igwmc

International Groundwater Modeling Center

Newsletter

Volume XX ISSUE 1 **Spring 2002**

MODFLOW 2001 and Other Modeling Odysseys

Golden, CO, USA, September 11-14, 2001

On the opening evening of MODFLOW 2001 and Other Modeling Odysseys conference, September 11 2001, we were all shocked by the events of the day. About half of the conference attendees had arrived and half were stranded in airports. Some never made it to the conference due to the paralyzed travel industry, while others made monumental journeys and arrived late. The atmosphere of the conference was warm and friendly as we rearranged the schedule daily to accommodate the erratic arrival of speakers. Many conference participants mentioned that they felt close to everyone who attended and had valuable technical conversations with people they might not have approached otherwise.

The conference was successful with 60% of those registered attending and 42% of the presentations given. Evaluations indicated it was an excellent conference. Thank you, organizing and technical committees for you hard work and thank you, presenters for the high quality of the papers, posters, and presentations. Exhibits, workshops, seminars, and software demonstrations were also top-notch.

It was particularly stimulating to have many analytical element modelers at the conference. The organizing committee wishes to emphasize that, although MODFLOW serves as a centerpiece of the recurring conference, we anchor on MODFLOW only because of its widespread use and its status as a modeling standard. We encourage participation of those using all types of models so that the modeling capability of our profession will evolve. MODFLOW serves as a standard to which all of the other models can be compared. The advantages and disadvantages of alternative codes can be reflected from MODFLOW with which nearly all modelers are familiar.

Our sincere thanks to all of the registrants who could not attend but donated their reimbursement to IGWMC to help us meet the already expended costs of the conference. These supportive sponsors include: Peter Andersen, Scott Anderson, Hale Barter, Dave Bennett, Daniel Burnell, Wen-Hsing Chiang, Serguey Chmakov, John Coleman, Gregory Council, Patrick Delaney, James Feild, Daniel Feinstein, Jon Fenske, Carl Gable, Mike Goodrich, Jonathan Green, Miln Harvey, Randy Hunt, Michael Kennard, Robert Knowlton, Eric LaBolle, Alan Lemon, Paul Martin, Alge Merry, Joseph Morrice, Steve Robertson, Dave Romero, Frans Schaars, Robert Schmidt, Jesse Schwalbaum, Jon Sykes, Peter Thibodeau, Patrick Wang, Song-Kai Yan, and Steve Young.

We have nearly completed the review of a series of papers from the conference for a special issue of Ground Water Journal. Watch for its publication in the coming year.

CALL for PAPERS: MODFLOW and MORE 2003: Understanding through Modeling

September 17-19, 2003, Ice-Breaker Evening of September 16

The MODFLOW conference series has become a tradition for the presentation of cutting-edge practical application of ground water models in all aspects of hydrologic work. MODFLOW, the USGS modular three-dimensional finite-difference, ground-water flow model, has become an international standard for ground-water modeling. MODFLOW serves as a centerpiece for the recurring conference, but we anchor on MODFLOW only because of its widespread use and its status as a community model. The conference organizing committee needs and encourages participation by users of all types of models in all kinds of applications, including those for which MODFLOW is not suitable, so that the modeling capability of our profession will evolve. MODFLOW is a basis from which other models can be considered. The advantages and disadvantages of alternative codes can be reflected from MODFLOW with which nearly all modelers are familiar.

The productive conferences "MODFLOW '98" and "MODFLOW 2001 and Other Modeling Odysseys" were held by the International Ground Water Modeling Center (IGWMC). Many registrants were disappointed by the travel problems in September of 2001, so the next conference is scheduled after only two, instead of three, years. The conference will include keynote speakers on a wide range of topics, contributed oral presentations and poster sessions (both oral and poster papers will be published in a proceedings volume), exhibitors, short courses, and software demonstrations.

