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USGS Directions in MODFLOW Development

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Introduction

The development and application of ground-water models has been an important component of USGS hydrologic investigations since the early 1970s. During the past 35 years, the USGS has developed a wide range of computer models to simulate saturated and unsaturated subsurface flow, solute transport, and chemical reactions. The most widely used of these programs is the MODFLOW model, which simulates three-dimensional (3D) ground water flow (GWF) using the finite-difference method (Harbaugh 2005). Although originally conceived solely as a ground water flow model, MODFLOW's modular structure has provided a robust framework for integration of additional simulation capabilities that build on and enhance its original scope. The family of MODFLOW-related models now includes capabilities to simulate coupled ground water/surface water systems, solute transport, unsaturated zone flow, parameter estimation, and ground water management (GWM) (optimization modeling). This column is intended to summarize some of the current directions for MODFLOW development within the USGS. This is an opportune time to provide such a summary because of the several MODFLOW-related programs that have been published during the past 2 years.

The USGS develops models as part of its overall mission, which is to provide unbiased hydrologic data and scientific analyses to support informed management of the nation's water resources. Typically, new capabilities for MODFLOW are developed to solve specific problems that arise during the course of our water resource assessment programs, such as a need to improve the simulation of ground water/surface water interactions in areas of thick unsaturated zones or simulation of salt water intrusion in coastal areas. MODFLOW's development within the USGS is distributed across several organizational units, with much of the overall coordination, prioritization, and support for the code's development done through the Office of Ground Water. This distributed format for code development is in large measure an outgrowth of one of the original intents of MODFLOW, which was to provide a programming structure that could be easily enhanced as new capabilities were needed. In our opinion, the USGS provides a unique environment in which to develop and test computer models because of the agency's national scope, the feedback that is possible between our research and applied programs, and the continuity of our data-collection and resource-assessment programs over time. USGS scientists also are fortunate to be able to work with colleagues outside of the Survey, and such collaboration has been particularly important in the development of new capabilities for MODFLOW during the past few years.

Recent Developments

The newest version of MODFLOW is MODFLOW-2005 (Harbaugh 2005). As of this writing, MODFLOW-2005 includes only the GWF and Observation Processes, but its scope is anticipated to expand with time. The primary change in MODFLOW-2005 from MODFLOW-2000 (Harbaugh et al. 2000) is the use of Fortran modules to declare data that can be shared among program subroutines. Although these modules will not affect the typical MODFLOW user, they provide a means to define multiple model grids in a single MODFLOW simulation, which is the basis for the new local grid refinement (LGR) capability developed by Mehl and Hill (2005). LGR allows the user to simulate flow in a higher-resolution local grid (referred to as a child model) within a larger, coarser-grid parent model. Locally refined grids often are needed for conditions where hydraulic gradients change substantially over short distances, for detailed representation of aquifer heterogeneity, or for site-scale simulation of contaminant transport. LGR uses a two-way iterative solution method that couples the parent and child models such that heads and flows are balanced across the shared interfacing boundary (Mehl and Hill 2005). Although formal parameter estimation and model sensitivity are not supported directly in the current version of MODFLOW-2005, automatic model calibration for MODFLOW-2005 (and other models) is provided by an updated version of UCODE (UCODE_2005; Poeter et al. 2005). Additional programs for sensitivity analysis, model calibration, uncertainty evaluation, and optimization are available with the JUPITER Application Programming Interface (Banta et al. 2006).

Several new MODFLOW packages and processes have been developed during the past 2 years that enhance the scope of MODFLOW. Because of space limitations, we focus on only a few of these recent developments—those related to unsaturated-zone flow, GWM, and variable-density flow and solute transport.

