step in the transport modeling project, then this is the approach that should be used to turn off solute transport. (On the other hand, the same objective can be achieved by using the Solute Transport checkbox in the Stresses/Solvers dialog box, but this will erase all information about transport that has been entered, which generally is not desired.)

The user may also export the *MOC3D* and *MODFLOW-96* input data files, but not execute the *MOC3D* or *MODFLOW-96* program. The model can then be run independently and outside of the Argus ONE environment, if desired. The checkboxes in the bottom half of the dialog box will turn export off or on for each of the input files required by *MODFLOW-96* and *MOC3D*. Turning export off for certain files speeds up the export process and is useful when only one aspect of a problem has changed and



- 1 Checkbox to run the flow model (*MODFLOW-96*) with or without solving the transport equation (*MOC3D*).
- 2 Button to edit project information (in the MODFLOW/MOC3D DataSets window).
- 3 Checkboxes controlling export of specific packages and files.

Figure 13. The Run MODFLOW/MOC3D dialog box.

thus only a few selected files need to be exported. The Edit Parameters button accesses the project information dialog boxes.

Clicking on OK in the Run Modflow/MOC3D dialog box brings up a window querying for the name of the "Export File" (Figure 14). The GUI does not require a name for the export file here (in fact, it is ignored). However, the directory in which all exported files will be saved is defined with this dialog box by browsing for the desired directory and clicking Save.



Figure 14. Dialog box for choosing directory in which exported files will be saved. Note that inputs for file name and file type are ignored when using the pre-processor for exporting files.

A barber pole window will appear as the files are exported. After the files have been exported the *MOC3D* or *MODFLOW-96* model is launched (a console screen appears with the data directory and executable path) using the files that were just exported. If requested, hit any key to exit the console window, and control is returned to Argus ONE. The completed model creates files in the directory specified in the Export File dialog box using the root name defined in the Output Files dialog box.

Files Created for *MOC3D* Simulations

Below is a list and explanation of file names that are created by the pre-processing PIE for *MOC3D*. *Rootname* refers to the file name

specified in the Output Files dialog box of the pre-processor.

MOC3D.BAT is a DOS executable created by the export template that contains a link to the executable for *MOC3D*. This is used to run the model from the directory in which the files were created (for example, if the model was not executed from within Argus ONE). Note that the GUI exports files to run *MOC3D* in *MODFLOW-96* "batch" mode (see description in Shapiro and others, 1997, under "Files Created for *MODFLOW-96* Simulations").

MODFLOW.BAT is a DOS executable created by the export template that contains a link to the executable for *MODFLOW-96*. This is used to run a model without simulating transport. Files must be exported with the "Run with solute transport" option in the Run MODFLOW/MOC3D Dialog Box unchecked for *MODFLOW.BAT* to be created and used.

Rootname.ERR is a file created by the export template that contains error information encountered during the export of *MOC3D* or *MODFLOW-96* files.

Rootname.MCN is the *MOC3D* name file.

Rootname.MOC is the main *MOC3D* input data file.

Rootname.CRC is the file containing information for the concentrations associated with the recharge package. This file is created only if the recharge package is chosen in the Stresses/Solvers dialog box.

Rootname.OBS is the file containing input information for *MOC3D* observation wells.

Files Created by Executing *MOC3D*

The output files that are optionally created by executing *MOC3D* are defined in the *MOC3D* Output + Dispersivities dialog box in the pre-processing PIE. Below is a list and explanation of file names that are created by executing *MOC3D* if the pre-processing PIE discussed in this report

is being used. *Rootname* refers to the file name specified in the Output Files dialog box.

Rootname.OUT is the main *MOC3D* listing file containing general information about the simulation. This file is always created by *MOC3D*.

Rootname{N}.OBA is the formatted text file containing the *MOC3D* observation well data. If the option to write observation well data to separate files is chosen (see IOBSFL in the Transport Subgrid dialog box), *N* is appended to the *Rootname* for each file, where *N* is a number from 1 to the number of observation wells defined. Otherwise, the file will be named *Rootname.OBA*.

Rootname.CNA and *Rootname.CNB* are the formatted text file and binary file, respectively, containing the calculated concentrations for the time steps or moves specified in the *MOC3D* Output + Dispersivities dialog box. If concentrations are not printed out to one or both of these separate files, they are printed in *Rootname.OUT*. The post-processing visualization of concentration that is described in this report uses the *Rootname.CNA* file. Generation of the *Rootname.CNA* file is the default mode.

Rootname.VLA and *Rootname.VLB* are the formatted text file and binary file, respectively, containing the calculated velocities for the time steps specified in the *MOC3D* Output + Dispersivities dialog box. If velocities are not printed out to one or both of these separate files, they are printed in *Rootname.OUT*.

Rootname.PTA and *Rootname.PTB* are the formatted text file and binary file, respectively, containing the particle location information for the time steps or moves specified in the *MOC3D* Output + Dispersivities dialog box.

VISUALIZING CONCENTRATIONS AND VELOCITIES

A post-processing PIE has been developed for *MOC3D* simulation results that have

used the pre-processing PIE in the Argus ONE application. The post-processing PIE uses the formatted text files for concentration and velocity data generated by executing *MOC3D* (the output control for these files is located in the *MOC3D* Output + Dispersivities dialog box). The concentration data file is given the name *Rootname.CNA* and the velocity data file is given the name *Rootname.VLA*, where *Rootname* is the file name specified in the Output Files dialog box. Note that the *MODFLOW* post-processing PIE should be used to visualize head and drawdown results for *MOC3D* simulations (see Shapiro and others, 1997).

The post-processing PIE for *MOC3D* is launched from within the Argus ONE application and uses information from the layer *MODFLOW* FD Grid. Therefore, it is necessary to have a project file open with the same finite-difference grid that was used to generate the *MOC3D* output files.

Launching the Post-Processor

To execute the post-processing PIE, choose *MOC3D* Post-Proc from the PIEs menu at the top of the Argus ONE window. A file dialog box appears; choose the *Rootname.CNA* (concentration) or *Rootname.VLA* (velocity) file that was created from the *MOC3D* simulation that used the finite-difference grid in the layer *MODFLOW* FD Grid of the current project file. The post-processing PIE reads the file that is chosen and a dialog box titled Available Data (Figure 15) appears giving a list of solutions.

If a concentration data output file is selected (this is the default file name), for each data set that is contained in the file, the layer, the stress period, the time step, the transport time increment (MOVE), and the data type (CONCENTRATIONS) are specified. In the Available Data dialog box (see Figure 15), stress period is abbreviated by SP, time step is abbreviated by S, and transport time increment is abbreviated by M (the

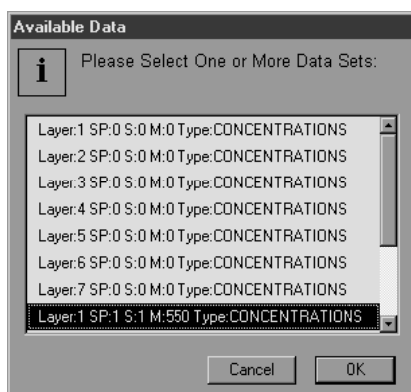


Figure 15. Data dialog box for the *MOC3D* post-processor. For each data set, stress period is abbreviated by SP, time step is abbreviated by S, and transport time increment is abbreviated by M (the initial concentration is always saved; the values of SP, S, and M are equal to 0 for this case).

initial concentration is always saved; the values of SP, S, and M are equal to 0 for this case). Select one or more of the solutions for each model layer and time level by clicking on one or more rows in the Available Data dialog box. De-select rows by clicking on them while they are highlighted. Clicking OK causes another dialog box to appear to specify the type of post-processing visualization. The types of post-processing methods are Contour Map, Color Map, 3D Surface Map, and Cross Section (these methods are described later in this section). Choose the type of map desired and click OK.

