

Variably Saturated Flow and Transport 2-D (VSAFT2)

The latest version of VSAFT should be downloaded from <http://tian.hwr.arizona.edu/yeh/downloads.html> VSAFT2 is constantly being refined and updated. Make sure you have the latest version.

1. GRID TAB

To create a new VSAFT2 model domain, first create a rectangular area which will encompass the active portion. By default a domain with constant width rows and columns will be created, but the size of each individual row or column can be edited manually to achieve any desired arrangement of spacings.

Rows:

The number of rows for the basic grid system to be created. All rows will be the same height by default.

Columns:

The number of columns for the basic grid system to be created. All columns will be the same width by default.

Row spacing:

Use to uniformly change all the heights of the rows in the domain. (unit of Length)

Column spacing:

Use to uniformly change all the widths of the columns in the domain. (L)

Accept Default:

This accepts the default grid system shown in the window as the active numerical solution domain. If variable width rows and columns are needed, or an irregular (non-rectangular) active domain is desired, you must modify it, as explained below.

Modify:

This function allows you to change the geometry of the basic grid system to any arbitrary row and column widths or active domain shape, for the numerical solution domain.

Add Element or Delete Element:

The add or delete options allows adding or deleting elements in the basic grid system to form the solution domain and this task can be accomplished by three different methods: element, window, or polygon (note right click cancels the previous point of the polygon). Select one of the methods first, then select add element or eliminate

element, and move cursor to the grid system to active the element or region of the solution domain from the basic grid system.

The Geometry function (see **FUNCTIONS IN THE MANUAL BAR** below) can be used to create a variable grid mesh for the solution domain.

Accept Changes:

After add or delete element, this option should be chosen to accept changes done to the basic grid system or the solution domain (if it has already defined) as the solution domain for the following simulation.

Next: advance to Problem Definition tab.

2. PROBLEM DEFINITION TAB

Title:

Title for identification of the simulation.

Restart:

This option should be chosen, if you want to restart the simulation from the end of a previous simulation due to **1)** continuation of the simulation for a longer period time with different boundary or source or sink values (e.g., different stress periods) or **2)** previous simulation did not converge.

If the solution did not converge in the previous simulation, the restart option enables a new simulation that continues from the solution obtained from the time step before the divergence occurred. If this is a steady flow simulation, the value of the boundary condition should be changed (for example, a smaller infiltration rate) such that convergence of the solution can be obtained. Once the solution converges for the small flux, the restart option then allows the next simulation to use a larger flux with the last converged solution as the initial guess solution. Restart, in essence, allows a successive approximation the true non-linear solution. If this is a transient flow problem and the solution did not converge, you should redefine (reduce) the initial time step size and try it again. In general, a small time step size will allow convergence but it will then take a long time to complete the simulation.

The restart option also allows change boundary conditions to simulate time-varying boundary conditions. If you create a new project to restart the simulation, you should copy the restart file from the previous project to the new project so that the simulation will start with the previous result.

Problem type:

1. Steady state flow (steady state saturated, unsaturated, or variably saturated flow)
2. Transient flow:
3. Steady state flow with transient solute transport
4. Transient flow and solute transport

Flow type:

1. Horizontal plane flow (depth-average flow)
2. Axisymmetric flow (cross-sectional view of radial flow)
3. Vertical plane flow (vertical cross-section flow)

Next: continue to **simulation control** tab

Back: return to previous **grid** tab

3. SIMULATION CONTROL TAB

Iteration Scheme:

The Picard or Newton-Raphson iteration scheme are used to solve the nonlinear unsaturated flow equations. Newton-Raphson is the default. In general, the Newton-Raphson iteration scheme provides rapid convergence to the solution.

Storage Scheme:

Diagonal lumping, as in Finite Difference (Default)

Lumped Scheme

Consistent Scheme

The diagonal lumping scheme makes the diagonal terms in the stiffness matrix more dominant and leads to a matrix with a better conditional number and the solution converges faster.

Variation:

Indicates the variation of conductivity and moisture capacity within an element for the integration of element matrices: constant (equal to average of nodes) or linear variation. Constant is the default.

Maximum Number of Iteration:

The maximum number of iterations allowed in the nonlinear solver (Picard or Newton-Raphson scheme). If the number is exceeded, the program either reduces the time step size automatically (if it is transient flow) or declares that the solution diverges if this is a steady flow simulation. If the total number of reductions in the time step during a transient flow simulation is exceeded, then the transient case will said to have not converged.

