VS2DTI—A Graphical User Interface for the Variably Saturated Flow and Transport Computer Program VS2DT

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VS2DTI -- A Graphical User Interface for the Variably Saturated Flow and Solute Transport Computer Program VS2DT

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ABSTRACT

VS2DTI is a graphical user interface for the U.S. Geological Survey's variably saturated ground-water flow and solute transport computer program, VS2DT. VS2DTI provides a windowsbased modeling environment that allows the user to generate input data sets, run the VS2DT program, and display simulation results. Computer program VS2DT solves the finite difference approximations to Richard's equation for flow and the advection-dispersion equation for transport. Problems can be simulated in one or two dimensions using cartesian or radial coordinate systems. VS2DTI consists of a preprocessor, the VS2DT program, and a postprocessor. The preprocessor allows the user to view and edit spatially varying input data. Grid design and model domain boundaries can be changed independently of hydraulic parameters. This feature greatly facilitates resizing and refinement of the model grid. There are several options for setting time-varying boundary conditions. Numerical values can be entered into tables and model options can be selected from menus. The postprocessor can display contours of simulated pressure head, moisture content, saturation, or concentration for each time step, thus creating a simple animation of model results. This report provides an overview of the features and capabilities for VSDTI. The current version of the software contains an on-line help manual that gives detailed instructions and a tutorial on how to use the software.

INTRODUCTION

VS2DTI is a graphical user interface for simulating water and solute transport through variably saturated porous media with the computer program VS2DT (Healy, 1990; Lappala and others, 1987). The interface consists of a preprocessor and a postprocessor. The user selects simulation options and enters the input data required by the model in the preprocessor. VS2DT can then be executed from within the interface, and results, in terms of contour plots of pressure heads or other variables, can be displayed as functions of time in the postprocessor.

VS2DT is a finite-difference model for simulating water and solute movement through variably saturated porous media. It has been applied in a variety of field studies (for example, McCord and others, 1997; and Halford, 1997). The approximating equations that it solves are based on Richard's equation for flow and the advection-dispersion equation for transport. The model can analyze problems in one or two dimensions using either cartesian or radial coordinate systems. Several boundary conditions that are specific to flow under unsaturated conditions are available, including infiltration with ponding, evaporation, plant transpiration, and seepage faces. Solute transport options include first-order decay, adsorption, and ion exchange. The program is written in standard Fortran 77.

In the VS2DTI preprocessor, options are selected from pull-down menus and various buttons, check boxes, and text fields. Numerical data that are independent of space in the simulation are entered into tables. Data that vary spatially are entered and edited graphically with tools that are commonly found in other graphical user interfaces for hydrologic models. The

preprocessor creates an ASCII format input file that is passed to VS2DT. Once all required data have been entered, the user can run VS2DT within the graphical user interface and display results in the postprocessor. The postprocessor graphically displays results as they change over the duration of the simulation time. Overall errors in fluid and solute mass balance are also displayed.

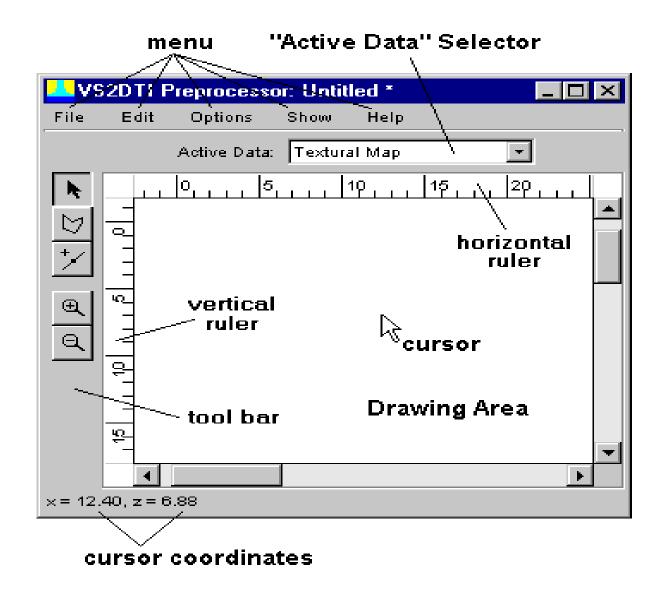


Figure 1. -- Main window of VS2DTI preprocessor.