If a velocity data output file is selected, for each data set that is contained in the file, the layer, the stress period, the time step, and the direction (COLUMN, ROW, or LAYER) are specified to indicate the time level and the directional component of the velocity vector in the data set. Select *pairs* of solutions by clicking on two rows in the Available Data dialog box (for example, COLUMN and ROW). The post-processor will use the two directions chosen to create a vector object (arrow) at each node in that layer using the magnitude of the velocity in each of the two directions for that node.

Using the post-processing methods described above results in two layers being added to the project file. These layers are titled MOC3D Data and MOC3D Post Processing Charts, and can be seen in the list of layers in the floating layers window. The layer MOC3D Data is an Argus ONE data layer. These data appear as discrete points located at the center of the grid cells, and can be used for calculations with other data layers or exported to a text file. For example, concentration solutions in the layer MOC3D Data can be compared with the initial concentration, if such information has been entered into geospatial information layers. It is then possible to create and visualize a new parameter linked to the finite-difference grid that gives the change in concentration for the simulation.

The layer MOC3D Post Processing Charts is an Argus ONE map layer, which consists only of drawn objects. Making the layer MOC3D Post Processing Charts the active layer shows the post-processing objects that have been created--it may be necessary to hide other layers in order to clearly see the post-processing charts that were created. It may be helpful to rename the MOC3D Post Processing Charts layer to preserve its contents before using the post-processing PIE again (each time the post-processing PIE is used the MOC3D Data and MOC3D Post Processing Charts layers are overwritten).

Similar maps of head and drawdown can be made using the *MODFLOW* post-processing PIE (Shapiro and others, 1997). Double-clicking on a post-processing object in the layer MOC3D Post Processing Charts will bring up a dialog box that can be used to alter the appearance of the map. Additional information on creating and modifying the appearance of post-processing objects in Argus ONE is given in the Argus ONE User's Guide. A brief description of the post-processing methods available for concentration data follows.

Contour Map

Selecting the contour map option produces a contour map of concentration in the selected layers for the selected time steps in the selected stress periods. If only one layer is selected, the concentration contour map will overlay the finite-difference grid. If a transport subgrid has been defined, the contour map will overlay the area of the grid so defined. If more than one layer is selected, the selected contour maps will be scaled and placed in the layer MOC3D Post Processing Charts.

Color Map

Selecting the color map option produces a colorized interpolation of concentration in the selected layers for the selected time steps in the selected stress periods. If only one layer is selected, the concentration color map will overlay the finite-difference grid. If more than one layer is selected, then the selected contour maps will be scaled and placed in the layer MOC3D Post Processing Charts.

Three-Dimensional Surface Map

Selecting the three-dimensional surface map option produces a colorized three-dimensional perspective map of concentration in the selected layers for the selected time steps in the selected stress periods.

Cross Section

Selecting the cross-section option produces a plot of the concentration as a function of distance along a line through the modeled domain. The concentration from more than one layer can be included on the cross-section by choosing more than one layer in the Available Data dialog box in the *MOC3D* post-processor. The orientation of the line and other attributes of the plot of the cross section can be adjusted by double clicking on the post-processing object.

STEP-BY-STEP *MOC3D* SAMPLE PROBLEM USING THE GUI

This section provides an illustrative example of analyzing a simple problem using the pre- and post-processors. The following step-by-step examples are intended to be followed in sequence. We ran the example problem on a Micron workstation running Windows NT version 4.0 and having 32MB RAM and a 133 MHz Pentium processor.

The two-dimensional sample problem is based loosely on the ground-water contamination problem documented at the Rocky Mountain Arsenal, Colorado (Konikow, 1977). For use as an example for the application of modeling techniques, the properties and boundaries of the physical system have been approximated and greatly simplified. The results of this example problem, therefore, should not be taken to have any direct bearing on the actual field situation in Colorado. All of the information needed to define the problem are presented in the base map (Figure 16) and in Table 1. The area is bounded on two sides by impermeable bedrock, which act as no-flow barriers. The boundary at the top of the map is dominated by a freshwater lake, which can be assumed to represent a fully penetrating constant-

Table 1. Parameter values for two-dimensional sample problem

Parameter	Value
hydraulic conductivity	0.0001 m/s
storage coefficient	0.0
effective porosity	0.20
saturated thickness	12 m
longitudinal dispersivity	30 m
horizontal transverse dispersivity	3 m
initial concentration	0.0 mg/L
total simulation time	20 years

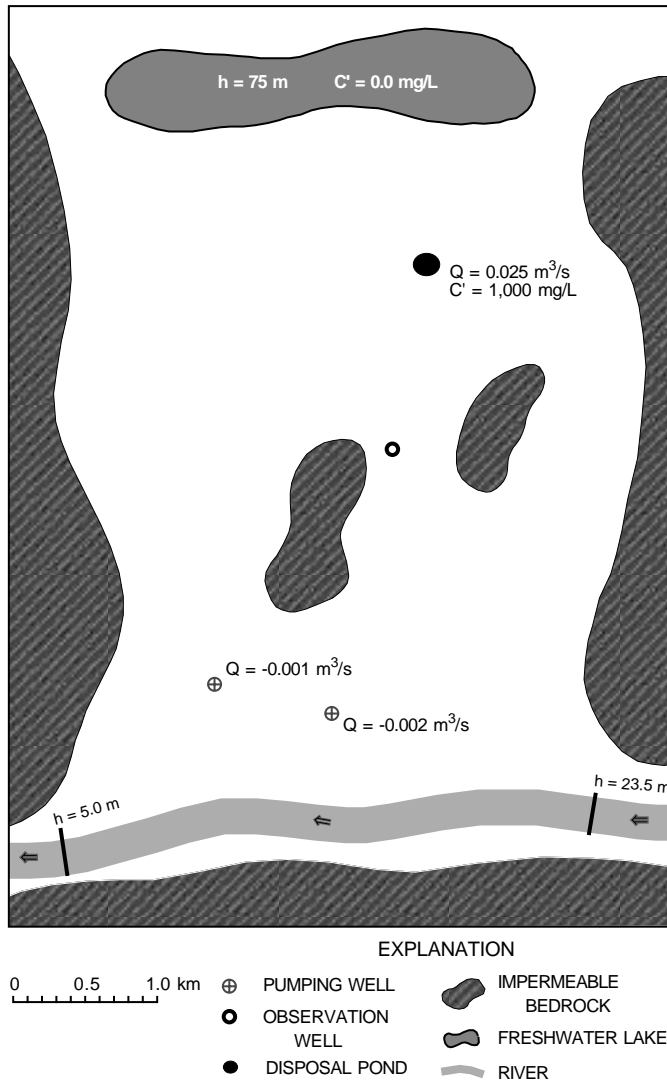


Figure 16. Base map for a two-dimensional sample problem.

head boundary. A river acts as a constant-head boundary along the bottom edge of the map, but the river also slopes to the left. The saturated thickness is assumed to be constant, so the aquifer can be represented as confined. The aquifer is also discontinuous because of two bedrock islands. The source of contamination is assumed to be an unlined disposal pond. Flow is assumed to be at steady state and will to simulate solute transport in the aquifer for a period of 20 years.

