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Software Spotlight/ Chunmiao Zheng, Software Editor

# Recent Developments and Future Directions for MT3DMS and Related Transport Codes

reviewed by Chunmiao Zheng

## Introduction

MT3DMS is a three-dimensional (3D) multispecies contaminant transport model with a modular structure to permit simulation of solute transport processes independently or jointly (Zheng and Wang 1999; Zheng 2009). MT3DMS interfaces directly with the U.S. Geological Survey's finite-difference ground water flow model, MODFLOW, for the flow solution, and supports all the hydrologic and discretization features of MODFLOW (McDonald and Harbaugh 1988; Harbaugh et al. 2000; Harbaugh 2005). MT3DMS is unique in that it contains several transport solution techniques in a single code, including the fully implicit finite-difference method (FDM), the particle-tracking based method of characteristics (MOC) and its variants, and a third-order total-variation-diminishing (TVD) scheme that conserves mass while limiting numerical dispersion and artificial oscillation.

Since its first release in 1990 as MT3D for single-species mass transport (Zheng 1990), MT3DMS has been widely used in research projects and practical field applications. In recent years, continuing development efforts have significantly expanded the simulation capabilities of MT3DMS through new extensions and related codes. This column provides a brief overview of the recent developments and future directions in the MT3DMS family of transport-modeling tools.

## Recent Developments

### Coupled Geochemical and Transport Modeling

By itself, MT3DMS is primarily intended to simulate physical transport processes, that is, advection, dispersion, molecular diffusion, and various fluid sinks/sources. Although it contains basic functionalities for modeling sorption and simple kinetic reactions, an add-on reaction module must be incorporated into MT3DMS for multispecies reactive transport modeling. A number of reactive modules have been developed for this purpose, including MT3D'99 (Zheng 1999), RT3D (Clement 1997, 2003), and SEAM3D (Waddill and Widdowson 1998; Widdowson 2002), among others. MT3D'99 is a special version of MT3DMS implemented with biodegradation kinetics and parent-daughter chair reactions. RT3D couples MT3DMS with several preprogrammed reaction modules for common biologically mediated reactions. In addition, the user has the option to program any arbitrary kinetic reactions. SEAM3D is similar to RT3D in concept but is more specifically focused on sequential electron acceptor-based biological reactions.

The most comprehensive tool in this category is the PHT3D code (Prommer et al. 2003), which couples MT3DMS with the geochemical modeling program PHREEQC-2 (Parkhurst and Appelo 1999) for simulation of complex multicomponent reactive transport processes. Most of the geochemical modeling capabilities of PHREEQC-2 are retained in PHT3D, including equilibrium-controlled aqueous complexation/speciation, kinetic reactions of aqueous components such as biodegradation of organic compounds, mineral precipitation/dissolution, ion exchange, and surface complexation reactions. Recent applications of PHT3D to complex field-scale reactive transport systems include water-quality changes during managed aquifer recharge (Prommer and Stuyfzand 2005; Greskowiak et al. 2006), fate of oxidisable organic contaminants in ground water (Barry et al. 2002), isotopic fractionation processes (Van Breukelen and Prommer 2008), and impact of mass transfer processes on uranium fate (Ma et al. unpublished data). Figure 1 shows the results of a modeling study that investigated microbial dynamics and geochemical changes in a metal bioprecipitation experiment (Prommer et al. 2007).

### Variable-Density Flow and Transport Modeling

The use of MT3DMS with MODFLOW is based on the "decoupled" approach that allows flow and transport