The simulation domain of MODFLOW has been expanded substantially by the recent development of two new packages and a new process to simulate flow in the unsaturated zone. These new capabilities provide improved methods for representing surface-subsurface hydrologic connections in MODFLOW such as soil zone infiltration, ground water recharge, and surface water/ground water interactions. The two packages—the Streamflow-Routing (SFR2) and Unsaturated-Zone (UZF1) packages—simulate one-dimensional (1D) vertical flow and storage in the unsaturated zone using a kinematic-wave approximation to Richards' 3D flow equation. Both packages are based on the assumption that unsaturated flow occurs in response to gravity potential gradients only and ignore negative potential gradients. The SFR2 Package (Niswonger and Prudic 2005) simulates unsaturated flow beneath streams that have become hydraulically disconnected from underlying aquifers, whereas the UZF1 Package (Niswonger et al. 2006b) simulates flow, storage, and evapotranspiration in the unsaturated zone in response to infiltration at land surface (Figure 1). In contrast to the SFR2 and UZF1 packages, the Variably Saturated Flow (VSF) Process (Thoms et al. 2006) uses a finite-difference approximation to solve the full 3D form of Richards' equation, and includes packages to simulate seepage faces, surface ponding, bare-soil evaporation, and root-zone evapotranspiration. The VSF Process offers a more rigorous, but also more computationally demanding, approach for simulating unsaturated zone flow than is provided by the UZF approach (Niswonger et al. 2006b; Thoms et al. 2006).

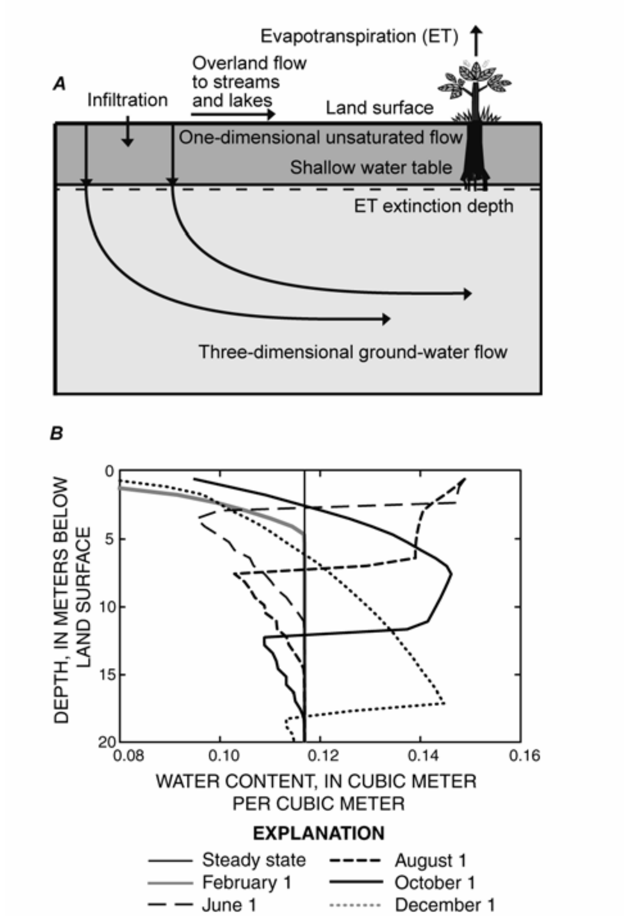

Figure 1. (A) 1D unsaturated zone flow simulated with the new UZF1 package for MODFLOW-2005 and (B) representative water-content profiles calculated by UZF1 for a model cell in a test simulation with time-varying infiltration rates at land surface. Figures modified from Niswonger et al. (2006b).

