Summary of VS2DRTI

NAME

vs2drti - A graphical software package for simulating water flow and heat and reactive solute transport in variably saturated porous media

ABSTRACT

VS2DRTI is a graphical software package for simulating flow and transport in variably saturated porous media. This software package consists of two components:

- VS2DRTI, for simulating water flow and heat and reactive solute transport,
- a standalone postprocessor, for viewing results saved from previous simulation runs.

VS2DRTI combines a graphical user interface with a numerical model (VS2DRT) to create an integrated, window-based modeling environment. Users can easily specify or change the model domain, hydraulic and transport properties, initial and boundary conditions, grid spacing, and other model parameters. Simulation results can be displayed as contours of pressure head, moisture content, saturation, concentration or temperature, and velocity or flux for each time step, thus creating a simple animation.

VS2DRT links the U.S. Geological Survey's computer models VS2DT (for solute transport), VS2DH (for energy transport), and Phreegc (for geochemical reactions). VS2DRT is a finite-difference model that solves Richard's equation for fluid flow, and the advection-dispersion equation for heat solute transport. The model can analyze problems in one or two dimensions using either cartesian or radial coordinate systems. Relations between pressure head, moisture content, and relative hydraulic conductivity may be represented by functions developed by van Genuchten, Brooks and Corey, Haverkamp and others, or by data points. Initial hydraulic condition can be specified as static equilibrium, specified pressure head, or specified moisture content. Boundary conditions include specified pressure or total head, specified flux, infiltration with ponding, evaporation, plant transpiration, and seepage faces. Solute transport processes include advection and dispersion, as well as a complete implementation of the chemical reactions available in Phreeqc.

VS2DRT is written in Fortran 90 and C++.

A Windows executable version of VS2DRT (vs2drt.exe) is included in the download package for user who would prefer to run simulation in batch mode.

METHOD

For the flow equation, spatial derivatives are approximated by central differences written about grid-block boundaries. Time derivatives are approximated by a fully implicit backward scheme. Nonlinear conductance terms, boundary conditions, and sink terms are linearized implicitly. Relative hydraulic conductivity is evaluated at cell boundaries by using full upstream weighting, the arithmetic mean, or the geometric mean of values from adjacent cells. Saturated hydraulic conductivities are evaluated at cell boundaries by using distance-weighted harmonic means. Nonlinear conductance and storage terms can be represented by algebraic equations or by tabular data.

For the advection-dispersion equation, either central or backward

differences may be selected for the spatial and time derivatives.
Thermal conductivity is assumed to vary linearly with moisture content.
The matrix equations produced for the flow and transport equations are
solved sequentially using the strongly implicit procedure.

An operator-splitting approach is used in VS2DRT, whereby the flow
and transport equations are solved independently of the geochemical
reactions. At each time step, the flow, heat, and solute transport
equations are solved, allowing simulated concentrations to be transported
by advection and dispersion. Component concentrations for each model cell
are then transferred to PhreeqcRM; geochemical reactions are simulated;
and updated component concentrations are returned to each cell.

HISTORY

Version 1.6.0 Date: March 20, 2020
 VS2DRTI Graphical Package version 1.6
  Includes recent revisions to PhreeqcRM.
  Updates JRE/JDK download url.
  Adds missing runtime merge modules.

Version 1.5.0 Date: February 14, 2019
 VS2DRTI Graphical Package version 1.5
  Includes recent revisions to PhreeqcRM.

Version 1.4 Date: December 15, 2017
 VS2DRTI Graphical Package version 1.4
  The new computer program VS2DRT links existing USGS computer models VS2DT,
  VS2DH, and PhreeqcRM. VS2DRT allows simulation of water flow, heat transport,
  and reactive solute transport in variably saturated porous media. VS2DRT was
  originally constructed by Haile (2013).
  The VS2DRTI graphical user interface (GUI) is a revised version of the
  VS2DI GUI that supports the new VS2DRT model.