The "Drawing Area" is where graphic input are viewed. The "Active Data" selector is used to switch among different types of spatial data to be entered or edited on the drawing area. Spatial data include the model domain, textural map, initial and boundary conditions, observation points, grid, and site map. The toolbar contains buttons for data entry and editing. Menus are used for file management, displaying and editing data, selecting options, and accessing the help manual. Horizontal and vertical rulers show the coordinate axes system. The cursor coordinates are displayed in the lower left corner of the window and give the position of the cursor with respect to the model origin. These features are explained more fully in the following sections.

Pull-Down Menus

Five pull-down menus are located at the top of the main window: "File", "Edit", "Options", "Show", and "Help" (fig. 1).

File

The "File" pull-down menu allows the selection of a new ("New") or existing ("Open") file as the VS2DTI input data file. It also allows the current input data file to be saved ("Save") or renamed ("Save As"). Note that the input data file to VS2DTI is not the same as the input data file to VS2DT. The latter is an ASCII file generated by the interface based on the simulation set up. This file is automatically generated when the postprocessor is invoked, but it can also be saved to a user-specified directory by using the "Export" menu item. Exported data can be used to run VS2DT outside of VS2DTI. (Note that the current version of this software does not allow existing VS2DT input data sets to be imported into the interface.) Selection of the "Print" menu item prints whatever is currently displayed in the Drawing Area. The "Exit" item in the menu terminates the program.

Edit

The "Edit" pull-down menu allows selection of several common editing tools, such as "Undo", "Redo", and "Delete". The actual items that appear in this menu depend on how the "Active Data" is set and are discussed in the subsequent section on Spatial Data Types.

Options

The "Options" pull-down menu has two items: "Drawing..." and "Model...". Selection of "Drawing..." opens the **Drawing Options** dialog box which is used to set the size and scales of the drawing area as well as the location of the origin and ruler units. Selection of the "Model..." item opens the **Model Options** dialog box. This box contains five or seven, if transport is simulated, tabbed panels within which the user selects and sets various options.

The **Basic** panel allows selection of *length*, *time*, and *mass units*. It is recommended that the user set these units as the first step in constructing a simulation and that they never be changed. Any set of units can be used, but consistency must be maintained in using those units when entering values for hydraulic and transport properties (such as hydraulic conductivity) and boundary conditions. If units are changed after data have been entered, then the user must reenter the affected data. VS2DTI does not automatically convert data to different units. The **Basic** panel also allows selection of *radial coordinates* (as opposed to cartesian coordinates) and *simulation of solute transport*, *evaporation*, and *plant transpiration*.

The **Flow** panel allows three options for setting initial conditions for the flow equation:

1) *Equilibrium profile* - the initial pressure head equals negative elevation head above a water table, 2) *Pressure head* - as input by the user, and 3) *Moisture content* - as input by the user. (Selection of actual values for initial conditions is discussed in the section on Initial Hydraulic Conditions under Entering Spatial Data.) In this panel the user can also select the method for calculating intercell relative hydraulic conductivity. *Arithmetic mean* is the preferred method, but

users may also select *geometric mean* or *upstream weighting*. Four methods are allowed for representing hydraulic characteristic function: the *van Genuchten model*, the *Haverkamp model*, the *Brooks-Corey model*, and *tabular data*. Details on these methods are given in Lappala and others (1987) and in the on-line help manual in VS2DTI.

The **Transport** panel appears only if the *Simulate transport* option was selected on the **Basic** panel. On this panel there are two options each for space and time differencing. *Centered in space* differencing is preferred; *backward in space* is less accurate, but can be used to avoid oscillations when coarse spacing is used. *Centered in time* differencing (Crank-Nicholson scheme) is more accurate than *backward in time* (fully implicit scheme) but can cause oscillations. There are several options for adsorption and ion exchange. Users may select one and only one of these options. Details on the available adsorption isotherms and ion exchange reactions as well as definitions for the required parameters are contained in Healy (1990) and in the on-line help manual in VS2DTI.