Two new MODFLOW processes that can be applied to GWM problems have been developed in collaboration with university colleagues. The first of these is the GWM process for simulation-optimization modeling (Ahlfeld et al. 2005). GWM can be applied to several types of linear, nonlinear, and mixed-binary linear GWM (optimization) problems, such as limiting ground water level declines or streamflow depletions and conjunctively using ground water and surface water resources. The basis of GWM's solution process is the new Response-Matrix Solution package, which calculates response coefficients between management problem decision variables and physical system state variables, and solves the management problem using either the simplex or branch and bound algorithms. The second contribution is the Farm Process (FMP1) (Schmid et al. 2006), which allows MODFLOW users to simulate a wide range of the water supply and water demand components of irrigated agriculture. FMP1 uses a multi-step algorithm of crop water demand, surface water availability, and water rights hierarchies to determine the net amount of ground water pumping that is necessary to satisfy total farm water delivery requirements. FMP1 also calculates the amount of excess water that is not effectively used for crop growth, which becomes either overland runoff or ground water recharge.

Constant-density solute transport can be simulated with the Ground Water Transport (GWT) Process of MODFLOW (formerly referred to as MOC3D; Konikow et al. 1996). In some hydrogeologic settings, however, an assumption of constant ground water density may not be valid. In such cases, the SEAWAT-2000 program (Langevin et al. 2003; Langevin and Guo 2006), which combines MODFLOW-2000 with MT3DMS (Zheng and Wang 1999), can be used to simulate variable-density GWF and solute transport. SEAWAT-2000 uses a modified version of the GWF Process of MODFLOW-2000 (referred to as the Variable-Density Flow Process) to solve a variable-density form of the GWF equation using equivalent fresh water heads as the dependent variable. SEAWAT-2000 has been applied to a wide range of variable-density ground water problems, including salt water intrusion in coastal aquifers, saline ground water movement in inland areas, quantification of submarine ground water discharge to marine estuaries, aquifer storage and recovery, and the transport and fate of wastewater injected into deep saline aquifers.

Future Directions

Although it is difficult to look too far into the future to predict the development of specific simulation capabilities for MODFLOW, we present here some of the ongoing USGS model development efforts that should be available soon and speculate on some future needs. To a large extent, these efforts build upon some of the recent developments described previously.

Most hydrologic simulation models that are currently available focus on either ground water or surface water resources; yet, many of today's most important issues related to water supply, water quality, and the health of aquatic ecosystems cannot be adequately addressed without properly accounting for all of the processes that affect water flow through the surface-subsurface hydrologic continuum. In an effort to improve the simulation of coupled surface-subsurface systems, the USGS has been developing and testing a fully integrated ground water and precipitation-runoff (watershed) model that can be applied to water resource problems at the scale of a watershed—that is, on the order of 100 km^2 or larger (Niswonger et al. 2006a). The basic components of the integrated model are MODFLOW-2005 and the USGS precipitation-runoff (watershed) modeling system (PRMS) (Leavesley et al. 1983). PRMS is a modular, distributed-parameter modeling system that partitions daily precipitation in the form of rain or snow (or a mixture of both) among several watershed hydrologic compartments (interception by vegetation, surface evaporation, overland flow, infiltration to the soil zone, and so forth). Hydrologic connections between the surface and subsurface zones are through the soil zone and surface water bodies (streams and lakes), and the recent development of the SFR2 and UZF1 packages for coupling saturated flow conditions simulated by MODFLOW's GWF Process with unsaturated zone flow beneath streambeds and the soil zone, respectively, has been an important part of the integration of the two models.

Initially, the integrated ground water/surface water model is anticipated to be used to better understand flow and storage processes within watersheds, such as the timing and magnitude of ground water recharge, the role of ground water discharge to overland runoff and streamflow generation, and the effects of land-use changes and climate variability on ground water and surface water resources. With time, however, advancements to the integrated model will be needed to account for the transport and reactions of chemicals that are released at land surface, move into the subsurface, and discharge into streams (Sanford et al. 2006). Further developments also will be needed to address biogeochemical and ecological aspects of the interaction between surface water and ground water, particularly at the scale of individual stream reaches.