Version 1.3 Date: March 28, 2012
 VS2DI Graphical Package version 1.3
  Preprocessor:
     1. Compatibility with Windows 7 and Vista (32 and 64 bit)
     2. Gravity drain boundary condition.
     3. Rossi-Nimmo hydraulic functions for simulation of very
        dry conditions.
     4. Evapotranspiration period parameters can be
        imported/exported from or to a text file.
  Java Runtime Environment:
     The JRE bundled with the application has been updated to
     Version 1.7.
  VS2DT and VS2DH versions 3.3:
     1. Gravity drain boundary condition.
     2. Rossi-Nimmo hydraulic functions for simulation of very
        dry conditions.
     3. Revised formats for ascii output files - higher
        resolution; wrap around lines eliminated.

Version 1.2 Date: October 12, 2004

 VS2DI Graphical Package version 1.2
  Preprocessor:
    1. Source or sink points may be specified in the model domain.
    2. The x-z (or x-r) coordinates at a vertex of a domain
       boundary, textural zone, or contour may be explicitly
       specified by right-clicking on the vertex.
    3. Multiple, consecutive recharge periods can be added,
       edited, or deleted in the Recharge Period Window.
    4. Boundary condition at a domain boundary segment may be specified by
       double clicking the segment.

5. Boundary condition data (for example, specified pressure) for may be imported from file.
6. Comments are added to the model input files generated for VS2DT and VS2DH Versions 3.2.

Postprocessor:

1. The boundary between textural zones may be displayed.
2. The mass/energy balance calculation has been revised to correctly account for instantaneous changes in mass/energy within the simulated domain due to instantaneous changes in boundary conditions.

Java Runtime Environment:

The JRE bundled with the application has been updated to Version 1.4.2.

VS2DT and VS2DH versions 3.2:

1. Conversion of VS2DT and VS2DH to Fortran 90. This removes all limits on number of rows and columns, number of recharge periods, number of texture classes, number and size of seepage faces, iterations per time step, number of observation points, and output times.
2. Modification to mass balance calculations to list changes in mass due to changing boundary conditions as separate items.
3. Option has been added for enhanced precision (14 digits) in print out to observation and mass balance output files. This option is selected by setting input variable NUMT equal to the negative number of time steps (input line A-5).
4. Output to observation file can be made at selected times only (as opposed to every time step) by setting NOBS (input line A-15) equal to the negative number of observation points.
5. Output to mass balance file can be made at selected times only (as opposed to every time step) by setting NMB9 (input line A-17) equal to the negative number of observation points.
6. Requested output times are now matched exactly, even if this requires a time step size less than the minimum size.
7. Column labels have been added to mass balance output file.
8. Evaporation allowed to occur from cells other than those representing land surface.
9. Corrected bug in loop of ET cycle.
10. Corrected bug in use of interpolation tables for hydraulic properties.
11. Corrected bug in storage term for finite difference transport equation.

Version 1.1 2000/02/09 - extended to work with VS2DH; improved postprocessing capabilities. This release contains revised versions 3.0 of VS2DT and VS2DH, which allow runtime selection of hydraulic function and adsorption type. The VS2DI postprocessor has the capability to run on input files created with earlier versions of VS2DT and VS2DH.

Version 1.0 1999/07/28 - Initial release

DATA REQUIREMENTS

A conceptual model of the geometry and boundaries of the region to be simulated is of prime importance. Initial conditions in terms of pressure heads or moisture contents for flow simulations and concentrations or temperatures for transport simulations are needed. Hydraulic and transport properties of the porous media are also required. These values can be different for different sediments. Flow simulations require values for saturated hydraulic conductivity and for relative hydraulic conductivity and moisture content as functions of pressure head. Solute transport simulations require values for dispersivity and molecular diffusion. Energy transport simulations require values for heat capacities of water and soil and

thermal conductivity. Solute transport simulations require a Phreeqc data file and a Phreeqc input file, which can be created with the PhreeqcI software package (Charlton and Parkhurst, 2002; https://wwwbrr.cr.usgs.gov/projects/GWC_coupled/phreeqc/). Other information may be needed, depending on the program options that are selected.

