8 Modeling Fractured Rock

Groundwater flow and chemical transport models can help to characterize and remediate fractured rock sites at all scales. It is critical that any modeling be performed by modelers with experience in fractured rock, and with the specific application in fractured rock, because this modeling is significantly different from modeling in unconsolidated media. Models are tools that efficiently perform simple to complex calculations describing physical and chemical processes. A common tenet in modeling is that the overall value of a model depends on the quality of the input parameter values, and how well those parameter values reflect actual site conditions. This principle applies to modeling of fractured rock.

The complexity of fractured rock requires diligent focus on site characterization to develop data for the model. Although any model is an approximation, a well-designed model can help support decision making. Models, however, should not be considered as perfect predictors of future behavior. Based on initial model results and sensitivity analyses, specific data collection actions can be identified that further refine the model and further improve its usefulness.

Two types of goals often apply when using models:

- interpretive modeling to improve understanding of key processes or site characteristics, with the intent of improving the CSM or identifying significant data gaps for additional characterization
- predictive modeling to help with long-term site management, such as prediction of contaminant plume velocity or remediation timeframes with consideration of matrix diffusion or design of a hydraulic containment system.

Predictive modeling in fractured rock settings is difficult and is best suited to assisting the modeler in understanding various outcomes that may happen, rather than a definitive prediction of what will happen.

Applying a model requires simplifying the modeled setting by applying average input properties over some scale (such as site-wide) or identifying and simulating key major parameters in a more exact context (such as significant transmissive fractures). While most models incorporate simplified representations relative to the actual site complexity, they can be used to qualitatively or quantitatively evaluate site conditions or support remedial or corrective actions (MDEQ, Feb. 2014).

ASTM has compiled standards providing guidance on groundwater modeling. Many of the principles described in these standards are relevant to models of fractured rock systems (ASTM 1994, 1994b, 1994c, 1995a, 1995b, 1996, 1998).

8.1 Comparisons Between Modeling of Fractured Rock versus Unconsolidated Porous Media

Figure 1-1 illustrates some of the key similarities and differences between fractured rock and unconsolidated porous media. The factors shown in this figure have significant implications for groundwater flow and solute-transport modeling, and should be accounted for when considering or undertaking modeling of fractured rock sites. For example, using a standard soil porosity in an estimate of flow velocities in fractured rock can result in errors on the order of 1000%.

8.1.1 Groundwater Flow Modeling

Modeling of groundwater flow for water-balance purposes is similar in both types of media. Such models apply general representations of recharge and discharge boundaries, bulk hydraulic conductivity and storage parameters, and hydraulic stresses such as pumping wells. However, plan-view anisotropy may be more extreme in fractured rock than in porous media, particularly in situations with a dominant dipping fracture set. The SRSNE case study presents an example where the plan-view anisotropy was estimated as 1:20 in a system of dipping bedding-plane fractures; calibration of modeled particle-tracking results confirmed that the anisotropy estimate was reasonable. Also, in some cases, relatively discrete flow zones in fractured rock—such as fracture zones and faults—may require a finer model grid design in some parts of the model domain.

8.1.2 Solute Transport Modeling

Solute transport modeling in fractured rock is significantly different from modeling in unconsolidated porous media. Solute-transport models for unconsolidated deposits often use a bulk retardation factor to account for sorption-based retardation. This approach does not apply in fractured rock because these models do not explicitly simulate the extreme hydraulic conductivity of fractures and do not explicitly simulate matrix diffusion.

Solute-transport models for fractured rock typically represent fractures as discrete flow zones and the unfractured matrix as a low-permeability, diffusion-dominated storage zone (such as in a dual-porosity formulation). Dual porosity formulations can capture the physics of transfer from flowing and storage zones; however the transfer coefficients are challenging to parameterize.

Characterizing fractured rock sites for modeling purposes should focus on fracture orientations and hydraulics (including hydraulic aperture estimation) and matrix storage capacity (such as porosity, bulk density, and organic carbon content). Solute transport modeling of metals also may require characterizing select geochemical parameters.