Those interested in presenting a paper or poster should submit a 200-word abstract via http://www.mines.edu/research/igwmc/events/modflow2003/abstract_form.shtml by April 20, 2003. Abstracts must include sufficient detail to permit a thorough review by the Technical Committee. If the abstract is accepted for an oral or poster presentation, the author will be notified by May 20, 2003; he/she is then required to submit a short paper for publication in the proceedings by July 20, 2003. IGWMC will sponsor travel and registration for the student submitting the abstract judged to be the best. Format information for papers will be sent with the abstract acceptance notice. Topics include:

* MODFLOW-2000, latest developments and related issues
* links for simulating processes not included in MODFLOW
* MODFLOW limitations and directions for future development
* typical problems encountered in modeling and their solutions
* data collection/monitoring for model calibration
* model calibration and parameter estimation
* uncertainty reduction and quantification
* parameterization approaches in ground-water modeling
* weighting of observations for model calibration
* estimating recharge
* constraining ground-water models using hydrogeologic information
* new geologic approaches to benefit groundwater modeling
* groundwater modeling for interpreting geology
* stochastic approaches and applications
* new analytic approaches and applications
* surface-water/ground-water interaction modeling
* fracture flow modeling
* contaminant transport modeling
* reactive transport modeling
* coupling flow and reactive transport modeling
* bioremediation modeling
* unsaturated zone and multiphase modeling
* variable density modeling
* ground-water management and remediation design optimization
* ground-water modeling for mining applications
* ground-water modeling for agricultural applications
* code testing/performance and case studies

continued on page 4

Modeling Flow in Fractured Media with TOUGH2

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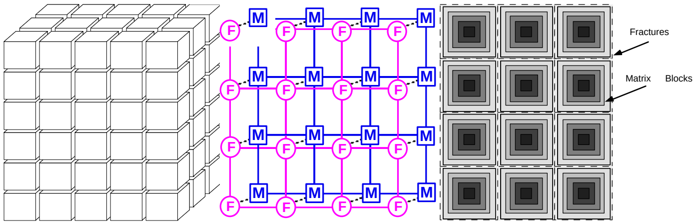
"Fractured media" come in a wide variety of geometric and hydrologic characteristics. Processes of interest to modelers range from single-phase isothermal flow of ground water to flow and transport of multiphase, multicomponent fluid mixtures under non-isothermal conditions, as in thermal methods for remediating NAPL contamination. In many applications advective and/or diffusive exchanges (of fluids, solutes etc.) between fractures and rock matrix are of interest.

The TOUGH2 (Pruess et al, 1999) code uses an integral finite difference technique for space discretization, which can accommodate a variety of modeling approaches for fractured media through built-in preprocessing of geometric data. Conceptually, the simplest approach involves an explicit representation of fractures, which are described as more-or-less planar regions of large permeability and porosity, with "small" spatial extent perpendicular to the fracture plane. Such explicit representation of fractures is feasible only for flow systems with a small number of fractures. For flow systems with ubiquitous interconnected fractures, their explicit representation is neither practically possible nor desirable, and continuum representations are used instead. TOUGH2 includes 3 alternative approaches: double-porosity (DPM), dual permeability (DKM), and multiple interacting continua (MINC); see Fig. 1.



(a) (b) (c)

Figure 1. Illustration of concepts used for modeling of multiphase flow in fractured rocks: (a) double-porosity model (DPM; after Warren and Root, 1963); (b) dual permeability model (DKM), with global flow in both fractures (F) and matrix continua (M); (c) MINC sub-gridding for resolution of gradients in the matrix blocks (after Pruess and Narasimhan, 1982, 1985). References available upon request to K_Pruess@lbl.gov.

The DPM considers that global flow in the system occurs only through the network of interconnected fractures, while fractures and matrix rock of generally low permeability may exchange fluid, solutes, and heat locally. The fracture system is characterized and modeled with customary porous medium parameters. At each point (or grid node) of the system, two sets of thermodynamic parameters are defined to characterize the state of the flow system: one set involves an average over the fractures, the other an average over the matrix rock. "Interporosity flow" between the fracture and matrix continua is assumed to be proportional to the difference in the average values of the intensive quantities driving flow and transport, such as differences in pressures, solute concentrations, or temperatures, between fractures and matrix.

For flow systems in which both the fracture and matrix continua contribute to global flow, the DPM is generalized to allow global fracture-fracture as well as matrix-matrix flow, in addition to fracture-matrix exchange DKM (Fig. 1b). This type of approach is applicable for multiphase (or unsaturated) flow in fractured-porous media, where global flow of the gas phase may occur through the fracture network, while global flow of the aqueous (wetting) phase may involve matrix-to-matrix flow.