To start the Argus ONE program, double click on the Argus ONE icon or on the name of the Argus ONE executable code. From the PIEs

menu at the top of the Argus ONE window, select New MODFLOW/MOC3D Project. This opens a window titled MODFLOW/MOC3D DataSets. The data sets (comprised of a series of dialog boxes) will allow the user to enter *MODFLOW-96* and *MOC3D* general simulation parameters and control the packages and geologic units used in the simulation. For now, click OK; we will return to this window shortly.

Control is returned to a new Argus ONE window (titled "untitled1"). It is the window in which the model will be designed, run, and evaluated. When a new project was created, a number of layers that hold model information were created. These can be seen in an additional window titled "Layers of untitled1"; this is referred to as the floating layers window. The floating layers window allows the user to control which of the layers will be visible (those with an open-eye icon) and which layer is 'active' and therefore available for input or editing (a check-mark will appear to the left of the 'eye'). Clicking on an 'eye' icon will toggle the layer visibility, and clicking to the left of the eye will make it 'active' (see Figure 7).

The page-size base map shown in Figure 16 was saved as a DXF file. First, we will import this DXF file into a map layer. In the floating layers window, click to the left of the "eye" icon next to Map Unit1. This will make that layer active. Under the File pull-down menu in the main Argus ONE window, choose Import Map Unit1, and drag the mouse to the selection arrow to the right edge of the menu, which opens a sub-menu listing file types. In the sub-menu, select DXF File. That will open a dialog box to specify which file to open. After selecting the desired file name (*rma_map.dxf* for this example), click Open. This will import the DXF file. The *rma_map.dxf* file is in units that do not fit within the default Argus ONE scale; a dialog box appears asking if the

drawing size should be extended to accommodate the figure. Click OK. Then select Scale and Units from the Special pull-down menu. Change the label for units to "m" (see Figure 17). Click OK. If necessary, expand the size of the Argus ONE window to get a reasonably-sized image on the screen (Figure 18). Note that the scale at the bottom of the map indicating 1 km matches 1000 units (in meters) on the Argus ONE rulers.

Now we are ready to begin defining the problem. We will present the steps in a sequence that we feel is logical, though there is not a fixed order in which tasks must be completed.

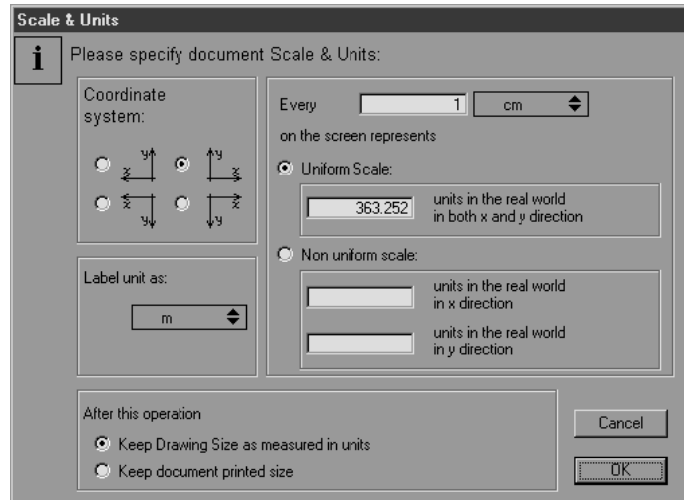


Figure 17. The Scale and Units dialog box.

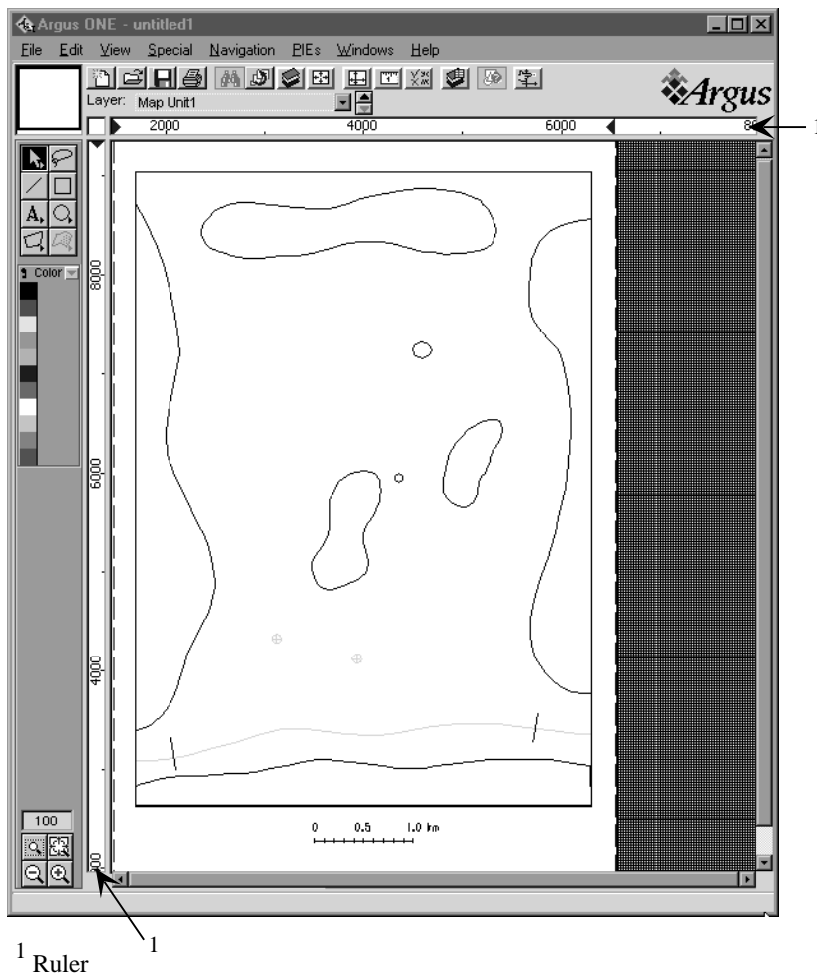
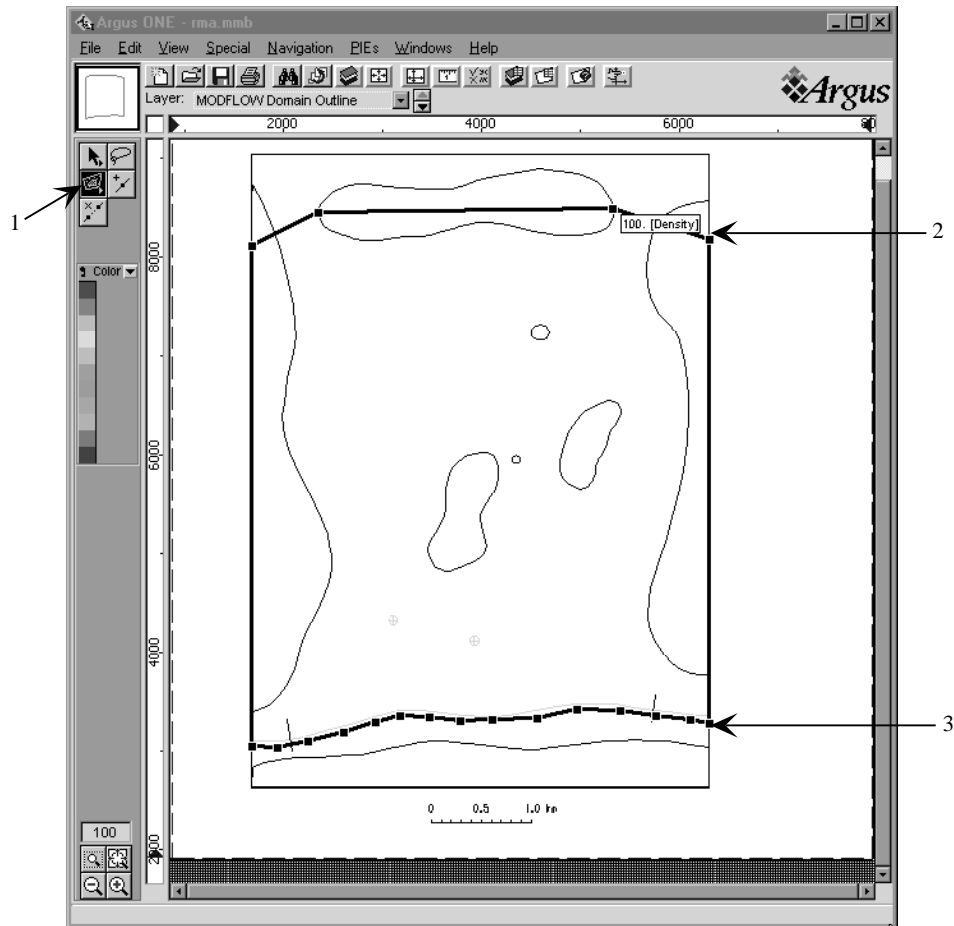