8.2 Types of Fractured Rock Models

An analytical model is typically a simple equation (often referred to as a scoping calculation), which may be easily applied using spreadsheet software. Analytical models are typically one-dimensional and offer a simplified or small-scale representation of site conditions. For example, one analytical model presents a simple solution for evaluating the diffusive flux into or out of a rock matrix (Parker 1994). Numerical models refer to the solution of more complex mathematical equations, which allow for representation of more sophisticated site conditions than is typically possible with an analytical solution.

A common historical modeling approach for fractured sites has been to use an equivalent porous media (EPM) framework. This approach assumes that the fractured system behavior is equivalent to porous media behavior and can be represented by an equivalent porous medium, with equivalent hydraulic conductivity in a certain area. EPM models do not directly account for preferential flow in fractures, but approximate the larger-scale conductivity of the fracture network, often with anisotropy in plan view and vertical perspective. EPM modeling approaches are useful in fractured rock settings for large-scale flow/water-balance assessment and capture-zone analysis for hydraulic containment systems. The applicability of EPM approaches is a function of scale, and increases with increasing scale. EPM approaches have even been demonstrated to be suitable for water resources management decisions in regional groundwater flow in karstic systems (Scanlon 2003).

Discrete fracture pathways and mass transfer between mobile (generally fractures) and immobile (generally matrix) porosities can be modeled with many hydrogeologic modeling codes; however the large degree of uncertainty in these parameters at most sites requires modeling to be performed in a stochastic or probabilistic framework and not as a single deterministic simulation. The level of accuracy and effort required for modeling depends on how well the selected numerical approach can be parameterized and discretized, given financial, technical, and schedule constraints (Selroos 2002). Modeling approaches that explicitly represent fractured rock systems include the Discrete Fracture Network (DFN) approach (Long 1983; Robinson 1984; Dershowitz 1985), the Hybrid Equivalent Porous Media (EPM)/DFN approach (Bordas 2005; Dershowitz 2006; Neuman 1987; Bruine 2003; ITRC 2003), and channel network (CN) approaches (Watanabe 1997). Reviews of these models and concepts can be found in the literature (Evans 1987; Haneberg 1999; Faybinshenko 2000; Berkowitz 2002; Selroos 2002; Dershowitz 2004; Ijiri 2009; ITRC 2003). DFN models are available through commercial, government, and academic sources, but are not used as commonly as equivalent porous media type models, even though DFN models offer advantages for modeling fractured rock systems.

8.3 Choosing the Right Model

To achieve modeling goals, it is critical to have well-defined and reasonable objectives for the modeling task, as well as the right model. Without a clear framework based on achievable objectives, modeling programs may not deliver the required results, may result in significant re-work, or may fail all together. The choice of a model to be used depends in a large part on the goals and specific objectives of the modeling. Table 8-1 presents some common objectives for modeling, and identifies suitable modeling approaches for each.

Table 8-1. Suitable modeling approaches for various objectives

Potential Model Objective	Potentially Suitable Approach
Estimating and tracking the possible migration pathway of groundwater contamination	DFN, EPM/DFN, CN
Designing and evaluating hydraulic containment and pump-and-treat systems	Analytical, DFN, EPM, EPM/DFN, CN
Designing and evaluating groundwater monitoring networks	Analytical, DFN, EPM, EPM/DFN, CN
Estimating the possible fate and migration of contaminants for risk evaluation	DFN, EPM/DFN

Potential Model Objective	Potentially Suitable Approach
Estimating contaminant removal rate and cleanup time	Analytical, DFN (with dual porosity), EPM/DFN (with dual porosity)
Evaluating the potential impact to downgradient receptors such surface water bodies or potable water supply wells	EPM with appropriate anisotropy coupled with particle tracking, DFN, EPM/DFN
Predicting contaminant concentrations for natural attenuation remedies	Analytical, DFN (with dual porosity), EPM/DFM (with dual porosity)
DFN – Discrete Fracture Network, EPM – Equivalent Porous Medium, CN – Channel Network	

