ROBIN

Win32 computer program for 3D contaminant transport modeling using the deterministic Streamline Method based on 2D Dupuit-Forchheimer groundwater flow

Version 0.1

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2   Version

Robin version 0.1

3   Manual

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5   Introduction

Robin is a 3D reactive transport simulator using the deterministic Streamline Method (1). In the Streamline Method the 3D transport domain is discretized into a set of streamlines. These 1D streamlines are described using the travel time, or time-of-flight τ, of a particle traveling along the streamline. The reactive transport is then computed by solving the Advective-Dispersive-Reactive Equation in τ-space.

The streamlines are defined by tracking particles through the transport domain. The groundwater flow solution supporting the particle tracking is obtained using the Analytic Element Method

(AEM) (2; 3; 4). The advantage of AEM compared to finite element or finite difference based methods is that the groundwater velocities can be computed everywhere in the domain without the need for interpolation. The AEM implementation used here is the Dupuit-Forchheimer steady-state groundwater simulator SPLIT (5). A mass balance on water is used to approximate the vertical velocity generated by recharge (6) and by flow under streams.

6   Where to Obtain and How to Use Robin

To obtain the current version of ROBIN, visit www.groundwater.buffalo.edu and go to the Software page. ROBIN does not contain a Graphical User Interface (GUI). ROBIN is a mathematical engine only that takes two ASCII input files (one prepared manually and the other prepared by the groundwater simulator SPLIT (5)) and prepares a number of output files which are formatted for use in MS EXCEL and SURFER. The input and output files used by ROBIN are described later in this document. The current version of ROBIN is in the beta-testing phase, and is thus not fully tested. Any software problems or suggestions should be directed to the author (see contact information above).

7   Implementation and Limitations

In ROBIN rectangular source zones (either vertical or horizontal) are used to introduce contaminants into the domain. Unlike other Streamline Method implementations where the whole domain is covered by streamlines, streamlines are only started at source zones. Each source zone is subdivided into a set of rectangles of equal area, and a streamline is started in the center of each of the rectangles. The streamline and the four corners of the rectangle (the extent of the streamtube) are then tracked through the domain using particle tracking. The flow velocities needed for particle tracking are computed within ROBIN using the element coefficients supplied by SPLIT. The streamlines are tracked until they are captured by a flow sink or until they leave the transport domain. The particle locations and the velocities are recorded at user-specified intervals ($\Delta\tau$), leading to a discretized streamline. The transformed Advective-Dispersive-Reactive Equation (ADRE) is then solved using a 1D Petrov-Galerkin Finite Element Method along the streamline and a Crank-Nicholson Finite Difference Method to advance the solution in time. Reactions are handled using either a sequential or alternate Operator-Splitting approach. All reactions are formulated as kinetic reactions and are solved using LSODE (7). The process of tracking the streamline and then solving the ADRE is repeated for all the streamlines of all the source zones. The fluxes generated by each streamline are added at the end of the simulation.

One of the main limitations of this implementation of the Streamline Method, is that transverse dispersion is neglected, because there is no communication between the streamlines. Two additional limitation stem from the use of the AEM groundwater simulator SPLIT: the hydraulic conductivity is constant in depth, and conductivity has to be piecewise constant in the horizontal (no gradual changes). A further limitation is that streamlines should not intersect other source zones, as streamlines will not adhere to the boundary conditions of other source zones.

8   Parallel Processing

The independence of the streamlines makes the algorithm used by ROBIN very suitable for parallel processing. The streamlines are divided among the processors and no communication is necessary

until the simulation has finished and the contaminant fluxes are computed. The Message Passing Interface (MPI) (8) is used for communication between the processors.

The currently distributed version of ROBIN is compiled to run on a single processor. Versions for parallel processing are available on request.

9 Input ASCII Files: *robin.dat* and *flow.dat*

ROBIN requires two ASCII-formatted files to be present in the working directory to run. The first input file has the name *robin.dat* and contains all the information pertaining to the reactive transport (e.g. sources, model discretization, output control, ...). The second input file, *flow.dat*, contains the flow information (i.e. the element geometries and coefficients). While *robin.dat* is constructed manually by the user, *flow.dat* is written by the 2D steady-state groundwater flow simulator SPLIT (5).

9.1 Description of *robin.dat*

The commands used in *robin.dat* are typeset in bold, are case insensitive, and do not have to appear in any particular order. The commands can be divided into four categories: output control, domain specifications, sources, and reactions.

9.1.1 Output control

OutTimes: specifies output interval. If omitted output is written for each time step.

WriteReceptors: specifies that contaminant fluxes across receptor planes and into flow sinks are written.