The **Solver** Panel allows entry of values for parameters that affect the iterative matrix solver in VS2DT. The *Relaxation parameter* should generally be in the range of 0.4 to 1.2. The *Minimum and Maximum number of iterations* control the range in number of iterations that the solver will attempt. If convergence is not achieved in the allowed number, then the solution is restarted for the time step with a reduced time-step size. If convergence is not achieved after three consecutive time-step reductions, the simulation is considered to have reached convergence failure. When this occurs, the action taken by VS2DT depends on whether the user selected the option to *Stop simulation at convergence failure*. If so, then the program is terminated. If not, then the simulation proceeds to the next time step after printing a warning. It is recommended that the *Stop simulation at convergence failure* option be selected. The simulation will also halt if the *Maximum number of time steps* is reached. *Closure criteria for head and concentration* are used by the matrix solver to test for convergence. If the maximum change in head or concentration at any node between successive time steps is less than the criterion, then convergence is assumed. In general, as these criteria are decreased, the accuracy of results is improved and the computational effort is increased.

The **Output** panel controls the writing of VS2DT output files. Specific information on these files is contained in the Files section of this report. There are five *Output Variables* that may be selected. If selected, then values for these variables at every node will be printed to the main output file at selected *Output Times*. (Note that if the *Print Result* option of the **Recharge Period** window is selected, these values will be printed for every time step in the recharge period.) *Mass Balance Output* may be printed to the main output file at selected *Output Times* or after every time step. *Output Times* can be selected to coincide with regular time intervals or they can be set by the user.

The **Fluid Balance** panel allows selection of any combination of fluid balance components to be written to the auxiliary output file, "file09.out". For each selected component, three entries are written: total for simulation, total for time step, and rate for time step.

The **Solute Balance** panel appears only when the *Simulate transport* option is selected on the **Basic** panel. It allows selection of solute mass balance components in exactly the same manner as described for the **Fluid Balance** panel.

Show

The "Show" pull-down menu allows the user to select spatial data to display in the Drawing Area. One or more of these data types can be displayed at a time. The user may also select display of the "Postprocessor" and three windows that specify attributes of the spatial data: the **Textural Class** window, the **Evapotranspiration** window, and the **Recharge** window. The **Textural Class** window is linked to the Textural Map spatial data type and is discussed in that section. Similarly, the **Recharge Period** window is linked to the Boundary Conditions spatial data type and is discussed in that section. The **Evapotranspiration** window is presented in the following paragraph. Selecting the "Postprocessor" opens the **Postprocessor** window, which is discussed in a later section.

The **Evapotranspiration** window contains a table of parameters for each evapotranspiration period. It can be displayed only if either or both of the *Simulate evaporation* or *Simulate transpiration* options are selected on the **Basic Model Options** panel. The columns of the table are divided into two tabbed panels - one for evaporation, the other for plant transpiration. The user may enter the evapotranspiration (ET) period length, add new ET periods, or edit parameters in existing ET periods.

Help

The "Help" pull-down menu has two items: "Contents..." and "About...". When "Contents..." is selected, an HTML browser window is opened to the table of contents of the online help manual. This manual contains extensive information on how to use VS2DTI. There are manual pages for all windows and spatial data types. The manual is organized so that the table of contents can be used to navigate to any desired page. The order in which material is presented in the table of contents is designed to guide new users through all steps of creating a new simulation. There is also a tutorial that new users will find useful before constructing their own simulations. The "About..." item displays the version number of VS2DTI.

Entering Spatial Data

Eight different types of spatial data are discussed in the following paragraphs. To enter or edit a particular data type, it must be selected as the "Active Data" in the main window (fig. 1).