The choice of a numerical modeling approach and the specific numerical model to use depends on the system to be modeled, the intended use of the model, available financial, human, and data resources, and the abilities and experience of the modeling team. The first and most crucial step in the process is to start at the end and identify what the goals of the modeling are and what decisions will be made based on the outcomes of the modeling project. Very different model choices (and approaches) would be made for goals such as designing a pump and treat system in a fault-dominated granite, versus designing a compliance monitoring network in a limestone, versus examining chemical process dependence for an injection-based remedy in an argillaceous setting.

A common mistake when performing fractured rock modeling is to choose an overly complex model or modeling approach under the assumption that it provides more versatility and flexibility during the process. The default approach should not be "What numerical code should I use?" but rather "Do I need to use a numerical model at all?"

Analyzing contaminant mitigation and designing remediation solutions need not be complicated—even at complex sites. It is often worthwhile and cost effective to use simple scoping calculations to determine the level of analysis necessary for a given objective. At sites having evidence that a single discrete pathway dominates transport, an approximate analysis to identify and quantify the pathway hydraulic properties may be sufficient to estimate transport behavior. At other sites, the most important process may be the exchange between fractures and matrix, rather than transport within the fractures themselves. In those cases, if the question to be answered involves time-dependent behavior at a site scale, an analytical solution of mass exchange might provide an excellent indication of the time scales of site remediation.

If numerical modeling is performed, the default approach should be to use the simplest tool for achieving project objectives. Increasing sophistication and capabilities in the model choice should be directly tied to the level of site complexity and the availability of data to support model design. Given the number of choices, the modeling team should consider the range of available approaches and their limitations and parameter requirements. All modeling requires simplifications, and fractured rock modeling often requires drastic simplifications as compared to modeling in typical porous media settings. ASTM (ASTM 1998) provides further details regarding groundwater model code selection.

8.4 Parameterization (Data Needs)

A full description of a fractured rock system would include data on the size, orientation and hydraulic properties of each fracture and matrix block, the temporal variability of hydraulic head through the system, the spatial variation in the permeability and porosity of the matrix, boundary conditions, sources and sinks of water and contaminants, geochemical understanding of the interaction of the rock and the contaminants, and much more. Collection of such detailed information is infeasible and often unnecessary. The more detailed the site characterization and the more it focuses on the key parameters for the modeling task, however, the greater the probability of meeting the modeling objectives.

A detailed discussion on the parameterization of models is outside the scope of this document, but many existing references are available on this topic (NRC 2015; NRC 1996). Key parameters that are likely to be needed for modeling fluid flow in fractured rock are listed below:

- Boundary conditions are required for every numerical groundwater flow model and some analytical models. These conditions are constraints on the mathematical model. ASTM (ASTM 1994b) provides guidance on assigning boundary conditions.
- Bulk rock hydraulic conductivity is required for models that focus on site-scale water-balance analysis, capture-zone estimation, and generalized groundwater flow directions. These parameters can be measured using field hydraulic tests at wells and boreholes.
- Bulk rock anisotropy data is needed for the same purposes as above; these can be estimated based on multiwell pumping test analysis, resistivity survey data, seismic refraction data, fracture set orientations, or calibrating

particle tracking results to match observed tracer or plume migration directions.
- Fracture set orientations are used to help estimate the potential for anisotropy and probable direction of dominant fluid flow.
- Fracture apertures and fracture porosity data are used to simulate or calculate fluid flow rates and simulate particle-track velocities.
- Hydraulic heads and gradients are needed for a variety of modeling purposes.