Figure 18. The imported base map for the sample problem. The Argus ONE rulers have been scaled to show distances in meters (see Figure 17).

1. Define the MODFLOW Domain Outline: Make the MODFLOW Domain Outline layer active, and the Map Unit1 Layer visible. Choose the closed-contour tool from the tool bar on the left side of the Argus ONE window. Draw a contour similar to the one shown in Figure 19. The contour shown in the figure incorporates the lake as the northern boundary and the river as the southern boundary, but little area beyond that. A single click with the closed-contour tool defines a vertex on the contour. Drag the mouse to the desired location of the next vertex and click once. When the last vertex is reached, double click; this connects the first vertex to the last and completes the contour (Figure 19). This opens a Contour Information dialog box showing information about the contour (Figure 20). This will allow us to define the density of the grid, which is an Argus



- 1 Tool bar selection of the closed-contour tool.
- 2 First vertex of contour.
- 3 Last vertex of contour (double-click to close contour).

Figure 19. Using the closed-contour tool to define the model domain. In this example, we defined the domain by successively placing key points at desired boundary locations in a counter-clockwise direction.

ONE term analogous to the grid spacing. Click once in the Value field for Density and enter a value of 100, which will allow generation of a moderately fine grid having a grid spacing of approximately 100 m. Click OK.

2. Define constant head boundary conditions (lake and river): Make the Map Unit1 active in the floating layer window. Select both the lake and river objects by clicking on them while holding down the Shift key. Copy the objects by choosing Copy under the Edit menu. Then make the Prescribed Head Unit1 layer active. Paste the

objects into this layer. Double-click on the lake object, which opens a Contour Information dialog box describing that contour. Enter a value of 75 to represent the head in the lake. Click OK. The head in the river slopes, so more steps are required to define this spatially varying function. We want to build in a function that will approximate the slope of the river in the x-direction. On our base map the location in the river where $h = 23.5$ m is at $X = 5740$ m on the Argus ONE ruler (see Figure 21), and $h = 5$ m at $X = 2080$ m. This yields a simple linear equation ($h = 0.005X - 5.5$). (If the base map is placed on

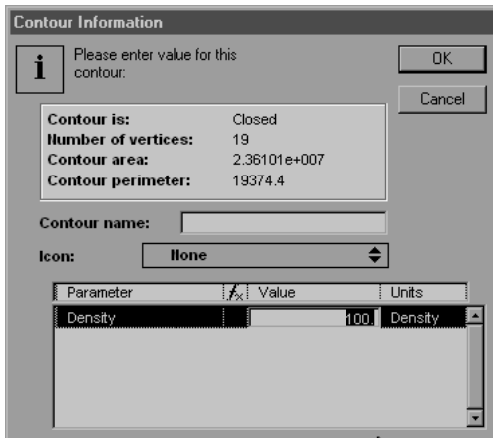


Figure 20. Contour Information dialog box for the domain outline contour. The value of density will be used to compute the cell size of the finite-difference grid.

the page differently, these locations may be slightly different, resulting in a different equation). We will now use this function to define a sloping background value for the layer. In the floating layers window, click on the Layers button. This opens the Layers dialog box (Figure 9). In the Layer Parameter table, click on the f_x button to the right of the Value column of the Prescribed Head Unit1 parameter. This opens the Expression dialog box. In the Functions list, select Mathematical. Then, scroll the right hand list until X is visible and double click on it. This places the function "X()" in the expression box. Then type "*0.005-5.5" after the "X()" in the expression box to complete the definition of the function (Figure 10). Click OK. Then click Done in the Layers dialog box. To have this background value apply to the river, we must null the contour value for the river object. This is done by double clicking the river object and deleting the existing contour value, then clicking OK. The value for the contour will vary, but the contour label will display the value of one of the vertices on the ends of the contour line. Use the mouse to check the value of head along the river and in the lake by placing the mouse pointer in the Prescribed Head Unit1 layer and observing the

value in the lower-left corner of the Argus ONE window.

3. Define regions of no flow: Copy the five objects in the Map Unit1 layer that correspond to impermeable areas in which there are no-flow zones (see Figure 16) and paste them into the Added Inactive Area Unit1. The default value (0) of the pasted objects defines them as no-flow barriers.

4. Define geologic units, packages, and general simulation parameters: Return to the MODFLOW/MOC3D DataSets window by selecting Edit Project Info from the PIEs pull-down menu. Clicking on the tabs at the top of this window allows access to the various data sets.

a. Project dialog box: Enter "Sample problem using MOC3D" for Project Name and Project Title. Add additional information as desired. Remember that you should advance to additional dialog boxes by using the tabs at the top of the window rather than clicking OK. The latter would return you to the main Argus ONE window.

b. Geology dialog box: Click on the Geology tab at the top of the window. The default specification for the *MODFLOW-96* GUI is to define three geologic units initially (see Figure 4). Because our sample problem is two-dimensional, we must delete the second and third geologic units. Select the line in the table labeled Bottom Aquifer and then click Delete. Repeat this process for the unit labeled Aquitard. The default properties of the remaining unit labeled "Top Aquifer" are acceptable for our problem.

c. Misc. Controls dialog box: Click on the Misc. Controls tab. Select CHTOCH for Misc. Control Option (see Harbaugh and McDonald, 1996, p. 16). This *MODFLOW-96* option is recommended whenever using the *MOC3D* model.