Domain

The domain is the region in which fluid flow and solute transport is simulated. The domain is surrounded by the exterior boundary. Regions inside the domain may be excluded by interior boundaries. Exterior and interior boundaries are represented by polygons with an unlimited number of vertices. There are six buttons available in the toolbar. From top to bottom, these buttons are used for editing (or moving) polygons, creating an exterior boundary, creating an interior boundary, adding additional vertices to a polygon, zooming in, and zooming out. Items available in the "Edit" pull-down menu are: "Undo", "Redo", "Select All", and "Delete".

Textural Map

The textural map shows the spatial distribution of textural class zones. Each zone represents a region in which flow and transport properties are assumed to be uniform. The properties for the textural classes are entered in the **Textural Class** window. Zones are represented by polygons that are drawn by the user. There are six buttons, once the domain is defined (otherwise five buttons), on the toolbar. From top to bottom, these buttons are used for selecting, moving, or reshaping a zone, adding a zone, adding a vertex to an existing zone, viewing a discretized version of the map, zooming in, and zooming out. Items under the "Edit" pull-down menu include "Select All", "Delete", "Bring to Front", and "Send to Back". These last two items are available because zones may overlap one another. When portions of the domain are covered by more than one textural class zone, the overlying (or topmost) class is used. Any portion of the domain that is not covered by a textural zone is assigned to the "inactive" textural class.

When the textural map is selected as the "Active Data", the **Textural Class** window is displayed (fig. 2). The window may also by displayed through the "Show" pull-down menu. The window contains the table of parameter values for each textural class. The table is divided into two tabbed panels, one for flow and one for transport, if transport is simulated. The parameters that appear in the table are dependent on the options that were selected by the user in the **Model Options** dialog box (such as which representation is used for the hydraulic characteristic function and whether adsorption is to be simulated). The parameters are defined in the on-line help files.

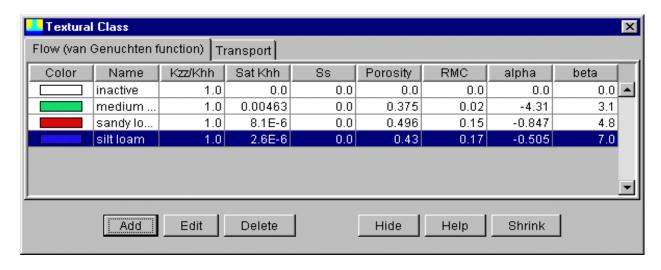


Figure 2. -- Textural Class window of VS2DTI.

Cells in the table are not directly editable. Instead, the buttons below the table may be used to add, edit, or delete a textural class. When the **Textural Class** window is opened for the first time, it will contain a single class named "inactive". This is the default class and represents regions of the domain that are impermeable (that is, water will not flow through zones that are assigned to this class). The parameters in this class are not editable. Before delineating a texture class zone on the "Drawing Area", the texture class must be added the table. To do so, the user must click the "Add" button. This will display the **Add Textural Class** dialog box. The user then selects a color for the new class and enters the required flow and transport parameters. Definitions

of all parameters are contained in Healy (1990) and in the on-line help manual. If the van Genuchten functions were selected to represent the hydraulic characteristics, the user has the option of selecting hydraulic parameters from a catalog of values for generic soil types. References for these parameter values are contained in Lappala and others (1987) and Carsel and Parrish (1988). Zones for any texture class can be delineated on the "Drawing Area" by highlighting the row of the desired texture class and using drawing tools available on the toolbar. Parameter values for existing textural classes may be edited by highlighting the appropriate row and selecting the "Edit" button. This will open the **Edit Textural Class** dialog box and allow the user to change any values.

Initial Hydraulic Condition

Initial hydraulic conditions may be specified in terms of pressure head, moisture content, or an equilibrium profile. This selection is made in the **Flow** panel of the **Model Options** dialog box. The spatial data type for the initial condition depends on this selection and is titled "Initial Pressure Head", "Initial Moisture Content", or "Initial Equilibrium Profile". When initial conditions are specified in terms of pressure head or moisture content, the user may draw contour lines of equal value across the model domain. The buttons on the toolbar allow the user to select or edit contour lines, add closed or open contours, add a vertex to a contour line, display the discretized initial conditions, view labels on the contour lines, and zoom in and out. Options available in the "Edit" pull-down menu include: "Undo", "Redo", "Select All", "Delete", "Contour Value..." (to edit contour values), "Interpolation Method..." (for selecting an alternative interpolation method), and "Color Scale" (for modifying the color scale).