WriteConc: specifies that concentrations along each streamline are written.

WriteTopNodes: specifies that a top-view of the nodes should be written (*nodes_top.bna*).

WriteXNodes: specifies that cross-sections along the x-axis the nodes should be written (*nodes_xcrs.bna*).

WriteYNodes: specifies that cross-sections along the y-axis the nodes should be written (*nodes_ycrs.bna*).

9.1.2 Domain specifications

Domain x_{min} y_{min} x_{max} y_{max}**:** horizontal extent of the transport model. The vertical extent is given by the flow model.

MaxTau τ_{max}*:* grid resolution in τ-space.

DeltaT Δt*:* time step for transport computation.

NTimes N_t*:* number of time steps of transport computation ($\Delta t * N_t$ = total transport duration).

Dispersivity α_l*:* longitudinal dispersivity of the domain.

AddSpecies *ID Name:* adds a species with *ID* number and *Name* to the transport domain.

Initial *ID Concentration***:** initial concentration in the domain for species *ID*. The default initial concentration is zero.

Receptor *Name*: creates a rectangular plane receptor identified by *Name*. Receptor is a multi-line command with four lines.

$x_1\ y_1$: (x,y) location of the starting point of the receptor plane.

$x_2\ y_2$: (x,y) location of the starting point of the receptor plane.

$z_{bottom}\ z_{top}$: top and bottom depth of receptor plane.

9.1.3 Sources

Source *Shape Orientation* $N_{streamlines}$: Creates a source zone. Currently the only supported *Shape* is *rectangular*. The *Orientation* is either *vertical* or *horizontal*. $N_{streamlines}$ gives the number of streamlines that will be started in the source zone. The *Source* command is a multi-lined command. Depending on the *Orientation* the next three (*vertical*) or five lines (*horizontal*) give the geometry of the source zone. For *horizontal* the next five lines are:

$x_1\ y_1$: x and y coordinate of the first corner.

$x_2\ y_2$: x and y coordinate of the second corner.

$x_3\ y_3$: x and y coordinate of the third corner.

$x_4\ y_4$: x and y coordinate of the fourth corner.

z: depth of the source zone.

For *vertical* the next three lines are:

$x_1\ y_1$: x and y coordinate of the first corner.

$x_2\ y_2$: x and y coordinate of the second corner.

$z_{bottom}\ z_{top}$: bottom and top depth of the source zone.

The lines identifying the geometry are followed by one or more lines specifying the contaminants released in the source zone, with one line per species:

ID Concentration Type: *ID* is the species ID of the contaminant. *Concentration* is the influent concentration. *Type* is the boundary condition type (1 = constant concentration, currently the only type)

After the line of the last contaminant of the source zone a line containing the symbol "&" ends the input for a particular source zone.

9.1.4 Reactions

SeqDecay $N_{species}$: sequential decay involving $N_{species}$. The *SeqDecay* command has four lines.

$ID_1\ ID_2 \ldots\ ID_N$: The second line gives the species IDs for the species involved, starting with at the top of the reaction chain.

$k_1\ k_2\ \ldots\ k_N$: The third line lists the decay rates.

$Y_{2-1}\ Y_{3-2}\ \ldots\ Y_{(N-1)-N}$: The fourth line contains the stoichiometric yield coefficients.

Nitro: nitrogen transport involving 13 species (12 mobile and 1 immobile). See Appendix 1 for reactions. The *Nitro* command has eight lines.

$ID_1\ ID_2 \ldots\ ID_13$: The second line gives the species IDs for the species involved, in the following order: H^+, OH^-, CO_2, HCO_3^-, CO_3^{2-}, CH_2O, O_2, NO_3^-, N_2, Ca^{2+}, Mg^{2+}, Cl^-, and $CaCO_3(s)$.

$K_{H_2O}^f\ K_{H_2O}^b$: forward and backward rate constants for reaction $H_2O \leftrightarrow H^+ + OH^-$

$K_{CO_3^{2-}}^f\ K_{CO_3^{2-}}^b$: forward and backward rate constants for reaction $CO_3^{2-} + H^+ \leftrightarrow HCO_3^-$

$K_{HCO_3^-}^f\ K_{HCO_3^-}^b$: forward and backward rate constants for reaction
$$HCO_3^- + H^+ \leftrightarrow CO_2 + H_2O$$

$K_{CaCO_3}^f\ K_{CaCO_3}^b$: forward and backward rate constants for precipitation/dissolution reaction
$$CaCO_3(s) \leftrightarrow CO_3^{2-} + Ca^{2+}$$

$k_{max,O_2}\ K_{O_2,S}\ K_{O_2,E}$ maximum rate, and substrate and electron acceptor half saturation constants for aerobic degradation.