Pressure Head Tolerance:

This criterion determines the convergence of the solution. That is, if the maximum value of change in the pressure head solution at every node of the solution domain during two successive iterations is less than this specified tolerance, the solution is considered converged.

Next: continue to **time step** tab

Back: return to the **problem definition** tab

4. TIME STEP TAB

These parameters control how the program dynamically allocates time step sizes. That is, if the convergence can be achieved rapidly, the time step size will increase automatically. On the other hand, if the solute diverges, the time step size will be reduced.

Initial value of time step:

Initial time step size for the simulation.

Maximum allowable time step size:

This specifies the maximum time step size allowed during the simulation. As a rule of thumb, for infiltration events where sharp wetting fronts are expected, a small maximum allowable time step size is suggested; during redistribution a large maximum allowable time step size can be used.

Multiplier of the time step size:

The value must be equal to or greater than one. This allows the initial time step size to be increased by this factor. If convergence of a solution takes less than 5 iterations, the time step size for the next time level will be multiplied by this factor. As a rule of thumb, a small multiplier (e.g., 1.01) will facilitate convergence.

Maximum simulation time:

The time span for the entire simulation.

Maximum number of reduction:

If the solution diverges during a time step in a transient flow simulation, the program automatically restarts the simulation from the last time step with a reduced time step size ($\frac{1}{2}$ of the previous time step size). The number entered here specifies the maximum number of the reduction of the time step size. If this number is exceeded, the program terminates the simulation and declares the divergence of the solution. The restart option in **problem definition** tab then can be used with a smaller initial time step size.

Next: continue to **material** tab

Back: return to **simulation control** tab

5. MATERIAL TAB

Import:

Allows the import of material files if they already exist in VSAFT2 format.

Define Material Zone:

Use this option to define material zones in the solution domain.

Step 1, select the number of material zones in the solution domain.

Step 2, select the material zone number.

Step 3, select either element or polygon option (again, right click cancels the previous point of the polygon) to define the material zone in the solution domain.

Delete allows removal of the zone already defined. Repeat Steps 2 and 3 to complete the definition of all material zones in the solution domain.

Total Number of Zones:

Enter the total number of material zone to be used in the simulation domain.

Working Zone: Selected the zone to be defined.

Properties Definition: (if this is a new project)

Use this option to specify hydraulic and transport properties for each material zone. Each zone can be either homogeneous or heterogeneous. A homogeneous zone means that every element in the material zone will have the same hydraulic or transport properties. In a heterogeneous zone, these properties of each element in the zone will be generated by a random field generator.

Homogeneous material zone:

1. Saturated hydraulic properties: these includes

K_{sx} : saturated hydraulic conductivity in x direction (L/T)

K_{sy} : saturated hydraulic conductivity in y direction (L/T)

n: porosity (unitless)

S_s : specific storage (1/L)

2. Constitutive Model: Four different models for unsaturated hydraulic properties:

a. Van Genuchten unsaturated hydraulic property model

b. Exponential model (default)

c. Gardner-Russo model

d. User specified model

3. *Relative hydraulic conductivity parameters*

- α_x : inverse of air entry value in the x direction (1/L)
- β_x : slope parameter for the relative conductivity in the x direction
- α_y : inverse of air entry value in the y or z direction (1/L)
- β_y : slope parameter for the relative conductivity in the y or z direction

Different values for α and β in the x and y or z direction yield moisture-dependent anisotropy (Yeh, et al., WRR, 1985). If the exponential or Gardner-Russo model is chosen, the values of β_x and β_y are ignored.

4. *Moisture release curve:*

- α_m : inverse of the air entry value (1/L)
- β_m : slope parameter for the moisture release curve.
- Wcs: saturated water content, or porosity (unitless)
- Wcr: residual water content. (unitless)

If the exponential or Gardner-Russo model is chosen, the value of β_m is ignored.

5. *Solute transport and chemical reaction properties.*

- DLONG: Longitudinal dispersivity for material 1 (L)
- DTR: Transverse dispersivity for material 1 (L)
- DMOL: Apparent molecular diffusion (L²/T)

The following properties are assumed to be constant.

- AK1: Forward (Adsorption) rate coefficient (1/T)
- AK2: Backward (Desorption) rate coefficient (1/T)
- AK3: Equilibrium constant (1/T)
- VLAMDA: Decay constant (1/T)
- PULSE: =1 if initial concentration is a pulse input; =0 otherwise

Note that VSAFT solves the *variably saturated* flow and transport equations, and pre-specified unsaturated hydraulic properties are given as default. If your simulation only concerns saturated flow problems, only the default values for saturated hydraulic properties need to be modified to your specifications and you can leave the default values for unsaturated hydraulic properties unchanged.