The DPM entails a quasi-steady approximation for interporosity flow. In some cases the characteristic times for interporosity flow may be large, and the quasi-steady approximation becomes inaccurate. This may occur for diffusion of solutes or heat into or out of matrix blocks, as well as for capillary-driven imbibition when matrix permeabilities are small and/or fracture spacings large. Under these circumstances it may be necessary to resolve the gradients driving fracture-matrix exchange, which can be accomplished by sub-gridding of matrix blocks into a series of continua defined according to distance from the matrix block surface, the so-called MINC-concept (Fig. 1c).

Pruess, K., C. Oldenburg and G. Moridis. TOUGH2 User's Guide, Version 2.0, Lawrence Berkeley National Laboratory Report LBNL-43134, Berkeley, CA, November 1999.

Some Thoughts on Modeling Flow in Fracture Rocks

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"Continuum or discrete-fracture model?" This is probably the most-commonly asked question about modeling flow in fractured rocks. Historically, the two modeling approaches have been portrayed as diametrically opposed to each other--the continuum approach represents the fracture network as an equivalent porous medium, whereas the discrete-fracture approach considers flow through each individual fracture.

To focus on this difference, however, is to miss that fact that both modeling approaches share the same underlying physical principles. For example, both approaches require that fluid mass must be conserved, and that flow rate be proportional to head gradient (Darcy's Law). If one examines that part of a computer program that solves for hydraulic head in a continuum model versus a discrete-fracture model, one would find many common elements. In principle, a discrete-fracture model may be set up to appear like a continuum model by using 3 set of mutually perpendicular and regularly spaced fracture sets that extend throughout the model domain, thus mimicking a finite-difference grid. Conversely, a continuum model may be set up to appear like a discrete-fracture model by using a fine grid with a highly variable distribution of hydraulic conductivity (K) such that grid cells with high K are connected in a fashion to mimick fracture network. Viewed from this vantage point, continuum and discrete-network models might appear to have more similarities than differences.

The key difficulty in modeling flow in fractured rocks is dealing with a medium that is highly heterogeneous. This problem is often treated with a two-pronged strategy. First is to explicitly characterize those large-scale features (e.g., major faults and fracture zones) that strongly control the overall flow pattern. These features are then explicitly represented in a continuum model by high K cells, or in a discrete-fracture model by highly transmissive fractures. Second is to find some means of representing the regions away from the large-scale features. It is here that that one sees a divergence between the continuum and the discrete-fracture approach. In the continuum approach, the emphasis is on K. A common approach is to divide the rock into several homogeneous zones and to determine the effective K for each zone by model calibration. A more sophisticated approach is to employ stochastic theory to generate spatially varying K fields based on stochastic parameters inferred from numerous hydraulic tests in the field. In contrast, the discrete-fracture approach places a large emphasis on fracture mapping. Statistics of fracture parameters such as orientation, lengths, and spacing are used to generate a fracture network through which fluid flows.

If a fracture network is viewed as an alternative way to characterize K, then the difference between the continuum and the discrete-fracture approach boils down to different ways of generating the spatial distribution of K. There is a lack of consensus on which is the better approach. The continuum approach might be criticized for simulating a flow field that tends to be more diffuse than the actual fractured rock. The discrete-fracture approach might be criticized for an over-emphasis on fracture geometry whereas field observations indicate that only a small percentage of fractures participate in fluid transmission. As with groundwater modeling in general, improvements in model results arise less from the selection of the model code, then from better characterization of the field.

Fracture Network Modeling

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Discrete Fracture Network (DFN) modeling endeavors to realistically incorporate the geology and geometry of fracture networks into a groundwater simulation. DFN modeling is appropriate to problems where fractures dominate the flow system. By neglecting the matrix (or reducing it to a dual-porosity system) the numerical model consists of a framework of two-dimensional plates that link in three-dimensional space to form the fracture network. Each plate is, effectively, its own aquifer having a transmissivity, storativity, and transport aperture, all of which may be defined homogeneously or distributed heterogeneously within a single fracture. A finite-element mesh of a fracture network model displays features embedded in a rock matrix (Figure 1).