$k_{max,NO_3^-}\ K_{NO_3^-,S}\ K_{NO_3^-,E}$ maximum rate, and substrate and electron acceptor half saturation constants for denitrification.

AlternateSplitting: specifies that the alternate Operator-Splitting approach is to be used. The default approach is sequential Operator-Splitting.

9.2   Description of *flow.dat*

The input file *flow.dat* is generated using SPLIT with the line "TRANSSOL" in the input file *split.dat*. A detailed description can be found in the appendix.

10   Maximum Model Size

ROBIN is distributed with the following size restrictions. ROBIN versions with different parameters (e.g. larger sizes) are available on request.

Number of streamlines	2,000
Number of nodes	2,000
Number of time steps	1,000
Number of species	15
Number of rows per source	50
Number of columns per source	50
Number of vertical sources	10
Number of horizontal sources	10
Number of plane receptors	50

11   Output File Format

11.1   debug.out

The file *debug.out* is created for each run of ROBIN. It contains any errors encountered by ROBIN.

1 The run completed successfully without errors or warnings

-1 Error while reading *robin.dat*

-2 Error while reading *flow.dat*

-3 Error while creating streamline

-4 Error while computing advection / dispersion

-5 Error while computing reactions

11.2 concentration_XXXX_YY.csv

ROBIN generates one concentration profile for each streamline and each species ("XXXX" stands for the streamline ID and "YY" for the species ID). The columns give the spatial profile (horizontal distance along the streamline), while the rows give the temporal profile. If a streamline has more than 254 nodes only a fraction (every 2nd node, every 3rd node, ...) is written so that the files into MS Excel.

11.3 receptors_YY.csv

Contaminant fluxes across user specified receptor planes and into flow sink (i.e. linesinks and wells) are reported in the files *receptors_YY.csv*. One file is created for each species ("YY" species ID). The first column shows the time, the next set of columns shows the fluxes across the receptor planes followed by the fluxes into linesinks and fluxes into wells. The locations of the linesinks and wells receiving contaminants are reported at the bottom of the file.

11.4 Node visualization

ROBIN creates up to two Atlas files (*nodes_top.bna*, *nodes_xcrs.bna*, and *nodes_ycrs.bna*) to help visualize the 3D particle paths. *nodes_top.bna* contains the top view of the node location (x,y), while *nodes_xcrs.bna* and *nodes_ycrs.bna* contain a cross-section of the aquifer along the the x- or y-axis, respectively.

12 Acknowledgement

13 Example

A simple 3D transport problem is given here. The domain includes three head-specified streams and areal recharge in an unconfined aquifer. A conservative tracer is introduced in a horizontal source zone at the aquifer top. Some of the streamlines are captured by one of the streams, while the others pass under the stream.

Flow input file (*split.dat* to be run in SPLIT):

```
solveonly
CompareHeadOff
Transsol
Formatted
Precision 4
MaximumSolveIterations 500
MinimumSolveIterations 5
PotentialTolerance .000001
BaseAndThickness 0 30
Conductivity 1.0
Porosity 0.3
ReferencePoint 2450 50 24.5
AreaSink Recharge Zone example #1
 -150 -175
 250 -175
 250 225
 -150 225
& 0 0 -.0008 &
Head River example #1
 0 175 25.
 0 -125 25.
& Head River example #2
 100 175 24.6
 100 -125 24.6
& Head River example #3
 200 175 24
 200 -125 24
&
```

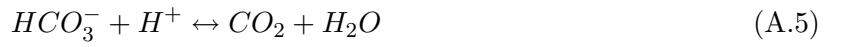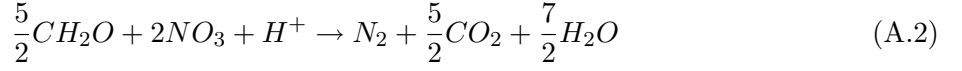Transport input file (*robin.dat*):

```
domain 0. 0. 190. 50.
maxtau 50
Ntimesteps 100
deltat 36.5
addspecies 1 Tracer
dispersivity 1.0
source rectangular horizontal 9
  50. 40.
  70. 40.
  70. 10.
  50. 10.
   25.
 1 1.0 1
&
WriteFlux
WriteXNodes
```