In addition to those listed above, key parameters for modeling solute transport in fractured rock include the following:

- Matrix permeability helps to interpret whether flow in the matrix needs to be explicitly simulated to represent solute transport with a reasonable degree of representativeness. If the matrix permeability is very low, mass transfer into and out of the matrix can be represented as diffusion.
- Matrix porosity and bulk density are needed, and if the solutes of interest are organic compounds, the matrix organic carbon content is also required.
- Geochemical parameters are used to simulate reactions that can affect mobility of metals and the viable degradation pathways of organics.
- Biologic parameters such as microbial populations support the conceptual model and simulation of degradation pathways for organics.
- Solute degradation half-life data are needed when simulating a reactive solute.

When possible, these parameters should be characterized within the dominant pathways, zones, or strata where flow and mass flux occur.

A particularly powerful use of models is to help identify areas of CSM uncertainty and sensitive parameters that may warrant further characterization. Model results may indicate areas of poor performance (calibration or prediction), where additional data may help reduce uncertainty or improve model estimations. The CSM (and translated numerical framework) is then updated based on the additional data, and the model run to assess the improved performance. Using models in this manner can help focuses field investigations, reduces the overall costs of site characterization, and improves confidence in the evolving CSM.

8.5 Model Calibration, Sensitivity Analysis, and Uncertainty

A thorough treatment of model calibration, sensitivity analysis, and assessment of uncertainty in fractured rock settings is beyond the scope of this document. An overview of these topics is provided here, however, so that modelers and the ultimate end-users of modeling can understand general approaches and limitations. For more information, refer to a modeling textbook such as *Applied Groundwater Modeling* (Anderson and R. Tokar 2015) and ASTM documents.

8.5.1 Model Calibration

Calibration is the process of refining the model representation of the hydrogeologic framework, hydraulic properties, and boundary conditions to achieve a desired degree of correspondence between the model simulations and observations of the groundwater flow system (ASTM 1994, 1995a, 1995b, 1996). Examples of hydrologic model calibrations at fractured rock sites include studies of potential sites for high level nuclear waste repositories such as Yucca Mountain (Zyvoloski 2003) (Mazurek 2003).

Some aspects of model calibration that are unique to fractured rock settings as compared to porous media include:

- *Potential for extreme heterogeneity*. Fracture zones, faults, or (in the case of carbonate rock or volcanics) karst-like conduits are likely to have hydraulic properties that differ extremely from those of the overall rock mass. If so, these types of features may need to be explicitly simulated to achieve a reasonable degree of agreement with measured site data.
- *Anisotropy* – Fractured rock may contain aligned fracture sets, which can impart a high degree of anisotropy to the hydraulic conductivity field, including in the horizontal and vertical planes. The SRSNE case study presents an example in which the plan-view anisotropy was estimated as 1:20 in a system of dipping bedding-plane fractures; calibration of modeled particle-tracking results confirmed that the anisotropy estimate was reasonable.
- *Low storativity*. Groundwater elevations in fractured rock settings can change quickly by significant magnitudes because of the low storativity of fractured rock formations, so that steady state model calibration may require collection and averaging of numerous water level measurements at calibration target wells.
- *Dual domain mass transfer and storage*. It may be necessary to explicitly simulate matrix diffusion effects rather

than using bulk sorption-based retardation approximations.

Calibration can be performed by trial and error, or with the aid of an automated parameter estimation code such as PEST or UCODE. The preferred approach to develop reasonable model inputs in the calibration process is as follows:

1. Identify reasonable ranges of input parameters.
2. Run predictive models within an automated parameter estimation framework, using various combinations of input parameters within the pre-defined ranges.
3. Identify the model input parameter combinations that produce output that is most consistent with site-specific observations and measurements.

Data used typically for model calibration targets include heads, measured flow rates, particle tracking of simulated groundwater flow directions (for comparison with mapped plume morphology), and geochemical measurements under natural and pumped conditions. Model input parameters are adjusted and model outputs are compared to site-specific measurements. Model results are then compared statistically to determine the relative degree of difference between the model output and site-specific measurements.

