

SOFTWARE REVIEW

Review of RT3D

by Mantha S. Phanikumar, Ph.D. – Michigan State University

RT3D (Reactive Transport in 3-Dimensions) is a public domain numerical code to simulate three-dimensional, multi-species reactive transport in saturated porous media. The finite-difference code written in Fortran-90 is based on the MT3D package (reviewed in *Southwest Hydrology*, March/April 2005) and shares several of its features. The flow solution comes from MODFLOW. A notable feature of RT3D is the use of an implicit reaction solver that gives it the flexibility to simulate complex user-defined reactions.

Released in 1997, RT3D is well-tested and can be used to simulate laboratory and field-scale experiments as well as to design remediation systems. RT3D has been successfully used to simulate natural attenuation, engineered in-situ bioremediation, chemical oxidation, and other reactive transport scenarios. Coupled chemical or biological reactions can be modeled using multiple mobile/immobile species following a kinetic framework.

A number of built-in reaction modules are included with the package, for example to simulate BTEX degradation using sequential electron acceptors, first-order decay of PCE and its daughter products, and aerobic/anaerobic chlorinated ethane degradation. These preprogrammed modules can be used either as is, or to set up more complex reaction scenarios. Sorption can be simulated using linear, Freundlich, or Langmuir isotherms. The code allows sorption parameters to be specified on a cell-by-cell basis and supports source/sink options (e.g., decaying sources) that are unique to RT3D.

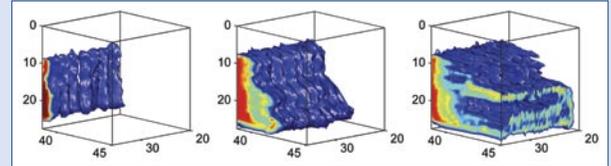
Input files can be edited using a text editor, and the file structure is similar to that of MT3D. The current version supports several new reaction solvers, including Runge-Kutta solvers and those that require an explicit Jacobian matrix

for stiff systems. For complex reactions, the analytical Jacobian matrix can be computed using a symbolic mathematics package such as MAPLE.

RT3D does not have a graphical user interface of its own but several choices are available to the user, including Groundwater Modeling System (GMS), GroundWater Vistas (GWV), and Visual MODFLOW. RT3D is developed and maintained by the Battelle Pacific Northwest National Laboratory.

Executables, source code, documentation, tutorials for GMS users, and a list of RT3D-related publications and GUIs are available at the RT3D Web page at bioprocess.pnl.gov/rt3d.htm.

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Ease of Use:

GUI: N/A

Application:

Output/Plotting: N/A

Documentation:

Speed:

OVERALL RATING:

Best Features

- User-defined reaction module
- Reaction solver options

Worst Feature

- Error reporting

Rating System



Excellent



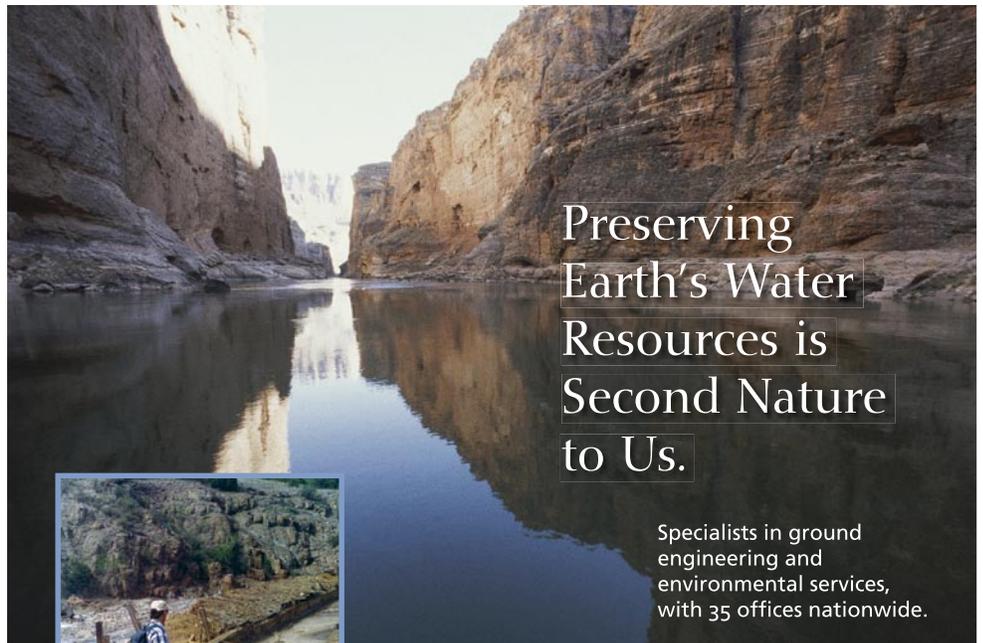
Poor



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