If an initial equilibrium profile is selected, pressure heads are set equal to the negative elevation head above a water table. The user must specify the *z coordinate of the water table*. The user may also replace the upper part of the equilibrium profile by a constant *Minimum pressure head*. In a new simulation, the user sets these values after opening the **Initial Equilibrium Profile** dialog box when "Initial Equilibrium Profile" is the "Active Data". This is done by clicking on the top most button of the toolbar or through the "Edit" pull-down menu. The region from the water table downward (the saturated zone) is colored blue. A red line is drawn at the z coordinate where the negative of elevation head above the water table equals the minimum pressure head. Pressure head below the red line is hydrostatic (uniform total head). Pressure head above the red line is equal to the minimum pressure head. The depth of the water table and the minimum pressure head may be modified by reopening the dialog box or by simply clicking and dragging the water table or red line.

Initial Concentration

These data are displayed only if solute transport is being simulated. Initial values for concentration are entered with contour lines in the same manner described for initial pressure heads and moisture contents.

Boundary Conditions

Boundary conditions must be specified for each recharge period. A recharge period is a time span during which boundary conditions and stresses remain unchanged. For each recharge period, boundary conditions must be assigned to each segment of the exterior boundary plus any interior boundaries. A segment is the straight line connecting two adjacent vertices on a boundary. A boundary condition applies to the entire segment. To vary the boundary condition along a segment, it is necessary to insert vertices on the segment to subdivide it into smaller pieces. Different boundary conditions can then be specified on the subdivided pieces.

Before boundary conditions can be assigned, recharge periods must be created. This is accomplished with the **Recharge Period** window which is automatically opened when "Boundary Condition" is the "Active Data". This window can also be opened from the "Show" pull-down menu. The window contains a table of recharge period parameters. Each row corresponds to a different recharge period. Columns contain parameter values. The values in the table are not directly editable. To add a new recharge period, the user must click on the row of the recharge period that the new period is to follow. Then the "Add" button should be selected at the bottom of the table. This will open the **Add Recharge Period** dialog box. The recharge period parameters can then be entered. Definitions and descriptions of these parameters are contained in Healy (1990) and in the on-line help manual. If the user wishes to modify parameter values, the recharge period row must be selected and the "Edit" button clicked. This will open the **Edit Recharge Period** dialog box.

Once recharge periods have been created, boundary conditions can be assigned. Both flow and transport boundary conditions must be specified. To specify boundary conditions, "Boundary Conditions" must be selected as the "Active Data". Next, the row of the recharge period of interest must be selected in the **Recharge Period** window. To assign boundary conditions, the user selects a boundary segment and clicks on it. Multiple boundary segments can be selected by holding the mouse button down and dragging the mouse across them. Selected segments will be highlighted in gray. Next, the user opens the **BC for Recharge Period** dialog box by clicking the "BC" button on the toolbar. In this box, the desired flow and transport boundary types may be selected. Users may also select the option to set this boundary condition for all subsequent recharge periods. Once a boundary condition is selected, it is colored according to the key displayed on the toolbar. Other buttons on the toolbar allow for display of labels of boundary condition values and zooming in and out. Items available in the "Edit" pull down menu include "Copy All To ..." which allows the user to copy all boundary conditions from one recharge period to another period, and "Corner Policy..." which allows the user to determine how boundary conditions should be applied at the vertices where boundary segments are joined.

Observation Points

Observation points denote locations where simulated total head, pressure head, moisture content, saturation, and concentration are written to output file, "file11.out", at every time step. Observation points can be added when "Observation Points" is the "Active Data" by using the second button from the top of the toolbar. The user then simply clicks on the desired location for the observation point. Points can be moved by using the top most button. Items in the "Edit" pull-down menu include "Select All" and "Delete".