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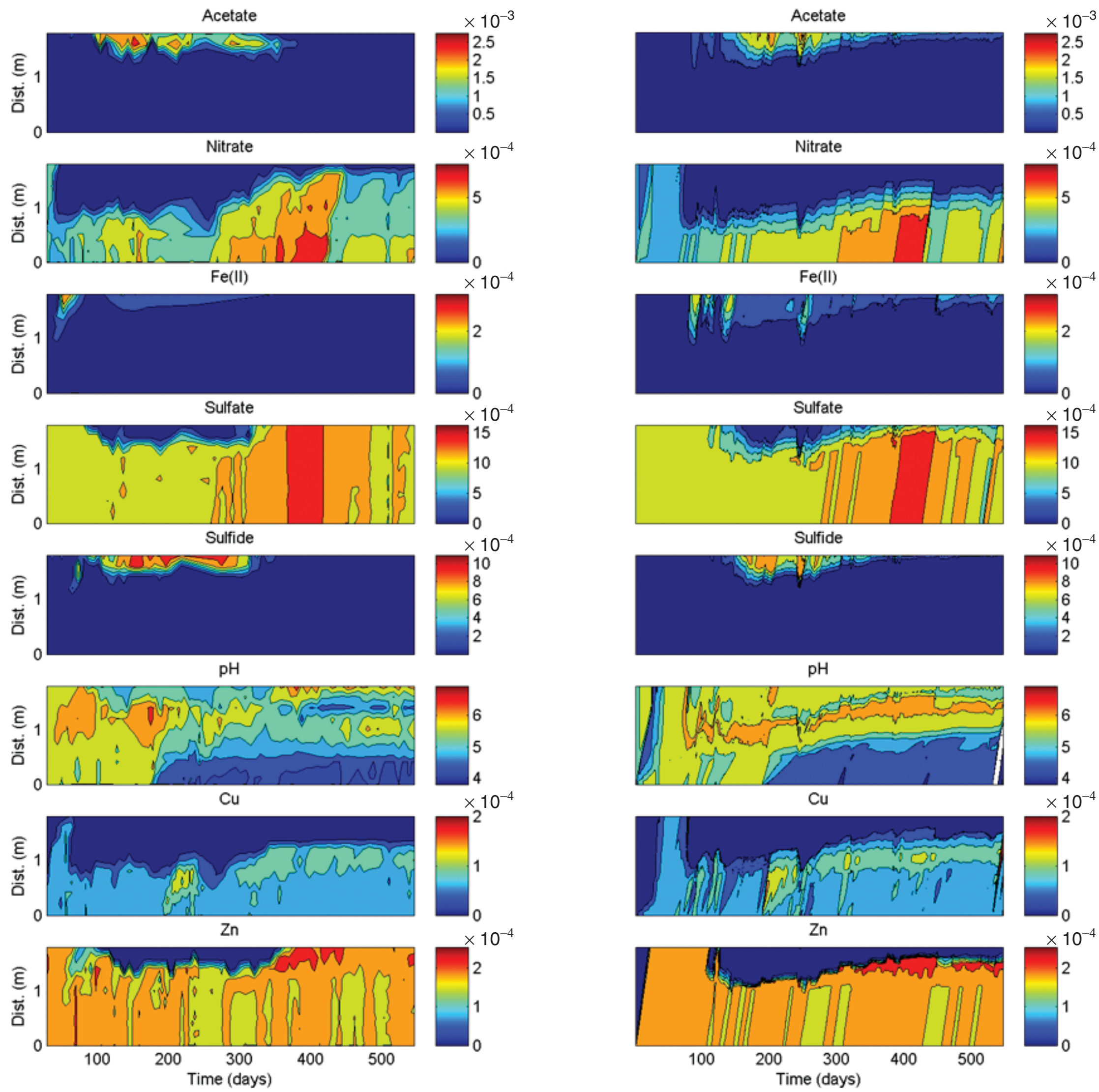


**Figure 1. Illustration of reactive transport modeling of in situ bioprecipitation of Zn and Cu using PHT3D. Reprinted with permission from Prommer et al. (2007). Copyright 2007 American Chemical Society.**

simulations to be completed independently of each other for greater computational efficiency. The intrinsic assumption is that solute concentrations are sufficiently small so that their effect on fluid density is negligible. While this assumption is valid in many contaminant transport-modeling applications, it is not in situations where there is substantial variation in fluid density, such as sea water intrusion or brine transport.

An area that has seen rapid development in recent years is variable-density flow and transport modeling through the SEAWAT series of codes (Guo and Bennett 1998; Guo and Langevin 2002; Langevin et al. 2007). SEAWAT combines MODFLOW and MT3DMS into a single code for flow and transport modeling under variable-density and variable-viscosity conditions. In the coupled approach, the flow solution is initially obtained and then passed to the transport solver for the concentration solution. The concentration solution is next used by the flow solver to update the fluid density and obtain the new flow solution. This iterative process continues until the end of the simulation period is reached. SEAWAT has found many real-world applications in sea water intrusion and other density-dependent flow and transport problems (e.g., Langevin 2001; Langevin and Guo 2006; Bauer-Gottwein et al. 2007; Post and Prommer 2007; Lin et al. 2009).