OUTPUT OPTIONS

Simulation results can be displayed as contours of pressure head, moisture content, saturation, concentration or temperature, and velocity or flux for each time step, thus creating a simple animation. The graphical displays may be printed or saved as bitmap files. Text (or ASCII) output can be obtained for pressure head, total head, volumetric moisture content, saturations, velocities, and solute concentrations or temperatures. Time histories and spatial profiles of the data can be obtained. In addition, the user may opt to view time histories of up to 72 mass balance parameters.

SYSTEM REQUIREMENTS

The VS2DRTI software package was developed using a combination of Java, C, and Fortran programming languages. This software has run successfully on the following operating systems: Microsoft Windows 7, XP, 2000, 98, and NT 4.0.
For other computer platforms, the usability of VS2DRTI depends on the availability of a Java Development Kit for that platform, and the ability to compile Fortran and C programs into dynamic or shared libraries that can be used by the Java program. Additional information on computer requirements can be found in the README file distributed with the software.

DOCUMENTATION

Parkhurst, D.L., and Wissmeier, L. 2015. PhreeqcRM: A reaction module for transport simulators based on the geochemical model PHREEQC. Advances in Water Resources 83: 176–189. DOI: 10.1016/j.advwatres.2015.06.001.

Haile, Sosina S. 2013. VS2DRT: Variable saturated two dimensional reactive transport modeling in the vadose zone. (Doctoral dissertation) Freiberg Online Geoscience 34: 1–152.

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An electronic version of this report can be downloaded from:
http://pubs.er.usgs.gov/pubs/wri/wri994130

Healy, R.W., and Ronan, A.D., 1996, Documentation of computer program VS2DH for simulation of energy transport in variably saturated porous media--modification of the U.S. Geological Survey's computer program VS2DT: U.S. Geological Survey Water-Resources Investigations Report 96-4230, 36 p.
An electronic version of this report can be downloaded from:
http://pubs.er.usgs.gov/pubs/wri/wri964230

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modifications to the U.S. Geological Survey's Computer Program VS2D: U.S. Geological Survey Water-Resources Investigations Report 90-4025, 125 p.
An electronic version of the report can be downloaded from:
http://pubs.er.usgs.gov/pubs/wri/wri904025

Lappala, E.G., Healy, R.W., and Weeks, E.P., 1987, Documentation of computer program VS2D to solve the equations of fluid flow in variably saturated porous media: U.S. Geological Survey Water-Resources Investigations Report 83-4099, 184 p.
An electronic version of the report can be downloaded from:
http://pubs.er.usgs.gov/pubs/wri/wri834099

REFERENCES

VS2DT and VS2DH have been used by scientists at the USGS and at various universities and consulting companies. Example applications are described in:

Bartolino, J.R., and Niswonger, R.G., 1999, Numerical simulation of vertical ground-water flux of the Rio Grande from ground-water temperature profiles, central New Mexico: U.S. Geological Survey Water-Resources Investigations Report 99-4212, 34 p.

Mills, P.C., and Healy, R.W., 1993, Water and tritium movement through the unsaturated zone at a low-level radioactive-waste disposal site near Sheffield, Illinois, 1981-85: U.S. Geological Survey Water-Supply Paper 2386, 72 p.

Halford, K.J., 1997, Effects of the unsaturated zone on aquifer test analysis in a shallow-aquifer system: Ground Water, v. 35, no.3, p. 512-522.

McCord, J.T., Gotway, C.A., and Conrad, S.H., 1997, Impact of geologic heterogeneity on recharge estimation using environmental tracers: Numerical modeling investigation: Water Resources Research, v. 33, no. 6, p. 1229-1240.

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Official versions of U.S. Geological Survey water-resources analysis software are available for electronic retrieval via the World Wide Web (WWW) at:

http://water.usgs.gov/software/

and via anonymous File Transfer Protocol (FTP) from:

water.usgs.gov (path: /pub/software).

See http://water.usgs.gov/software/ordering_documentation.html for information on ordering printed copies of USGS publications.

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