Figure 1.

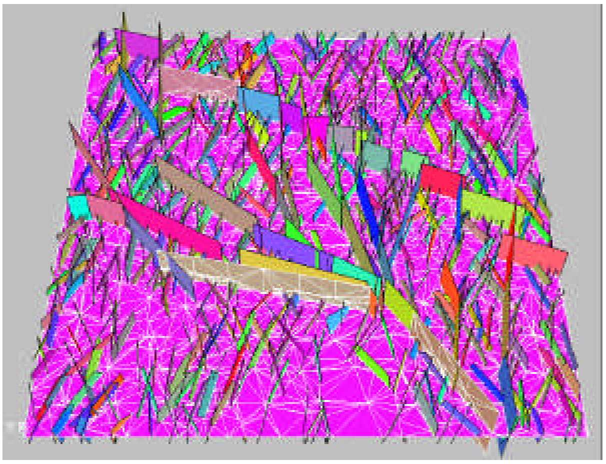
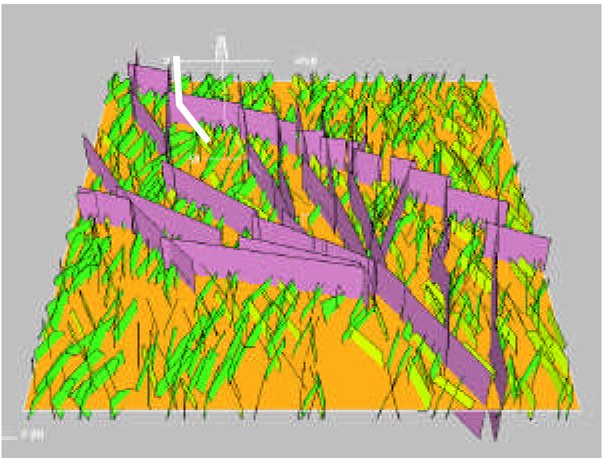


Figure 2.



Fracture network modeling traces its roots to David Snow's (1965) thesis work. Snow popularized the idea of treating individual fractures as aquifers or conductors and developing rock mass properties as an aggregation of the contributions of each fracture. The 1970's saw the development of statistical measures of fracture geometric and hydraulic properties with the motivation of risk-based analysis of rock mass stability. Fracture network models resulted from a marriage of Snow's concept of fractures as conductors, geometric statistics, and finite-element flow solvers (Long, et. al., 1983, Dershowitz, 1984).

The development of fracture network models received a major development boost in the 1980's and 1990's through applications at underground test facilities for radioactive waste disposal research. The Stripa Project (Fairhurst, et. al. 1993), Kamaishi Project (Japan), and Äspö Hard Rock Laboratory(Sweden) have promoted the evolution of DFN models into practical tools. A major conclusion of test facility work has been the recognition that DFN models should include major conductors (faults, fracture zones, etc.) as deterministic features, superposed on a background of stochastically generated features (Figure 2). For bedded or layered systems one may also include a bedding-plane fracture that incorporates matrix properties.

A fracture network model can be used in any of several ways. The network may be discretized and solved by direct simulation with the definition of appropriate boundary conditions to produce results like the simulated well test in Figure 3. Another alternative is to define continuum properties for a porous media solver like MODFLOW either by solving flow within the extracted network of each grid cell of the continuum model or by calculating a permeability tensor for each cell from the fracture geometries (Figure 4).

As with most models, defining the input parameters for DFN modeling is a significant challenge. For fracture network models it is important to recognize that the conducting network is generally a small subset of all geologically defined fractures. New tools from recent years, such as improved flow logging methods and borehole televiewers, greatly aid in defining this subset by identifying the conducting fractures and determining their geologic and geometric characteristics. Advances in well test analysis also provide data to constrain the overall network and provide data against which to test DFN model performance.

Figure 3.