Grid

The grid consists of vertical and horizontal grid lines forming a rectangular array of cells. To lay out the grid, the user selects "Grid" as the "Active Data". The grid may be edited on the "Drawing Area" or on the **Grid** window which may be opened by the button on the toolbar or through the "Edit" pull-down menu.

A uniform grid containing columns of equal widths and rows of equal heights can be created by selecting "Uniform Grid..." from the "Edit" pull-down menu. This opens the **Uniform Grid** dialog box, into which the user may enter values for the *number of columns* and *rows*. Clicking "OK" then causes the grid to be displayed. Buttons on the toolbar permit the user to move the entire grid, move individual grid lines, add new vertical or horizontal lines, show or hide the **Grid** window, display the "Drawing Area" as it will be discretized, and zoom in and out.

The **Grid** window can also be used to add additional vertical or horizontal grid lines. Additional items that can be selected from the "Edit" pull-down menu include "Subdivide..." for adding additional horizontal or vertical grid lines, "Select All..." for selecting all vertical or horizontal lines, and "Delete" for deleting grid lines.

Site Map

As an option, the user may load a site map in a "gif" or "jpg" graphics file. Such a map, although not editable, could be used to guide the drawing of graphical data. To load a map, the user must set "Site Map" as the "Active Data" and then select the third button from the top of the toolbar. This opens the **Load Site Map** dialog box, which allows the user to select the desired graphics file. The top most button on the toolbar can be used to move or resize the site map. The next button allows the user to stretch or compress the map in a manner that keeps one point fixed. This feature is useful for aligning the site map axes system with the rulers. Further details for resizing the site map are contained in the on-line help manual. The other buttons allow zooming in and out and bringing the map to the front or sending it to the back.

POSTPROCESSOR

The **Postprocessor** window contains tools to control the simulation and a display area that resembles the "Drawing Area" of the preprocessor. Simulation results are shown in the display area as contours plotted across the model domain. The postprocessor is interfaced with the numerical model VS2DT in such a way that as the model runs, the simulated pressure head, moisture content, saturation, or concentration are displayed for each time step, thus creating a simple animation of model results. The speed of the animation depends on the computation time needed for each time step. Overall errors in fluid and solute balances are also displayed.

Figure 3 shows a example of the **Postprocessor** window at the conclusion of a simulation. Contours of concentration are displayed along with a color scale. Below the contour plot is information on simulation time and mass balance errors. There are two pull-down menus at the top of the window: "Action" and "Option". Menu items under "Action" are "Run", "Stop", "Reset", "Print...", and "Done". If "Run" is selected, the model computes the solution for the next time step and continues until the entire simulation is completed. The "Run" button immediately below the "Action" menu performs the same function. Selecting "Stop" halts execution of the model and allows the user to print out the contour plot at the stopped time. The "Stop" button

performs the same function. "Reset" moves the clock back to the beginning of the simulation so that the simulation can be restarted. If "Print..." is selected, the screen as it appears at the current time is printed. Selecting "Done" closes the **Postprocessor** window.

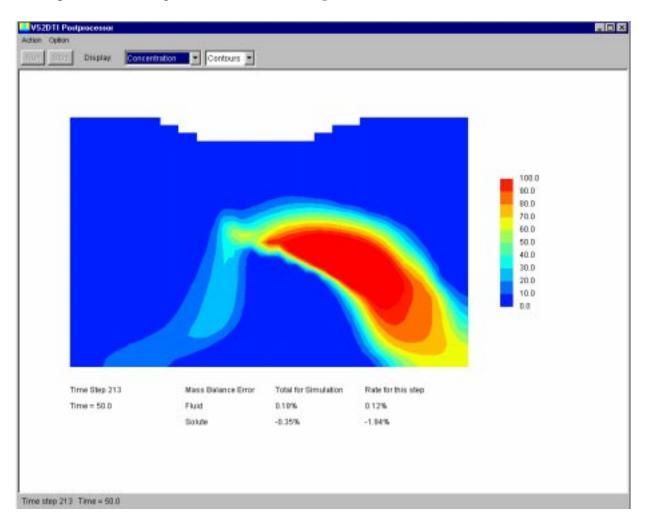


Figure 3. -- Postprocessor window of VS2DTI.