Heterogeneous material zone:

If the zone is selected as heterogeneous, each hydraulic property will be generated using a random field generator. Inputs for the field generator for each property include:

- Mean:* The natural logarithm of the mean value of the parameter
- Variance:* The variance of the natural logarithm of the parameter value.
- Seed:* Seed number used to generate the field. If the same seed number is used for different properties, the generated properties are perfectly correlated, i.e., identical pattern. Otherwise, they are uncorrelated.
- Covariance function:* Allows the selection of different covariance function for the random field generation.
- X correlation scale:* The correlation scale in the x direction.
- Y correlation scale:* The correlation scale in the y or z direction.

Modify: The same function as above.

Next: continue to **initial condition** tab

Back: return to **time step** tab

6. INITIAL CONDITION TAB

Initial head type:

Specify the initial and boundary head as pressure head or total head (pressure head plus elevation head).

Specify initial values for head, solute concentration, water flux, and solute flux at each node as needed.

Select one of the following: head, water flux, solute concentration, or solute flux. Select the **starting node** and the **ending node**. Then specify the **value**. Afterwards, click **apply** button to implement this specification.

Next: continue to **source and boundary** tab

Back: return to **material** tab

7. SOURCE AND BOUNDARY TAB

Specify source or sink location and strength for flow and solute transport

Source definition:

The source or sink is defined at the center of an element.

Add:

Click the add option; move the cursor to the solution domain. Move the new cursor to the element where the sink or source should be and click the mouse to finish. Enter a value for the sink (a negative value) or source (a positive value) in the window that pops up and click OK to finalize it.

Delete:

Click the delete option and then move the cursor to the existing source or sink. Then, click the mouse to delete. Undo in Edit can undo the delete action.

Edit:

Click the edit option and then move the cursor to the existing source or sink. Then, click the mouse to edit the specified value.

Change flux or head values for the existing boundary condition.

Boundary definition:

Define boundary locations in the solution domain.

Add:

Click the add option; move the cursor to the solution domain (the cursor changes to a “+”). Move the new cursor to the node where the boundary should start. Next move the cursor to the node where the end of this boundary should be and click the mouse to finish. For the first boundary condition defined, a third point between the two endpoints is needed. Select the prescribed water flux or head and its value (for solute transport, the solute flux or prescribe concentration must be specified) and click OK to complete it. Right clicking the mouse removes the red dot for the first node of a boundary.

Delete:

Select the delete option and move the cursor to the existing boundary to delete.

Edit:

Click the edit option and move the cursor to an existing boundary to change flux or head values of the existing boundary condition.

Next: continue to **output control** tab

Back: return to **initial conditions** tab

8. OUTPUT CONTROL TAB

Create output file:

Option to create a file which contains the input and all the simulated results.

Point observations:

This option allows addition or deletion of observation points to/from the simulation domain, where the simulated hydrographs or concentration breakthroughs are to be saved in files (hydrograph.dat and btc.dat).

Option for output time

1. Every time step
2. Output at the multiple of the time interval specified.
3. User specified N number of output times.

9. FUNCTIONS ON THE TOOLBAR

Edit: undo or redo button allows undo or redo a previous task.

Geometry: use add line or delete line to change the column and row widths at certain locations of the solution domain. The Line properties option can be specified by using the following options:

- Percent:* Percentage of the width of the grid
- Space:* The interval between lines in any physical unit (cm, m, etc)
- Line:* The number of subdivisions within a line segment.
- Value:* Value for the above three options.

Construct:

Add element
Delete element
Boundary
Zone
Source
Observation point

Run: VSAFT or Notepad

Calibration: Tools for model calibration

Load observed data: Input observation location data.

View: View calibration results in a scatter plot.

View:

Zoom:

zoom in or out to view the basic grid system, simulation domain, or material zone.

Geometry properties:

This option shows element, node, and material zone number at cursor location after clicking the left button of the mouse.