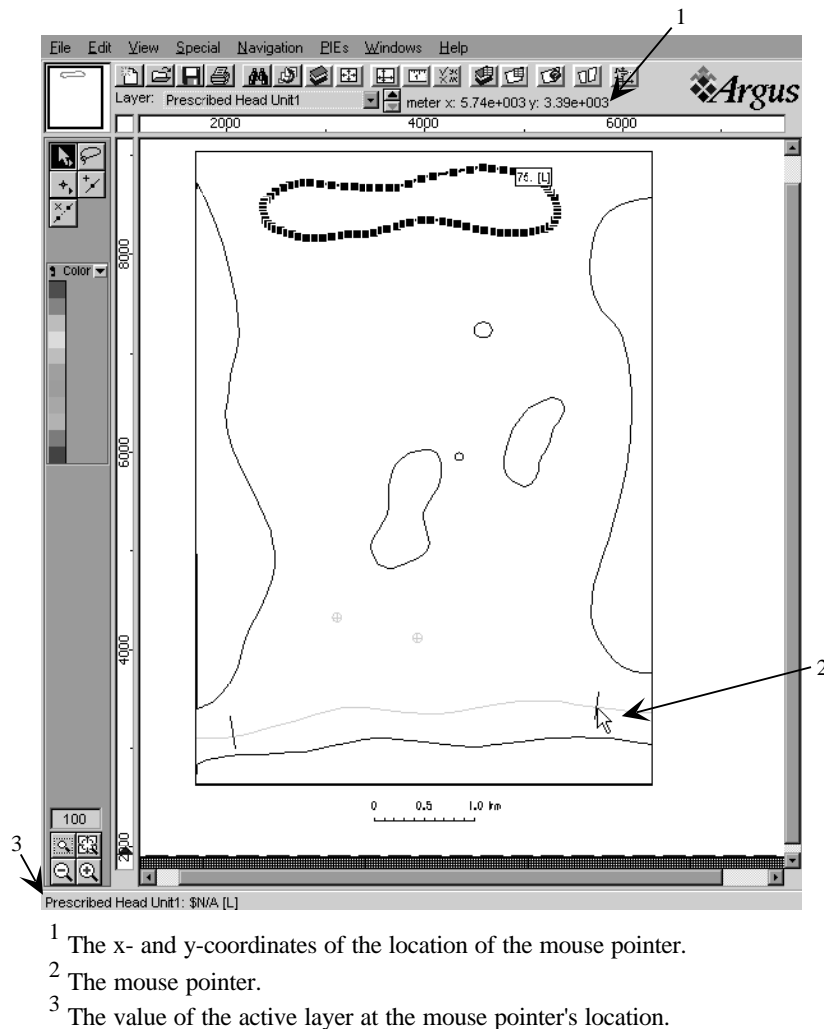


Figure 21. Using the mouse to point to the location on the base map (here, a point at which a measurement of head in the river was recorded) to verify the x- and y-coordinates for that location. Prescribed Head Unit1 is the active layer, while the basemap (in Map Unit1) is visible.

d. Stresses/Solvers dialog box: Click on the Stresses/Solvers tab. At the bottom of this window is the checkbox to include *MOC3D* in a simulation. Click on the checkbox next to Solute Transport to add *MOC3D* to the simulation. Also click on the checkbox to the left of the WEL package to add a Wells layer to the simulation. In this case, we chose to represent the river in our problem using the Prescribed Head layer rather than the River package. The default solver (PCG) is acceptable for this problem.

e. Time dialog box: Click on the tab labeled Time. This simulation assumes steady-state flow. For steady-state flow, *MODFLOW-96* treats a stress period as a unit length of time unless the time units and length of stress period are declared; the transport simulation, however, requires explicit definition of time. Click on the box next to "Time units" and choose Seconds. In the bottom half of the window, select the first and only stress period in the table. This loads the values from the selected stress period into the editable fields below. Click on the field next to Length (PERLEN) and enter a value of 6.31152E+8, which is the approximate number of seconds in 20 years, taking into account leap years. **You must click Modify to change the value in the table for the stress period.** Note that seconds are the unit of time and meters are the units of length for the simulation.

f. Output Files dialog box: Click on the Output Files tab. Enter "rma" for the root name of the simulation files. The default values for the other parameters are sufficient for the example problem.

g. Output Controls dialog box: Default values are acceptable.

h. PCG dialog box: Click on the PCG tab. Reduce the head change criterion (HCLOSE) to 0.0001 and the residual criterion (RCLOSE) to 0.0001 to ensure a numerically accurate solution.

i. Transport Subgrid dialog box: Click on the right arrow to scroll to the *MOC3D* dialog boxes. Click on the Transport Subgrid tab. This is where information describing the transport subgrid is entered, as well as several other *MOC3D* simulation parameters. Default values are acceptable. Note that if a subgrid is desired, the row and column extent of the subgrid should only be defined after the domain is discretized.

j. Particles dialog box: Click on the Particles tab. In this window, information about particles in *MOC3D* is entered. The default value of $NPTPND = 1$ should only be used for preliminary debugging runs, as the numerical accuracy using one particle per node is generally too low. For the test problem, set the number of particles per node ($NPTPND$) to 9.

k. *MOC3D* Output + Dispersivities dialog box: Click on the *MOC3D* Output + Dispersivities tab. Output options for *MOC3D* results are specified in the upper half of this box. The default values for the first two lines tell *MOC3D* to print concentration data at the end of every flow time step and velocity data at the end of every stress period to separate ASCII text files. These files will be used by the *MOC3D* post-processor to visualize concentration and velocity information. The values for second line will result in no separate file for calculated velocity output, but the velocity information will be printed to the main *MOC3D* output file at the end of every stress period. In the bottom half of the window, transport properties that vary for each geologic unit are entered. In our sample problem, there is only one geologic unit. Click on the first (and only) line in the table. In the fields below, enter a value of 30 for longitudinal dispersivity and 3 for transverse horizontal dispersivity. The transverse vertical dispersivity does not need to be designated because this is a two-dimensional horizontal-flow example. **Click the Modify**

button to enter these values into the table.

Click on OK; this saves all the information entered in the dialog boxes and returns to the main Argus ONE window. Note that the floating layers window contains a set of layers that has been modified by the data entered during this step. The MODFLOW/*MOC3D* DataSets dialog boxes can be viewed and edited at any time by choosing Edit Project Info under the PIEs menu.

5. Saving the project: Because a moderate amount of information has been entered, it is a good idea to save the project at this point. Save all the information and data in this project by opening the pull-down File menu, and clicking Save. This opens a dialog box in which you must specify a file name. In this dialog box, you also have the option to select a directory for saving the project. If you do not specify the suffix ".mmb" as a part of the file name, Argus ONE will automatically append it to the name you supply. We chose the name *rma.mmb*. This also becomes the title of the main Argus ONE window.

6. Defining layers having uniform values: For layer information that does not vary spatially, we will define background values for particular parameters using the Layers dialog box. Click on the Layers button in the floating layers window; this opens the Layers dialog box.

a. Elevation Top Unit1: For simplicity we will assume that the geologic unit is horizontal and that the elevation of its top surface is 51 m. Activate this layer by clicking on the name in the top table of the box; this highlights that line and loads the parameters for that layer in the bottom table. Click on the f_x button to the right of the Value column of the Elevation Top Unit1 parameter. This opens the Expression dialog box. Enter a value of 51 in the expression box. (NOTE: the MODFLOW FD Grid layer also contains a parameter named Elevation Top Unit1, as well as several of the parameters listed below.