Menu items under "Option" include "Color Scale...", "Speed...", "Zoom in", and "Zoom out". If "Color Scale..." is selected, the **Color Scale** dialog box is opened. In this dialog box, the user can set the upper and lower contour limits and the contour interval. Selecting "Speed..." opens the **Animation Speed** dialog box in which the user can enter a time-delay interval that insures that each time step in the model will be executed no faster than that increment. "Zoom in" and "Zoom out" perform the same functions as in the preprocessor.

The user can select which output variable to display (*pressure head, moisture content, saturation*, or *concentration*) in the left drop-down list box above the display area. The right drop-down list box allows the user to switch between *Cell* and *Contour* displays. When *Cell* is selected, the display consists of active cells each colored uniformly according to the color scale on the right. When *Contour* is selected, the display consists of contours with the regions between contours filled with a uniform color according to the color scale on the right.

Display of mass balance errors are included in the postprocessor to give an indication of the accuracy with which the finite difference matrix equations are being solved by the model. Mass balance error alone, however, may not be a valid indicator of simulation accuracy. A small mass balance error may not signify a high degree of accuracy, but a large mass balance error is usually indicative of low accuracy. As an example, backward differencing in the solution of the transport equation is mass conservative and can produce low mass balance errors, but for problems involving sharp concentration fronts, that scheme will not be highly accurate because of the introduction of artificial numerical dispersion.

FILES

The preprocessor creates an ASCII format file for input to the VS2DT model based on the data that have been entered by the user. ASCII output files are then generated by VS2DT. These files contain information in addition to that displayed in the postprocessor. Only brief information on these files is given here. The user is referred to Lappala and others (1987) and Healy (1990) for additional details on the VS2DT input and output files.

Input

An input file for VS2DT is created whenever the user exports data from the preprocessor. The user can give this file any name. An input file, "vs2dt.dat", is also created every time that the **Postprocessor** window is shown. This file is placed in the current working directory (the directory where the VS2DTI input file is located). These input files are identical in format with that described in Healy (1990) with the following two exceptions.

A new line of input follows line B-5 and contains two variables: "hydraulicFunctionType", which takes on a value of 1 for use of the van Genuchten functions, 2 for Haverkamp, 3 for Brooks-Corey, and 4 for tabular data; and "adsorptionType", which takes on a value of 1 for use of a linear isotherm, 2 for a Langmuir isotherm, 3 for a Freundlich isotherm, 4 for monovalent-monovalent cation exchange, 5 for monovalent-divalent exchange, 6 for divalent-monovalent exchange, and 7 for divalent-divalent exchange.

The other modification to the input file is that free format input is now allowed for importing initial conditions on input lines B-13 and B-25. Because of these modifications, previous versions of VS2DT will not read input files created with the preprocessor. A version of VS2DT that can be used with these input files outside of VS2DTI is included in the download package.

Output

There are five ASCII output files that are created by VS2DT in the current working directory. These are named "vs2dt.out" (the main output file), "file07.out", "file08.out", "file09.out", and "file11.out". These files are identical to those described in Healy (1990). The user can change the names of files to be created by VS2DTI by using a text editor to edit the file "vs2dt.fil" that is in the that directory. That file contains names for the input and output files.

HOW TO OBTAIN AND INSTALL VS2DTI

The software described in this report and an electronic version of this manual, along with instructions for downloading and installing the software, can be obtained from the web site http://water.usgs.gov/software/. Many other hydrologic computer programs are available at this site. Future updates to VS2DTI are planned to provide additional functionality in the postprocessor. The latest version of VS2DTI and a discussion of recent updates will also be available at that site.

Additional copies of this report and the reports by Healy (1990) and Lappala and others (1987) are available from:

U.S. Geological Survey Branch of Information Services Box 25286 Denver, CO 80225-0286

For additional information, write to the address on page ii of this report.

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