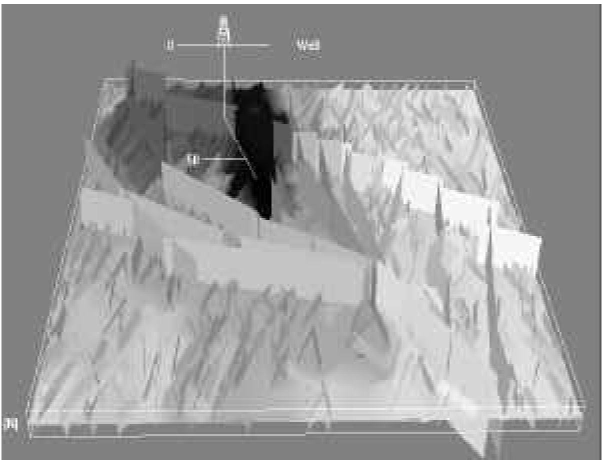
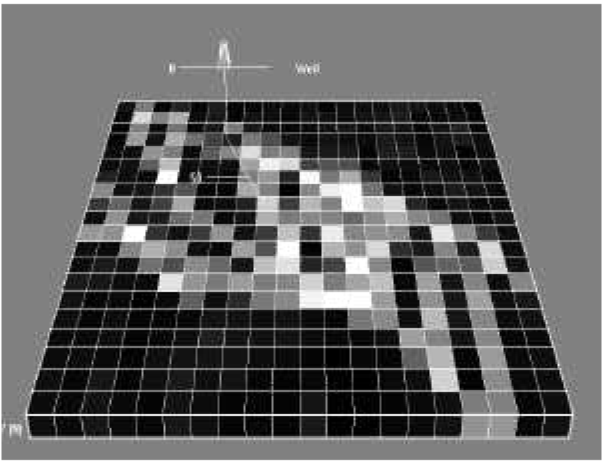


Figure 4.



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How important are horizontal fractures?

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The near-horizontal fractures that hydrogeologists detect in the subsurface or observe in outcrops in undeformed sedimentary rocks can dominate local and regional groundwater flow. Horizontal discontinuities occur in all types of sedimentary rocks. They can be either primary (bedding planes, facies changes, or other depositional features) or secondary (horizontal fractures, fracture zones, or solution features). Understanding the extent and hydraulic function of these heterogeneities can be critical to developing accurate and useful conceptual and numerical models of a hydrogeologic system.

How extensive can horizontal heterogeneities be? Our work in a dolomite aquifer in northeast Wisconsin suggests that thin (< 1 m) fracture zones related to bedding planes extend continuously for several kilometers and can be traced in the subsurface using hydrostratigraphic and geophysical techniques (Rayne and others, 2001; Muldoon and others, 2001). These thin but areally extensive features have significant transmissivity and control ground water flow and solute transport at local and regional scales. Investigators in Canada have reported very similar flow zones in dolomites near Niagara Falls (Novakowski and Lapcevic, 1988; Sayko and others, 2002). Similar features can be found in clastic sedimentary rocks (Michalski and Britton, 1997; Swanson, 2001).

Modern groundwater flow models can include these heterogeneities. Rayne and others (2001) used MODFLOW to simulate regional fracture zones by treating them as thin finite-difference layers having high hydraulic conductivity and low porosity. Figure 1 shows a cross section from a three-dimensional MODFLOW model along the flow path toward a municipal well. The particle tracks represent 100 days of travel from the indicated starting area at the water table. The particles move horizontally more than 5 km in 100 days, and these high simulated velocities are consistent with field observations such as tracer tests. Most of the advective travel occurs through the horizontal fracture zones. If the model did not include the fracture zones, it would have overestimated travel times to the well by a factor of 10 to 100.

On the basis of the field studies cited above, narrow but widespread fractures and other heterogeneities in sedimentary rocks are probably relatively common, and today's computer codes are capable of simulating many of these features. Ignoring the heterogenities, or assuming that they are insignificant at large scales of investigation, can lead to major errors in the prediction of groundwater flow rates, travel times, and movement of contaminants.