Hydrograph

Contour Toolbar:

FILES GENERATED IN THE PROJECT DIRECTORY

The program automatically creates a plot.dat output file which is the head at each node, at each time step listed in the output control tab. In addition, the following files are created when the graphic user interface is invoked. They are:

1. ***Geometry.mmoc:*** a binary file used by GUI and

2. Files for the VSAFT program, which includes:

Files.txt: A file contains the path and filenames to be read by the VSAFT. For example,

K:\Project2003\run00-6-1\grid.dat
K:\Project2003\run00-6-1\problem.dat
K:\Project2003\run00-6-1\simulation.dat
K:\Project2003\run00-6-1\sources.dat
K:\Project2003\run00-6-1\time.dat
K:\Project2003\run00-6-1\material.dat
K:\Project2003\run00-6-1\out.dat
K:\Project2003\run00-6-1\node.dat
K:\Project2003\run00-6-1\element.dat
K:\Project2003\run00-6-1\boundary.dat
K:\Project2003\run00-6-1\output.dat
K:\Project2003\run00-6-1\plot.dat

Boundary.dat The file contains the following information:

SymL is the variable name in the Fortran program.

SymL	FORMAT	COLUMN	DESCRIPTION
NBDY			Number of boundary nodes
N	I10	1-10	Node number of the first node on the boundary. Any corner can be taken as the starting point and direction of movement should be counter-clockwise.
KODE(N)	I5	11-15	=0 for prescribed flux (and all internal nodes) =1 for prescribed pressure head =-1 for nodes on unit gradient boundary
KODC(N)	I5	16-20	=0 if solute flux is specified at this node =1 if solute concentration is specified
INC	I10	21-30	If next few nodes have a constant increment in their numbers and same value of KODE, KODEC and AN, give the value of increment. (e.g., if nodes 1,4,7,10...22 lie on the boundary and have the same value of KODE, KODEC and AN, give INC=3. INC can be negative also.)
NEXT	I10	31-40	If increment is non-zero, this is the node number of the last node in the series of nodes subjected to increment INC (e.g., 22 for the above example). Make sure that (NEXT-N) is an integer multiple of INC.
AN(N)	E10.3	41-50	Angle made by the outward normal to the boundary at node N from direction 1. If N is a corner node, there may be 2 normals at that point. Use the normal along the predominant flow direction.

Element.dat

SYMBOL	FORMAT	COLUMN	DESCRIPTION
NUMEL	I10	1-10	Number of element
NODMAT(NUMEL,1)	I10	11-20	Node number of first node (counter-clockwise starting from any node) of this element. If rectangular element, first node is at bottom left.
NODMAT(NUMEL,2)	I10	21-30	Node number of second node
NODMAT(NUMEL,3)	I10	31-40	Node number of third node
NODMAT(NUMEL,4)	I10	41-50	Node number of fourth node (For triangular, blank or equal to third node)

NODMAT(NUMEL,5) I10 51-60 Material number for this element
 SANG(NUMEL) E10.3 61-70 Angles in degrees between x-coordinate
 and first principal conductivity for
 this element

Grid.dat This file stores the number of element and number of nodes of the
 solution domain.

Material.dat

SymbL	FORMAT	COLUMN	DESCRIPTION
SATK(1,1)	Free	--	First principal conductivity for the material 1 (L/T)
SATK(2,1)	Free	---	Second pr. cond. for material 1 (L/T)
POR(1)	Free	---	Effective porosity for material 1
SS(1)	Free	---	Specific storage for material 1 (1/L)
DLONG(1)	Free	---	Longitudinal dispersivity for material 1 (L)
DTR(1)	Free	---	Transverse dispersivity for material 1 (L)
DMOL(1)	Free	---	Apparent molecular diffusion (L*L/T)
BULKD(1)	Free	---	Bulk density for material 1 (M/L**3)

Repeat CARD 1 for material 2,3...NMAT.

ALPHAK(1,1)	Free	---	Alpha(x) for material 1 in the K-eqn. (1/L)
BETAK(1,1)	Free	---	Beta(x) for material 1
ALPHAK(2,1)	Free	---	Alpha(y) for material 1 (1/L)
BETAK(2,1)	Free	---	Beta(y) for material 1
IDM(1)	Free	---	Identification of constitutive model to be used for degree of saturation and conductivity for material 1. =1 for van Genuchten model =2 for exponential model =3 for Gardner-Russo =4 for a user specified model, which has to be defined in the subprograms

If solute transport is to be simulated, the file should include the following:

DLONG(1)	Free	---	Longitudinal dispersivity for material 1 (L)
DTR(1)	Free	---	Transverse dispersivity for material 1 (L)
DMOL(1)	Free	---	Apparent molecular diffusion (L*L/T)