## Direct Ground Water Age Simulation

Goode (1996) derived the governing equation for modeling ground water ages (or mean resident times), which in the simplest form can be written as:

$$\frac{\partial A}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial A}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(v_i A) + 1 \qquad (1)$$

where $A$ represents the age of an ideal tracer through the ground water flow system, $D_{ij}$ is the hydrodynamic dispersion tensor, and $v_i$ is the seepage velocity. Equation 1 is mathematically equivalent to the solute transport equation solved by MT3DMS,

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) - \frac{\partial}{\partial x_i}(v_i C) - \gamma \qquad (2)$$

where $C$ is the solute concentration, and $\gamma$ is the zeroth-order decay term. The zeroth-order decay term has been added to MT3DMS since version 5.2 released in 2006.

Because of the mathematical equivalency between Equations 1 and 2, MT3DMS can be used to simulate the ground water age distribution directly by setting the zeroth-order decay constant to $-1$, that is, a unit production, and by setting appropriate initial and boundary conditions. In so doing, the values of concentration calculated by MT3DMS represent the mean ground water ages or resident times. The ages computed through Equations 1 or 2 account for advection as well as hydrodynamic mixing of waters of different ages, and thus are more representative of the actual ages in the aquifer than those computed by particle tracking, which considers advective transport only. The age simulation capability of MT3DMS has been applied to some field problems (e.g., Zheng 2007; Konikow et al. 2008). It is expected that more applications will follow in the future as ground water age data become more widely available.

### Modeling Heat as a Ground Water Tracer

Heat is increasingly being recognized as an excellent ground water tracer because of its usefulness in identifying multiple hydrologic processes and recent availability of improved temperature sensors and measurement technologies (Anderson 2005). The mathematical equivalency between the heat and solute transport equations has been established in numerous studies (e.g., Healy and Ronan 1996; Kim et al. 2005; Prommer and Stuyfzand 2005; Greskowiak et al. 2006; Thorne et al. 2006; Bayer et al. 2008). As a result, MT3DMS can be used directly and efficiently to simulate heat transport with simple variable conversion. Figure 2 shows a heat plume from injection of cool water into warmer ground water as part of a pre-modeling exercise to guide the subsequent actual field heat tracer test.

The use of MT3DMS for heat transport modeling is based on the assumption that the changes in fluid density and viscosity induced by temperature variation are negligible so that flow and transport simulations can be decoupled for greater computational efficiency. However, when temperature causes significant changes in fluid density and viscosity, the SEAWAT code is more suitable because it can account for the effects of variable fluid density and viscosity during heat transport. Ma and Zheng (unpublished data) conducted a series of numerical experiments to quantify the conditions under which the effects of variable density and viscosity can be neglected without any significant loss of computational accuracy.

## Future Directions

### Transport in Unsaturated Zones

MT3DMS has already been linked with the hydrocarbon spill screening model (HSSM) (Weaver 1996) as part of its extension to the unsaturated zone. HSSM is a computer code that simulates the vertical migration of a light nonaqueous phase liquid (LNAPL) contaminant through the unsaturated zone and the formation of an oil lens on the water table. It also determines the rate of contaminant mass flux dissolved from the LNAPL source into ground water. Through a new time-varying source package (Zheng et al. 2009), the effect of one or more such LNAPL sources can be incorporated into three-dimensional (3D) advective-dispersive-reactive transport simulation using MT3DMS.