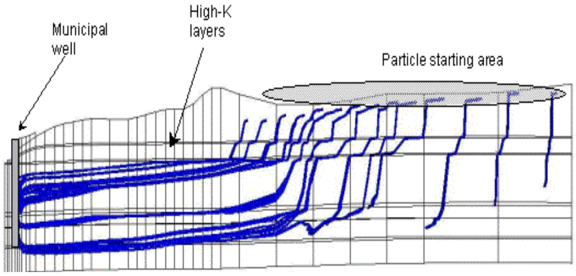

Figure 1. Cross section showing particle paths traced using MODPATH from the water table to a municipal well. Particles follow near-horizontal high-K layers; apparent deviation is caused by flow out of the plane of the section.

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Swanson, S.K. 2001. Hydrogeologic controls on spring flow near Madison, Wisconsin. Unpublished PhD dissertation, Dept of Geology and Geophysics, University of Wisconsin-Madison, Madison, WI. 436 p.

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continued from page 1

- * new developments in graphical user interfaces and visualization
- * database management and graphical information systems (GIS)
- * case histories involving unusual applications of ground-water models
- * educational issues in ground-water modeling
- * decision making and policy development through model application
- * use of models in resolving conflict
- * the sociology of groundwater modeling

The Conference will be held on the Colorado School of Mines Campus in Golden, Colorado, U.S.A. September 16-19, 2003. There are many hotels in the nearby Golden and Denver areas in which reservations can be made. Golden, Colorado is located at the foot of Lookout Mountain, 13 miles west of downtown Denver, on the majestic Front Range of the Colorado Rockies.

The Conference registration fee of $595 (US) includes proceedings, evening receptions, lunches, and breaks. A reduced fee applies for students registered for a degree. Address questions to IGWMC at 303/273-3103, fax 303/ 384-2037, e-mail: igwmc@mines.edu. Opportunities exist for exhibit/information booths as well as for corporate support of conference events. Such participation will be acknowledged publicly.

Important Dates

April 20, 2003 Abstracts Due
May 20, 2003 Notification of Acceptance
July 20, 2003 Manuscripts Due
September 17-19, 2003 Conference, Ice-Breaker September 16

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Modeling Chemical Transport over Regional Dimensions in Bedrock Aquifers: Hydrogeologic Complexity Doesn't Necessarily Warrant Complex Modeling

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In many environmental and engineering problems it is necessary to understand the potential for chemical migration over regional dimensions, which may encompass distances of hundreds of meters to tens of kilometers. Over such distances, the presence or absence of an individual fracture will not appreciably affect a regional volumetric water balance, and bulk hydraulic properties can be used to characterize the distribution of ground-water recharge, discharge and storage, provided that regional geologic structures affecting these processes are accurately incorporated. Regional ground-water flow models in fractured rock, however, are unlikely to provide an accurate characterization of the distribution of chemical constituents, because bulk hydraulic properties can not accurately characterize the hydraulic heterogeneity needed to represent a potentially irregular spatial distribution of chemical constituents, of which only a few sampling locations are available. Models of fractured rock that consider networks of fractures and assign hydraulic properties to fractures are also unlikely to provide accurate interpretations of chemical transport over regional dimensions, because of the uncertainty in the fracture properties and fracture connectivity over large dimensions.

A tracer experiment is needed to characterize the magnitude of in situ processes affecting chemical migration. Over distances of hundreds of meters to kilometers controlled tracer experiments are unlikely to be successful. For this reason, hydrogeologists have relied on naturally occurring (environmental) tracers, which are either chemical species or dissolved gases in precipitation recharged to the ground water. In relatively homogeneous unconsolidated porous media, fluid advection is assumed to control the spatial distribution of environmental tracers; the concentration of these tracers can then be directly translated to a ground-water age based on the assumed temporal history of the tracers in ground-water recharge. In bedrock aquifers, however, diffusion into low-permeability environments, such as the primary porosity of the rock, and dispersion, arising from the extreme variability in the fluid velocity, are likely to alter the concentration of the tracers as they migrate through the formation. Under such conditions, it is necessary to mathematically model the physical processes affecting chemical migration and not merely translate a tracer concentration into a ground-water age.

Because of the sparse chemical data, complex models of aquifer heterogeneity are not warranted in characterizing the spatial distribution of chemical constituents over regional dimensions, and instead simplified mathematical models of chemical transport processes should be considered as a means of placing bounds on the magnitude of processes affecting the fate of chemical constituents in ground water. Three types of hydrogeologic conditions are potentially applicable to simple mathematical modeling of chemical transport over regional dimensions in bedrock aquifers.