Parameter estimation codes are mathematically complex and require a highly skilled and experienced modeler; uninformed use of this approach can lead to incorrect interpretations. Many combinations of input parameters may yield output that is a good fit to observed conditions. A good fit, however, does not necessarily ensure that the model correctly represents the flow and transport conditions. Best practices include calibration to transient data or for a minimum of two different stress regimes (such as pumping and static conditions, or wet and dry seasons).

8.5.2 Sensitivity Analysis

Sensitivity analysis is a quantitative evaluation of the impact of variability or uncertainty in model inputs on the degree of calibration of a model and on its results or conclusions (Anderson 1992; ASTM 1994b). Sensitivity analysis in fractured rock settings generally progresses as it does in porous media. For several key types of input parameters, the input parameters are adjusted within a reasonable range of values and the model results are compared to the calibrated model in terms of the magnitude of changes to model calibration statistics. Input parameters selected for adjustment during sensitivity analysis are often those that have potentially large ranges in magnitude (such as hydraulic conductivity) or have not been well constrained by site-specific data (such as recharge, anisotropy values, or timing of contamination releases). Input parameters that are more sensitive produce larger changes in model results; those that are less sensitive produce smaller changes in model results. In this process, the modeler may find that a particular sensitivity run produces better calibration statistics than the previously identified calibrated model. If so, then the modeler may choose to replace the previously considered calibrated model with the revised model setup.

Analysis of the problem with initial scoping calculations often reveals ways to simplify numerical models. For example, some numerical model inputs have little effect on output. Quantitatively analyzing the sensitivity—or in this case, the insensitivity—of a model can be powerful because it can reveal what additional data may or may not constrain a model parameter and decrease model uncertainty. This type of insight is more valuable than that resulting from a single numerical model calculation.

8.5.3 Assessment of Model Uncertainty

Model uncertainty can arise from the following sources (NRC 2015):

- simplifications necessary to implement a conceptual model in a numerical model
- limitations of the understanding or implementation of physical-chemical-biological processes in the model
- errors in the numerical model implementation
- limitations in the match between measurements and model results

Quantifying these errors and uncertainties, to the extent possible, helps ensure that numerical models and the conclusions drawn from them are appropriately applied. Presentation and use of results from numerical models in fractured rock should be explicitly linked to the known uncertainties. Except for the simplest cases, providing an indication of the uncertainty in the model estimates, through methods such as box and whisker plots, provides the end user with an important understanding of the reliability and ultimate usefulness of the estimates.

Model uncertainty can be assessed in parallel with sensitivity analysis. However, uncertainty assessment often focuses on predictive model simulations, where hydraulic stresses or parameters are adjusted to reflect a hypothetical future condition (such as the operation of extraction wells, installation of hydraulic barriers, or removal of a constant-concentration source).

In uncertainty analysis, the results are compared before and after model input parameter adjustment to identify the degree of change in model results, and therefore the degree in model uncertainty, associated with that parameter change.

Just as examining the sensitivity of a model to input parameters can guide subsequent model development, so can quantifying the uncertainties that arise during the modeling process guide interpretation of model output. Structural uncertainties (fracture locations, size, and orientation) can be large and are often the most difficult to quantify and estimate when modeling fractured rock (NRC 2015). Formal statistical data analysis methods can be used to place bounds and characterize parameter distributions (normal, log normal) through statistical analysis of the data, if enough data are available. When data are limited, use experienced-based expert opinion with sound, documented explanations for the choices made.

8.6 Limitations

Models are conceptual descriptions, or approximations, that describe physical systems through the use of mathematical equations. Models are not exact descriptions of physical systems or processes. The applicability, or usefulness, of a model depends on how closely the mathematical equations approximate the physical system being modeled. For this reason, models that are based on a thorough understanding of the physical system and the assumptions embedded in the derivation of the mathematical equations produce better predictions (Michigan Department of Environmental Quality 2014).