A   Nitrogen transport reactions

A.1   Reactions

$$CH_2O + O_2 \rightarrow CO_2 + H_2O \tag{A.1}$$

$$\frac{5}{2}CH_2O + 2NO_3 + H^+ \rightarrow N_2 + \frac{5}{2}CO_2 + \frac{7}{2}H_2O \tag{A.2}$$

$$H_2O \leftrightarrow H^+ + OH^- \tag{A.3}$$

$$CO_3^{2-} + H^+ \leftrightarrow HCO_3^- \tag{A.4}$$

$$HCO_3^- + H^+ \leftrightarrow CO_2 + H_2O \tag{A.5}$$

$$CaCO_3(s) \leftrightarrow CO_3^{2-} + Ca^{2+} \tag{A.6}$$

A.2   Rates

$$R_{degr} = \phi_{O_2} k_{max,O_2} \left[\frac{(CH_2O)}{K_{O_2,S} + (CH_2O)} \right] \left[\frac{(O_2)}{K_{O_2,E} + (O_2)} \right] \tag{A.7}$$

$$R_{denit} = \phi_{NO_3^-} k_{max,NO_3^-} \left[\frac{(CH_2O)}{K_{NO_3^-,S} + (CH_2O)} \right] \left[\frac{(NO_3^-)}{K_{NO_3^-,E} + (NO_3^-)} \right] \tag{A.8}$$

$$R_{H_20}^f = K_{H_20}^f \tag{A.9}$$

$$R_{H_20}^b = K_{H_20}^b \left(H^+ \right) \left(OH^- \right) \tag{A.10}$$

$$R_{CO_3^{2-}}^f = K_{CO_3^{2-}}^f \left(CO_3^{2-} \right) \left(H^+ \right) \tag{A.11}$$

$$R_{CO_3^{2-}}^b = K_{CO_3^{2-}}^b \left(HCO_3^- \right) \tag{A.12}$$

$$R_{HCO_3^-}^f = K_{HCO_3^-}^f \left(HCO_3^- \right) \left(H^+ \right) \tag{A.13}$$

$$R_{HCO_3^-}^b = K_{HCO_3^-}^b \left(CO_2 \right) \tag{A.14}$$

$$R_{CaCO_3}^f = \phi_{CaCO_3} K_{CaCO_3}^f \tag{A.15}$$

$$R_{CaCO_3}^b = \phi_{CaCO_3} K_{CaCO_3}^b \left(CO_3^{2-} \right) \left(Ca^{2+} \right) \tag{A.16}$$

B   FLOW.DAT

Following is the description of the file format. For descriptions of the parameters please refer to the SPLIT manual.

Line 1: global constant, reference head

Line 2: x-coordinate of reference point, y-coordinate of reference point

Line 3: uniform flow in x-direction, uniform flow in y-direction

Line 4: number of strings, circles and ellipses in the model

Line 5: number of area sinks and wells in the model

Line 6: empty

Line 7: "aquifer data"

Line 8: aquifer base and aquifer thickness

Line 9: hydraulic conductivity and porosity

Line 10: empty

Line 11: "Strings"

This is followed by a list of all the strings. This block is repeated for each string.

Line S.1: string ID, number of line segments in string, string type

Line S.2: conductivity information for inhomogeneity boundaries, thin inhomogeneities and leaky walls. This line is skipped for all other string types.

Line S.3: counter variable, line segment ID, line segment order, and number of farfield coefficients

Line S.7: x,y location of start point and x,y location of end point of line segment

Line S.8: head or flux data for head or flux specified line elements, for other line elements this line is skipped.

Line S.9 to Line S.9+line order: line element coefficients

Line S.9+line order+1 to Line S.9+line order+1+number of farfield coefficients: farfield coefficients

This is followed by a list of all the circles. This block is repeated for each circle.

Line C.1: circle ID, circle order, and circle type

Line C.2: x-and y-coordinate and radius of circle

Line C.3: hydraulic conductivity for circular inhomogeneities or specified head for circular lakes

Line C.4 to C.4+circle order: circle coefficients

This is followed by a list of all the ellipses. This block is repeated for each ellipse.

Line E.1: ellipse ID, ellipse order, and ellipse type

Line E.2: x-and y-coordinate of center of ellipse

Line E.3 short and long axis and angle of ellipse

Line E.4: hydraulic conductivity for elliptical inhomogeneities, or specified head for elliptical lakes, or specified flux for elliptical reservoirs

Line E.5 to E.5+ellipse order: ellipse coefficients

This is followed by a list of all the area sinks. This block is repeated for each area sink.

A.1: area sink ID, number of control points, and strings associated with area sink

A.2: center of area sink

A.3 to A.3+number of control points: area sink coefficients

This is followed by a list of all the wells. This block is repeated for each well.

W.1: x- and y-coordinate of well

W.2: pumping rate and well radius

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