You should not change the value of these associated parameters. Make sure that you change the layer parameter in the appropriate layer, in this case, the Elevation Top Unit1 layer.) Click OK.

b. Elevation Bottom Unit1: Follow the same procedure as in step 6a, setting elevation of the bottom of the unit equal to 39 m. Note that the difference between the elevation of the top and bottom of this unit equals the saturated thickness (12 m).

c. Hydraulic Cond Unit1: Follow same procedure as in step 6a, setting $K_x = 1.0E-4$ (this value is in m/s). The value of K_z is not used in this two-dimensional areal simulation, so its value need not be modified.

d. Init Concentration Unit1: The default value is set to 0.0, which is the desired value in this case.

e. Porosity Unit1: The default value is set to 0.2, which is the desired value in this case.

f. Click Done.

7. Define wells: By definition, all wells are defined as points in the horizontal plane and lengths in the vertical dimension. In the base map the well locations are represented by symbols and the disposal pond by a closed contour that showed its areal extent. Because the disposal pond has a known leakage rate but the flux occurs over an area that may comprise of two or more cells of the finite-difference grid, we are choosing to represent the disposal pond as two injection wells. We will use the symbols on the base map for defining the location of the wells. Make the Wells Unit1 layer the active layer, and make sure the Map Unit1 layer is visible beneath it. Use the point tool to specify two wells to the left and right of the center of the disposal pond and one well at each of the locations of the two pumping wells (use the zoom tool if necessary). Placing a point

will open a Contour Information dialog box where the information associated with that well is entered (see Figure 22, which shows the values appropriate for each of the wells used to represent the disposal pond). Note that because the disposal pond is being represented by two separate wells, the stress rate must be divided between them to account for the known flux. (If a coarse grid is used and both wells fall within one cell, *MODFLOW-96* will account for both stress rates at a single node and the total flux will be consistent with the known value). Repeat this process for each well. Refer to Figure 16 for information associated with each well (use the

Contour Information

Please enter value for this contour:

OK Cancel

Contour is: One point
 Number of vertices: 1
 Contour area: 0
 Contour length: 0

Contour name:

Icon:

Parameter	Value	Units
Top Elevation	51	L
Bottom Elevation	39	L
Stress1	0.0125	L^3/T
Concentration1	1.000	

Figure 22. Contour Information dialog box displaying the values used for one of the two wells used to represent the disposal pond in the sample problem.

elevation values shown in Figure 22 for all of the wells). Stresses are negative in sign to represent withdrawals at the two pumping wells, and concentrations at these wells can be ignored because water is only removed. We also selected Sink icons for the pumping wells using the icon selection box in the Contour Information dialog box. When finished, values for four wells should have been entered.

At this point, the main Argus ONE window will show the location of all wells in the Wells Unit1 layer. The objects are labeled with the first parameter in the parameter list for the

layer. To change this label, enter the Layers dialog box and use the up- and down-arrows to the right of the parameter table to change the parameter order (we moved Stress1 into the first position). Figure 23 shows the main Argus ONE window with the Wells Unit1 layer active and the Map Unit1 layer visible. The well locations are flagged by their icons and the first value in the parameter list (Stress1). Note that the disposal pond on the map is covered up by the symbols for the two wells representing it. Double clicking on a well location while the Wells Unit1 layer is active opens the Contour Information dialog box for that well object, allowing you to edit the information associated with it.

8. Define Particle Regeneration Unit1: Particle

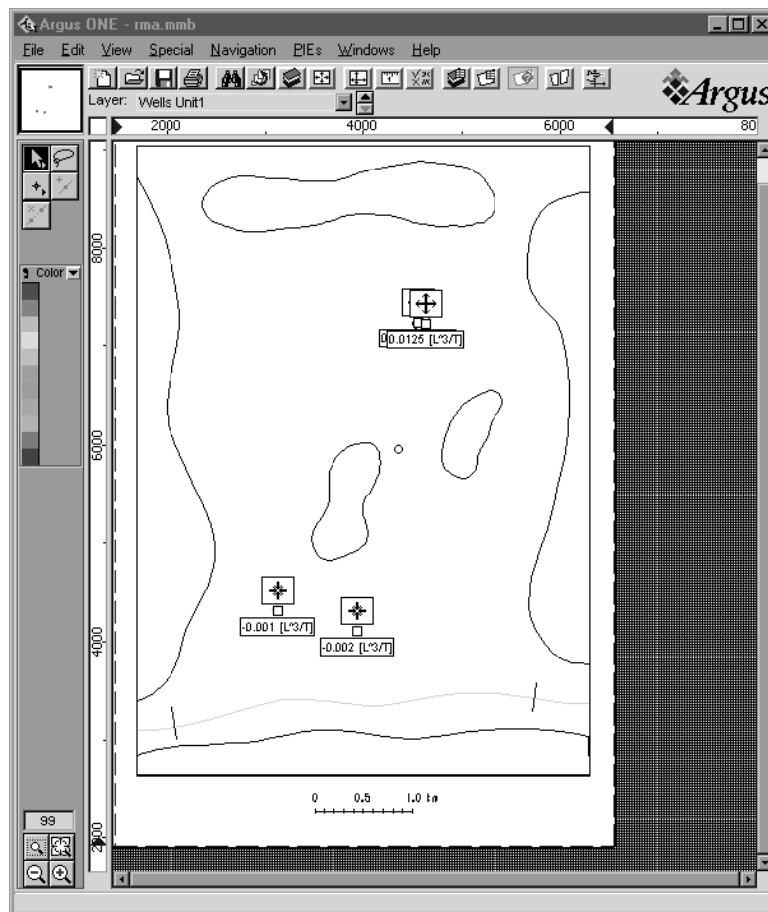


Figure 23. Map for the sample problem showing the placement of the disposal pond and pumping wells added using the Wells Unit1 layer. Note that the disposal pond is represented by two injection (recharge) wells.

regeneration must be flagged for all "strong" fluid sources and sinks (see Konikow and others, 1996, p. 76). *MOC3D* automates particle regeneration for constant-head cells (where $IBOUND = -1$); in our example the lake and the river were defined in this manner in the Prescribed Head Unit1 layer. Therefore, the only remaining *strong* fluid sources or sinks are the two wells representing the disposal pond (the pumping wells represent weak sinks). To add these locations to the Particle Regeneration Unit1 layer, select the two well objects representing the disposal pond in the Wells Unit1 layer and copy them. Activate the Particle Regeneration Unit1 layer in the floating layers window. Paste the objects into this layer, and double click on one of them. This opens a Contour Information dialog box, in which you

should change the value of the flag for particle regeneration to 1. Click OK. Similarly change the value for the second well location.

9. Define observation wells:

Activate the MOC3D Observation Wells layer. Choose the point-contour tool and place it over the location of the observation well visible in the Map Unit1 layer. Clicking once will open a Contour Information dialog box for this observation point. Define Elevation1 at some value within the range of the geologic unit. We used a value of 45. Note that the MOC3D Observation Wells layer allows the designation of up to five observation elevations at a single map location, which might be necessary in a three-dimensional problem. Click OK.