Node.dat

SymL	FORMAT	COLUMN	DESCRIPTION
N	I10	1-10	Node number
X(N)	E10.3	11-20	X (horizontal) co-ordinate of node (L)
Y(N)	E10.3	21-30	Y (vertical, if vertical flow) co-ordinate (L)
P1(N)	E10.3	31-40	Initial value of pressure head or total head at the node (L) (see IHEAD on group A (card 2))
Q(N)	E10.3	41-50	Flux into (+ive) or out of (-ive) the system at node N (L/T)
CP(N)	E10.3	51-60	Initial solute concentration at node (M/L**3)
SFLX(N)	E10.3	61-70	Solute flux into (+) or out of the system (M/L*L/T)

Problem.dat It stores the following information:

Title
 Problem type
 Flow type
 Initial head type

River.dat

Out.dat This file stores 1) create output option 2) point observation option for hydrographs and breakthrough curve points.

TIMKOD	Free	---	Code for detailed printout of results at different times. =0 if output desired at every time step =+t if output desired at times t,2t,3t...TMAX =-N if output desired at N time levels to be supplied on the next card(s)
MAXRED	Free	---	Maximum number of reductions allowed at one time step for DT when maximum number of iterations is exceeded. (See ITERMX on Group A, Card 2)

(Only if TIMKOD < 0 on the previous card)

NOUT	Free	---	Code for output file =0 output file is not created =1 output file is created (Program will prompt for the name of output file)
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Simulation.dat: This file stores inputs from the **simulation control** tab

SymL	FORMAT	COLUMN	DESCRIPTION
ITSCHM	Free	---	Indicates the iteration scheme to be used =1 for Picard iteration scheme =2 for Newton-Raphson iteration scheme
LUMP	Free	---	Indicates which scheme is used for storage terms =2 for Diagonal lumping, as in Finite Diff. =1 for Lumped Scheme =0 for Consistent Scheme
NVAR	Free	---	Indicates the variation of conductivity and moisture capacity within an element for the integration of element matrices =0 for constant (equal to average of nodes) =1 for linear variation
ITERMX	Free	---	Maximum number of non-linear iterations at each time step. If exceeded, DT is reduced to .5*DT for transient flow simulation and for steady state simulation results are dumped on tape 1.
XIF	Free	---	Time weighting factor for the flow equation (0.5 fully implicit)
XIC	Free	---	Time weighting factor for transport equation (0.5 fully implicit)
TOL	Free	---	Tolerance for pressure head Convergence (L)
EPSC	Free	---	Convergence limit for transport equation solver (1.0e-10)
EPSF	Free	---	Convergence limit for Flow equation solver (1.0e-10)
EPSV	Free	---	Convergence limit for velocity equation solver (1.0e-10)

Sources.dat

NSOURC	Free	---	Number of Source/Sinks (Each covers one element)
NBTC	Free	---	Total Number of Nodes where breakthrough data needs to be printed (concentrations at these nodes would be stored in file btc.dat at all time steps). NBTC=0 if KPROB =1 or 2.

Timestep.dat: This file stores inputs from the **TIMESTEP TAB**

DT	Free	---	Initial value of time step (T)
DTMAX	Free	---	Maximum allowable value of DT (T)
DTMUL	Free	---	If convergence is achieved in 5 or less non-linear iterations, DT is multiplied by DTMUL.
TMAX	Free	---	Maximum time of simulation (T). The final time for printout corresponds exactly to TMAX.

SYMBOL	FORMAT	COLUMN	DESCRIPTION

OUTTIM(1)	Free	---	First output time level (T)
OUTTIM(2)	Free	---	Second output time level (T)
.	.	.	.
.	.	.	.
(till OUTTIM(N), use as many cards as required)			

Output.dat: This file contains output from the simulation.

Plot.dat: This file is written as an input file for Tecplot. It prints out x, (y or z), pressure head, moisture content, velocity in the x direction, velocity in the y(or z) direction and concentration (if this simulation involves solute transport) for each requested output time step.

Hydrography.dat: If point observations for flow simulation are chosen, this file will contain the pressure head-time data for each observation location.

Btc.dat: If point observations for solute transport simulation are chosen for the simulation, this file will storage the concentration-time (breakthrough) data for each observation location.

SYMBOL	FORMAT	COLUMN	DESCRIPTION

NC(1)	Free	---	Node number of the first node where breakthrough data is to be printed
NC(2)	Free	---	Second Node for breakthrough data
.
.
till NC(NBTC). Use as many cards as required.			

Rstart.dat: This file contains information for restart the simulation.