Well-Defined Area of Recharge: If there is a single, small, well-defined area of recharge to the bedrock aquifer, then the distance to sampling locations can be identified and a simple one- or two-dimensional mathematical model of the physical processes affecting the tracer can be calibrated based on the known input at the recharge location and the measured response at sampling locations.

Regional Flow Lines: An alternative means of interpreting sparse geochemical information is to assume that sampling locations lie along a single flow line, and the distance between sampling points can be used in mathematical modeling of the physical processes affecting the changes in concentration between sampling locations (see, e.g., Plummer et al., 1990). It would be fortuitous, however, to assume that two sampling locations are located precisely along the same flow line. Nevertheless, this assumption is acceptable, if distances between sampling locations are large relative to the heterogeneity in the formation. Under such conditions, flow lines that are roughly parallel to each other will experience the same processes, and sampling locations on different flow lines can be interpreted as if they were from the same flow line.

Multiple Tracers: In instances where there is not a well-defined area of recharge, or the heterogeneity is significant relative to the distance between sampling locations, a third alternative is to interpret the migration of multiple tracers (see, e.g., Shapiro, 2001). In this conceptual approach, multiple flow lines are assumed to originate at the water table and extend through the bedrock. If there is an overlying unconsolidated material, it is assumed that all flow lines move through a similar distance in the overburden material regardless of their starting location. Also, after a sufficient distance in the bedrock, processes affecting chemical migration along one flow line are assumed to be similar to other flow lines. Therefore sampling in the bedrock and unconsolidated overburden is regarded as sampling at locations along an ensemble of similar flow lines, which, in turn, can be regarded as sampling one representative flow line at various distances from its origin; however, the distance from the recharge location to the sampling point along the flow line is unknown, and the relative distance between sampling locations is also unknown. Because distance along a flow line to a sampling location is unknown, the spatial distribution of environmental tracers needs to be removed from the modeling process to estimate model parameters. This is accomplished by interpreting the concentrations of multiple tracers moving simultaneously in the formation, and assuming that these tracers are subject to similar in situ processes. Concentrations from simulations of multiple tracers along a representative flow line can be plotted against each other (i.e., tracer A vs. tracer B), and model parameters can be varied to reproduce the measured relation between the tracers (i.e., tracer A vs. tracer B) from the sparse sampling locations.

The application of simple mathematical models of chemical transport to regional dimensions requires an intimate knowledge of the regional ground-water flow regime to assess if the hydrogeologic conditions are suitable for such modeling, and to provide constraints on the chemical transport (see, e.g., Shapiro, 2001). Simple, conceptual models of chemical transport that make use of sparse chemical data should be looked upon as a means of understanding large-scale spatial trends in chemical data, and for placing bounds on the magnitude of processes affecting the fate of chemical constituents; they should not be regarded as a mechanism for characterizing the explicit spatial distribution of chemical constituents in bedrock aquifers.

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MODFLOW 2003**

**Fracture Modeling
Issue**
featuring articles by:

Paul Hsieh
Tom Doe
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Karsten Pruess

IGWMC SHORT COURSES

COURSE (Descriptions are provided at http://www.mines.edu/igwmc/short-course/)	Instructors	Start Date No. of Days	End Date Times	Fee Late Fee/Date
Applied Environmental statistics **ID # 01-1**	Dennis Helsel Ed Gilroy	August 12, 2002 5 days	August 16 8am-5pm	$1495 $1595/July 26
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Subsurface Multiphase Fluid Flow and Remediation Modeling **ID # 01-5**	John McCray	October 31 2 days	November 1 8am-5pm	$795 $995/October 16
PHREQC Modeling : The Basics **ID # 01-6**	Geoffrey Thyne	October 31 2 days	November 1 9am-5pm	$795 $995/October 16

**PLEASE JOIN US! at the MODFLOW 2003 Conference
“CALL for PAPERS” Inside**

Update on Fracture Modeling: Hsieh, Shapiro, Pruess, Bradbury, Doe