10. Create finite-difference grid:

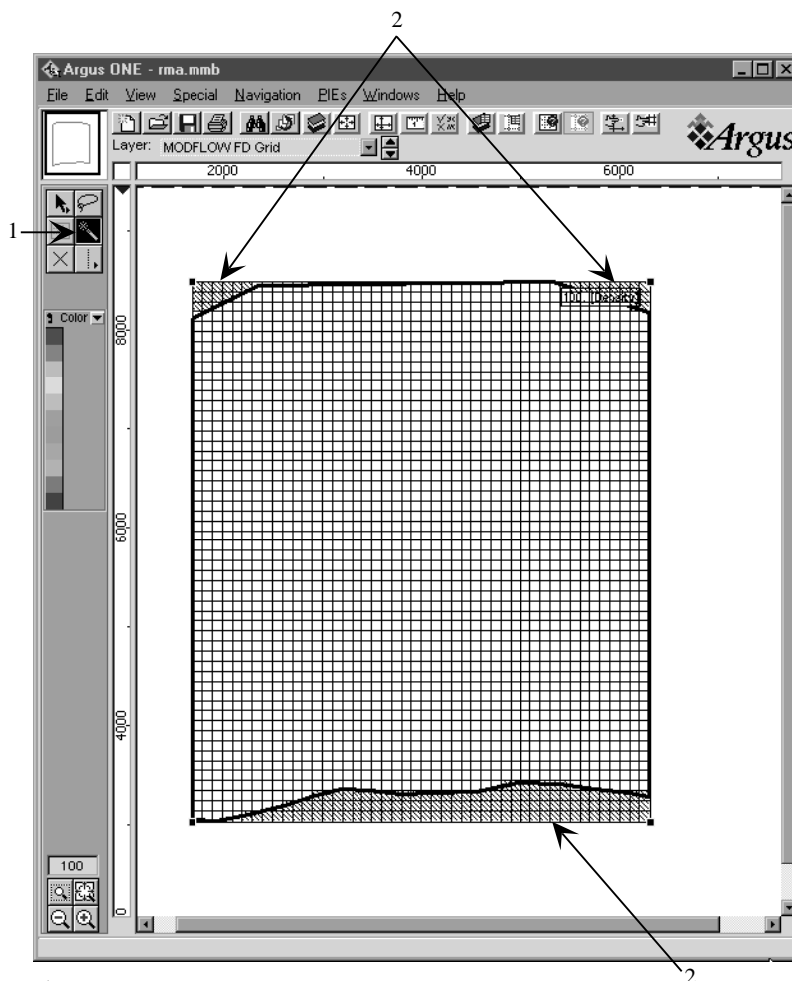
Activate the MODFLOW FD Grid layer from the floating layers window, and make sure the MODFLOW Domain Outline is visible. Choose the Magic Wand

tool from the tool bar near the upper left-hand corner of the map. Use the mouse to place the wand icon anywhere within the Domain Outline and click. This will open a Grid Angle dialog box. The default setting will automatically calculate the grid angle. This is desired, so click OK. The previously specified grid density of 100 (see step 1 above) will cause the gridding procedure to generate a grid having about 3,000 blocks (Figure 24). Note that the extent of the rectangular finite-difference grid is defined by the maximum and minimum x- and y-coordinates of the model domain. For our irregularly shaped domain, the areas outside of the domain that fall

within the rectangular grid area are automatically defined as inactive cells.

11. Visualizing and checking input: After completing steps 1 through 10, the data set should be complete and the model ready to run. It is good practice, however, to review the data set before running the model. The visualization capabilities of Argus ONE help to facilitate this. For example, if we want to view the IBOUND array to cross check the boundary conditions for the generated grid, we would first make sure the MODFLOW FD Grid layer is activated. A number of parameters are linked to this layer,

which enables color scale visualization within the grid. To list these parameters, click on the down arrow next to the color bar. Select IBOUND Unit1. This will color the grid to reflect the values of the IBOUND array. As seen in Figure 25, the 100-m grid spacing results in a reasonably close approximation to the geometry of the original geologic and hydrologic boundaries of the system. (Note: if there are isolated active cells "south" of the river boundary, they cannot interact with the main part of the active aquifer. These isolated cells should be eliminated by editing the contour you drew in the MODFLOW Domain Outline layer by dragging and (or) adding vertices, and then creating a new grid. See the Argus ONE User's Guide (Argus Interware, 1997) for information on editing contour lines.) To intensify the color, if desired, select Opaque Blocks under the View Menu. Similarly, you can check the Initial Head array, particularly to see that the sloping heads along the river were defined correctly, by choosing the Initial



- 1 The magic wand tool used to create the grid.
- 2 Areas of the grid that are inactive, designated with hatching.

Figure 24. The finite-difference grid in the MODFLOW FD Grid layer for the sample problem.

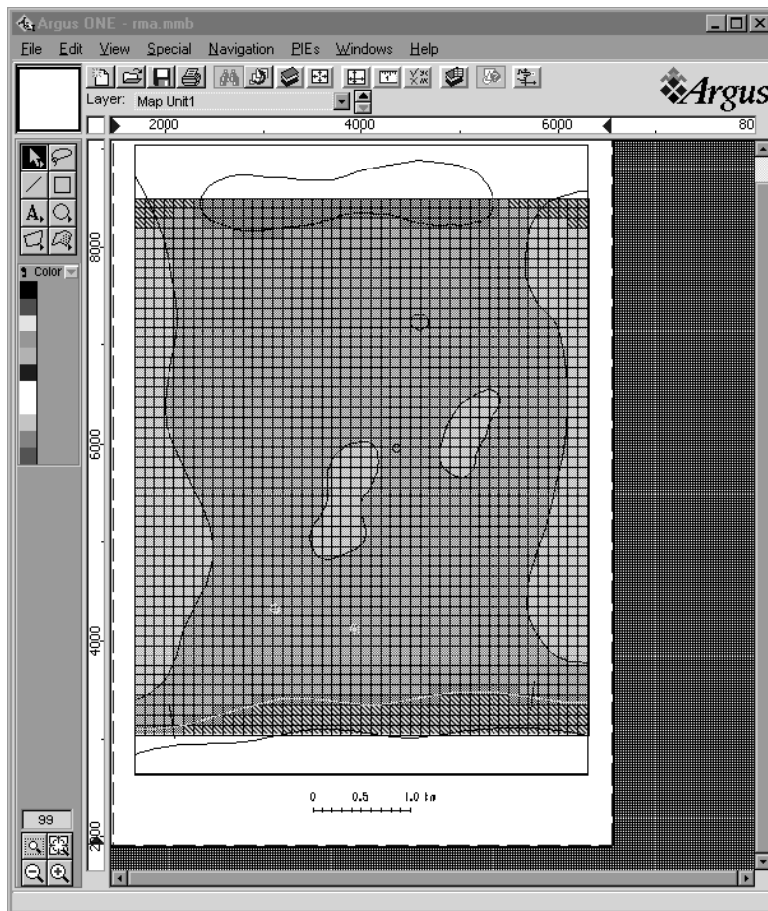


Figure 25. The MODFLOW FD Grid colored (shaded) according to the value of the IBOUND array in the sample problem.

Head Unit1 parameter from the color pull-down menu.