In addition to the integrated ground water/surface water model, we also see the need to continue model development and application in the areas of variable-density flow and solute transport, optimization modeling to support water resource management, and model prediction uncertainty. We anticipate that variable-density flow simulation will increase in importance in the years ahead as coastal areas of the nation continue to experience population growth, creating the potential for increased pumping that may result in salt water intrusion. Moreover, the emerging issue of using saline ground water as a source for desalination systems may require increased use of variable-density flow and solute-transport models to simulate the response of saline ground water (and hydraulically connected freshwaters) to ground water pumping.

Although tools for ground water optimization modeling have been available for nearly 20 years, the technique has yet to be routinely applied in ground water studies. This is unfortunate because simulation-optimization modeling provides a powerful tool for the analysis and management of hydrogeologically complex ground water systems and, in particular, the evaluation of tradeoffs between various hydrologic constraints and sustainable uses of ground water resources. In a similar manner, routine evaluations are needed to assess the effects of model design uncertainty on model prediction uncertainty, using techniques such as Monte Carlo analyses. By model design, we mean not only the uncertainty associated with model hydraulic properties and physical system stresses such as recharge that often are quantified using statistical inverse methods but also the other components of simulation models, such as forecasted water supply demands, estimates of future climate conditions, and the uncertainty associated with hydrologic constraints specified in management models.

Summary

The scope of MODFLOW has grown substantially since its first release in 1984. Its initial conceptualization as a ground water flow model capable of simulating a wide range of ground water features (wells, drains, rivers, and so forth) through the use of independent, modular programming packages has been expanded to the broader concept of simulation processes, wherein parts of the code solve a major equation or set of equations. Several processes are now available for MODFLOW, including solute transport, variable-density flow, parameter estimation, and ground water management, with the GWF Process remaining the core process on which other capabilities are built. Now, MODFLOW's scope is being extended further with the development of coupled models that integrate soil, vegetation, and atmospheric hydrologic processes with saturated and unsaturated subsurface flow. As noted by McDonald and Harbaugh (2003) in their discussion of the history of MODFLOW, as the scope of MODFLOW's capabilities expand, the challenge will be to ensure that the original design criteria for the program—that it be easy to understand, use, enhance, and modify—are maintained. This challenge will become more critical as the code is integrated with models from allied scientific fields.

Online Resources

The USGS maintains many of its computer models on the World Wide Web. Users can access these codes at URL http://water.usgs.gov/software/. A list of USGS reports related to MODFLOW is maintained online at http://water.usgs.gov/ogw/MODFLOW_list_of_reports.html and a bibliographic summary of additional USGS models is available at http://water.usgs.gov/ogw/pubs/circupdate.html.

References

Ahlfeld, D.P., P. M. Barlow, and A. E. Mulligan. 2005. GWM—A Ground-Water Management Process for the U.S. Geological Survey modular ground-water model (MODFLOW-2000). USGS Open-File Report 2005-1072. Reston, Virginia: U.S. Geological Survey.

Banta, E.R., E.P. Poeter, J.E. Doherty, and M.C. Hill, eds. *in press*. JUPITER: Joint Universal Parameter IdenTification and Evaluation of Reliability—An Application Programming Interface (API) for model analysis. USGS Techniques and Methods 6-E1. Reston, Virginia: U.S. Geological Survey.

Harbaugh, A.W. 2005. MODFLOW-2005, The U.S. Geological Survey modular ground-water model—the Ground-Water Flow Process. USGS Techniques and Methods 6-A16. Reston, Virginia: U.S. Geological Survey.

Harbaugh, A.W., E.R. Banta, M.C. Hill, and M.G. McDonald. 2000. MODFLOW-2000, the U.S. Geological Survey modular ground-water model—User guide to modularization concepts and the Ground-Water Flow Process. USGS Open-File Report 00-92. Reston, Virginia: U.S. Geological Survey.