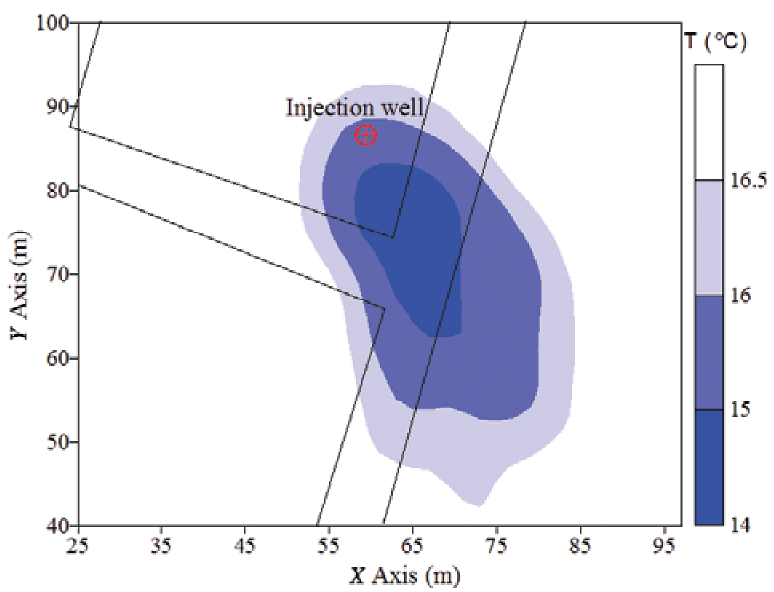


**Figure 2. Simulation of a heat plume following injection of cool water into warmer ground water using MT3DMS at the Hanford 300A site in Washington State.**

New work is going on to link MT3DMS and related codes directly with an unsaturated flow package for MODFLOW such as the unsaturated-zone flow (UZF) package (Niswonger et al. 2006) or the variably saturated flow (VSF) process (Thoms et al. 2006). The UZF Package simulates vertical one-dimensional (1D) unsaturated flow using the computationally efficient kinematic wave approximation, while the VSF process solves a fully 3D Richards' equation for unsaturated flow above the water table. The soil moisture contents and fluxes solved by UZF or VSF will be saved for use by MT3DMS to simulate the solute transport and reactions through the unsaturated zone.

#### Integrated Surface and Ground Water Modeling

Another area expected to have significant development activities is a closer integration with surface water modeling tools. This will build transport-modeling support in MT3DMS and related codes for newly developed or enhanced surface water packages such as stream routing and lakes. In addition, new flow processes for MODFLOW such as the farm process (Schmid et al. 2006) and conduit flow process (Shoemaker et al. 2007) can be supported to address water-quality issues during agriculture irrigation and ground water–conduit interaction. An example of the linkage between MT3DMS and a predecessor to the conduit flow process was described by Spiessl et al. (2007).

The long-term vision is to make MT3DMS a solute transport solver in fully integrated surface water–ground water modeling systems such as GSFLOW (Markstrom et al. 2008). This can only be accomplished through close collaboration and coordination between MT3DMS authors and other model developers, including those in the U.S. Geological Survey.

#### Solving Nonideal Transport Processes

MT3DMS is originally based on the classical advection-dispersion formulation for modeling solute transport through porous media. Since 1999, it has supported the dual-domain mass transfer formulation to accommodate preferential transport along high-conductivity pathways and mass exchange between the preferential transport pathways and less permeable matrix (Zheng and Wang 1999; Feehley et al. 2000). In recent years, more conceptual and mathematical model formulations have been developed for simulating solute transport in highly heterogeneous aquifers, including dual-domain multirate mass transfer (e.g., Haggerty and Gorelick 1995), fractional-order advection-dispersion (e.g., Benson et al. 2000), and continuous-time random walk (e.g., Berkowitz et al. 2002). One or more of these formulations will be implemented in MT3DMS to provide a wider selection of conceptual models to describe nonideal transport processes under complex field conditions.

## Summary

MT3DMS and its predecessor MT3D were developed as the transport companion to the U.S. Geological Survey's ground water flow model, MODFLOW. Since the 1990s, MT3D and MT3DMS have been widely used in research projects and practical field applications. In addition to solute transport, the MT3DMS code has also been applied to simulate ground water age distribution and heat transport. Continuing development efforts in recent years have significantly expanded the simulation capabilities of MT3DMS through new extensions and related modeling tools, especially in the areas of reactive transport, variable-density flow and transport, ground water age, and heat transport.

Future developments of MT3DMS and related codes will focus on extension to the unsaturated zone, a closer integration with surface water modeling components, and implementation of new conceptual and mathematical model formulations. Other related activities to make transport modeling more efficient and accurate will continue, including parameter estimation (e.g., Mehl and Hill 2001; Doherty 2004; Poeter et al. 2005), management optimization (e.g., Zheng and Wang 2002), local grid refinement (e.g., Mehl and Hill 2005), and parallelization to take full advantage of modern computer architecture.

## Our Mission

The goal of *Software Spotlight* is to help readers identify well-written, intuitive, and useful software. Independent reviewers from government, industry, and academia try out full working versions of software packages and provide readers with a concise summary of their experiences and opinions regarding the capability, stability, and ease of use of these packages.

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