12. Running *MOC3D*: Argus ONE must first transform the project information into the formats required by *MOC3D*. This process is called exporting, and it creates the input files that *MOC3D* uses. Then the simulation can be run (note that export can only take place when the MODFLOW FD Grid is active). Before exporting, it is a good idea to save the project. Choose Save from the File pull-down menu. After it is saved, in the PIEs pull-down menu, choose Run MODFLOW/MOC3D. The Run MODFLOW/MOC3D dialog box is opened. The default settings are acceptable, so click OK. This opens a dialog box allowing you to select a directory in which to put all input and output files for *MOC3D* (note that

entries in the export file name and file type boxes in this window are ignored by all processing). Click Save. This exports the data, showing a progress bar while the processing occurs (for our example, exporting took about 20 seconds). When that is completed, a DOS console window is automatically opened by the execution of *MOC3D*. When execution is completed, hit any key when prompted to close the console window (for our example, execution was completed in about 1.5 minutes).

13. Checking results: Use a text editor to examine the output listing files for *MODFLOW* (*rma.LST*) and *MOC3D* (*rma.OUT*) to check numerical convergence, fluid and solute budgets, and flow and solute mass balances. These files are created when *MOC3D* is executed and are located in the directory specified in step 12. Verify that the numerical accuracy is adequate for your needs.

14. Visualizing results: In a typical analysis, you may want to visualize the calculated heads, velocities, and concentrations. First turn off the present grid coloring; click on the down arrow next to the color bar and choose None.

- a. To contour the head distribution, select MODFLOW Post Proc under the PIEs pull-down menu. Open the appropriate file containing the calculated head data (*Root-name.FHD* where *Rootname* is the name entered in step 4f; in our case the file is named *rma.FHD*). This opens a dialog box showing the available data. In our case only one data set of head values exists, representing the steady-state solution of the flow equation. Choose this data set and click OK. This brings up the Chart Types dialog

box. Choose Contour Map and click OK. Because the contouring package includes the artificially high values specified for the no-flow cells, the initial contour interval is inadequate and must be modified. Make MODFLOW Post Processing Charts the active layer and double click anywhere on the post-processing object. This opens a Contour Diagram dialog box. Set the Minimum value to 0, the Maximum value to 80, and the Delta value to 2. To improve contrast when overlaying the heads on the concentrations, the colors can be turned off by clicking the Show Colors button. If desired, the title can be modified or deleted by clicking the Title tab and editing the title field. Click OK.

b. To create a vector plot of the calculated velocities, select MOC3D Post Proc under the PIEs pull-down menu. Open the appropriate file containing the calculated velocity data (these files have the suffix ".VLA"; in our case it is called *rma.VLA*). Select the COLUMN and ROW data sets, and click OK. Rename the MOC3D Post Processing Charts layer (by editing its name in the Layers dialog) to avoid overwriting the velocity vector map in the following step.

c. To create a color map of the calculated concentrations at 20 years, select MOC3D Post Proc under the PIEs pull-down menu. Open the appropriate file containing the calculated

concentration data (these files have the suffix ".CNA"; in our case it is called *rma.CNA*). Select the data set that represents the appropriate time level (in our case, the data was labeled for layer 1, stress period 1, time step 1, and move increment 325). De-select the data for the initial conditions unless you desire two maps scaled to fit the page size. Click OK. Choose Color Map from the Chart Types dialog box. Click OK. To view the visualization results with the heads overlaying the concentration and the original base map in the background, as shown in Figure 26, make the MODFLOW Post Processing

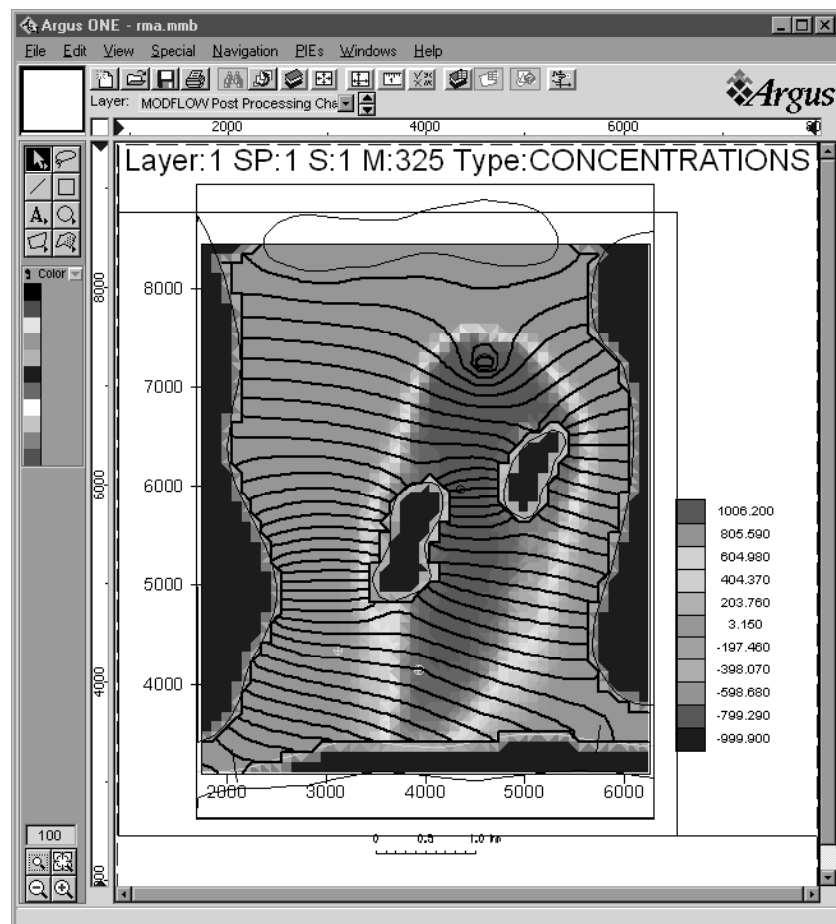


Figure 26. Post-processing layers generated with the *MODFLOW-96* and *MOC3D* post-processing PIEs using simulation results from the sample problem. The black contour lines represent calculated head values; the contour interval is 2 m. The color map (shown here in shades of gray) in the background represents calculated concentrations at the end of the simulation. Note that the concentration value of -999.9 in inactive cells is a flag that can be set within the pre-processor.

Charts the active layer and click the Show:None button in the floating layers window. Then make the Map Unit1 layer and MOC3D Post Processing Charts layer visible by clicking on their closed "eye" icons. Note that the results indicate that the leading edge of the plume has just started to enter the river.

CONCLUSIONS

The Argus ONE *MODFLOW-96* GUI with *MOC3D* capability offers an efficient and effective means to generate and visualize data sets for complex three-dimensional solute-transport problems. This interface is an enhancement of a previously published GUI for *MODFLOW-96* (Shapiro and others, 1997). The GUI is a Plug-In Extension to the commercially available Argus ONE software package.

Argus ONE associates aquifer properties with spatial coordinates using a geographic information system. This provides the basis for linking spatially varying system properties to a finite-difference grid and generating an input data set for *MOC3D*. Therefore, if it is desired to change the discretization of the finite-difference grid, it can be accomplished automatically and very efficiently. *MOC3D* can be executed from within the Argus ONE environment; however, *MOC3D* is a separate executable program. Because Argus ONE generates data files used by *MOC3D*, these data files can also be modified, if desired, outside of the Argus ONE environment. The results of a *MOC3D* simulation can be visualized using the post-processing capabilities of the GUI and Argus ONE. For example, velocity vectors can be plotted on top of concentration contours to illustrate the movement of a contaminant plume.

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