Konikow, L.F., D.J. Goode, and G.Z. Hornberger. 1996. A three-dimensional method-of-characteristics solute-transport model (MOC3D). USGS Water-Resources Investigations Report 96-4267. Reston, Virginia: U.S. Geological Survey.

Langevin, C.D., and W. Guo. 2006. MODFLOW/MT3DMS-based simulation of variable-density ground water flow and transport. *Ground Water* 44, no. 3: 339-351.

Langevin, C.D., W.B. Shoemaker, and W. Guo. 2003. MODFLOW-2000, the U.S. Geological Survey modular ground-water model—Documentation of the SEAWAT-2000 version with the Variable-Density Flow Process (VDF) and the integrated MT3DMS Transport Process (IMT). USGS Open-File Report 03-426. Reston, Virginia: U.S. Geological Survey.

Leavesley, G.H., R.W. Lichty, B.M. Troutman, and L.G. Saindon. 1983. Precipitation-runoff modeling system—User's manual. USGS Water-Resources Investigations Report 83-4238. Reston, Virginia: U.S. Geological Survey.

McDonald, M.G., and A.W. Harbaugh. 2003. The history of MODFLOW. *Ground Water* 41, no. 2: 280-283.

Mehl, S.W., and M.C. Hill. 2005. MODFLOW-2005, The U.S. Geological Survey modular ground-water model—Documentation of shared node local grid refinement (LGR) and the boundary flow and head (BFH) package. USGS Techniques and Methods 6-A12. Reston, Virginia: U.S. Geological Survey.

Niswonger, R.G., S.L. Markstrom, R.S. Regan, D.E. Prudic, G. Pohll, and R.J. Viger. 2006a. Modeling ground-water/surface-water interaction with GSFLOW—A new USGS model. In *MODFLOW and More 2006 Conference Proceedings*, 99-103. Golden, Colorado: International Ground Water Modeling Center.

Niswonger, R.G., and D.E. Prudic. 2005. Documentation of the Streamflow-Routing (SFR2) Package to include unsaturated flow beneath streams—A modification to SFR1. USGS Techniques and Methods 6-A13. Reston, Virginia: U.S. Geological Survey.

Niswonger, R.G., D.E. Prudic, and R.S. Regan. 2006b. Documentation of the Unsaturated-Zone Flow (UZF1) Package for modeling unsaturated flow between the land surface and the water table with MODFLOW-2005. USGS Techniques and Methods 6-A19. Reston, Virginia: U.S. Geological Survey.

Poeter, E.P., M.C. Hill, E.R. Banta, S. Mehl, and S. Christensen. 2005. UCODE_2005 and Six Other Computer Codes for Universal Sensitivity Analysis, Calibration, and Uncertainty Evaluation. USGS Techniques and Methods 6-A11. Reston, Virginia: U.S. Geological Survey.

Sanford, W.E., J.S. Caine, D.A. Wilcox, H.C. McWreath, and J.R. Nicholas. 2006. Research opportunities in interdisciplinary ground-water science in the U.S. Geological Survey. USGS Circular 1293. Reston, Virginia: U.S. Geological Survey.

Schmid, W., R.T. Hanson, T. Maddock, III, and S.A. Leake. 2006. User guide for the farm process (FMP1) for the U.S. Geological Survey's modular three-dimensional finite-difference ground-water flow model, MODFLOW-2000. USGS Techniques and Methods 6-A17. Reston, Virginia: U.S. Geological Survey.

Thoms, R.B., R.L. Johnson, and R.W. Healy. 2006. User's guide to the Variability Saturated Flow (VSF) Process for MODFLOW. USGS Techniques and Methods 6-A18. Reston, Virginia: U.S. Geological Survey.

Zheng, C., and P.P. Wang. 1999. *MT3DMS—A modular three-dimensional multispecies transport model for simulation of advection, dispersion, and chemical reactions of contaminants in ground-water systems; Documentation and User's Guide*. Jacksonville, Florida: U.S. Army Corps of Engineers.