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Superfund Ground Water Issue

Contaminant Transport in Fractured Media: Models for Decision Makers

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The Regional Superfund Ground Water Forum is a group of ground-water technical specialists, representing EPA's Regional Superfund Offices, organized to exchange up-to-date information related to ground-water remediation at Superfund sites. Site characterization of fractured rock sites, and modeling ground-water flow and contaminant transport in fractured media, have been identified by the EPA Regional Superfund Ground Water Forum as major issues of concern for decision-makers at many Superfund sites. The ability to reliably predict the rate and direction of ground-water flow and contaminant transport in fractured rock systems would be of great value in planning and implementing the remediation of contaminated aquifers. This paper summarizes the current status of modeling ground-water flow and contaminant transport in fractured rock systems. A companion paper summarizing the status of site characterization at fractured rock sites is in preparation.

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Summary

Mathematical models have a potentially useful role to play in arriving at a decision on the remedial action to be taken at a contaminated site. Where there is a need for a quantitative estimate of the threat to public health resulting from a particular course of action, of the estimated cost and time of clean-up for a particular remediation strategy, or of the results of other actions to be taken at a contaminated site, mathematical models have a greater potential to provide the needed information than any other approach to the problem. For contaminated sites in fractured rock, however, this potential has yet to be realized.

The development of predictive models for ground-water flow and contaminant transport in fractured rock systems is an active area of research, but field-validated models that are directly applicable to the remediation of contaminated sites are not yet available. Nonetheless, when used with appropriate site characterization data, the available models can be helpful in developing a qualitative understanding of the behavior of the fractured rock system and the interactions of contaminants with the system.

Selection of a suitable model requires the model user to have a specific objective in mind. For example, is the purpose of the modeling effort to determine the location of additional monitoring wells, to design optimal well placement for hydraulic control during site remediation, to interpret existing data, or to determine sources or predict the fate of a pollutant? No single model will serve all purposes. The choice of model will depend on the system conditions, the decision to be made, and the extent and availability of site characterization data.

Before ground-water models can be applied to any system, fractured or not, it is necessary to have extensive data about that system. Data are needed to (1) select or develop an appropriate model based on the processes acting on the system; (2) define boundaries in space and time of the domain in which these processes are acting; (3) determine the state of the system at some point in time from which predictions, either forward or backward in time, can be made; and (4) estimate the effects of future stresses or inputs to the system (Konikow and Mercer, 1988). Modeling and data collection are complementary activities, neither being a substitute for the other. Not only are data necessary for successful modeling, but modeling results may be used to guide data collection efforts.

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Because of the heterogeneous and anisotropic nature of fractures in the subsurface, the data requirements for modeling the movement of water and contaminants in fractured media are somewhat different than the requirements for modeling more homogeneous unconsolidated porous media. The development of techniques to characterize the hydrogeologic properties of fractured rock systems has proceeded in parallel with the development of models. These techniques are often more complex and more difficult to interpret than analogous techniques used in unconsolidated media.

There are at least four categories of models to describe flow and transport in fractured rock systems. (1) Models developed for use in unconsolidated porous media have been successfully applied to certain fractured rock systems. These models consider the fractured rock system as an equivalent porous medium (EPM). EPM models are more likely to accurately predict ground-water flux than to correctly predict solute transport (Endo, et al. 1984). (2) A second category of fractured rock models explicitly considers discrete fractures. The extensive data required by discrete fracture models for fracture system characterization limit their use to sites with a relatively small number of well defined fractures. (3) A third category of models represents the fractured system by a set of matrix blocks of well defined geometry. Such models are largely research tools that are useful for enhancing our conceptual understanding of pollutant transport in fractured rock. (4) A fourth category of models uses a stochastic approach to describe the fracture distribution. At the present time these are research models. It is important to note again that the choice of an appropriate model depends on the conditions present at the site, and on the decision to be reached by using the model.

Before discussing models in more detail, Section II provides some basic information on ground-water flow and contaminant transport in fractured rock systems. Section III briefly discusses methods of characterizing contaminated fractured rock sites. Site characterization and modeling are complementary activities and each is essential to the other. The last part of the paper discusses the conceptual basis of ground-water models and gives some specific examples of the types of models that are publicly available.

Fractured Rock Systems

Development of the theory of flow through porous media began with experimental work by Henri Darcy, published in 1857. The study of fluid flow through fractured rock was first developed in the petroleum industry. These studies resulted from observations that oil and gas production could be significantly increased by fracturing the producing formations near the well bore (Duguid and Lee, 1977). Gale (1982) notes that the first comprehensive experiments on flow through artificial fractures were conducted in the early 1950's. During the past decades, the amount of research on flow and transport in unconsolidated porous media has greatly exceeded that devoted to fractured media. This is due in part to the complexity of fractured rock systems and the lack of economic incentives.

Most fractured rock systems consist of rock blocks bounded by discrete discontinuities comprised of fractures, joints, and shear zones, usually occurring in sets with similar geometries (Witherspoon, et al., 1987). Fractures may be open, mineral-filled, deformed, or any combination thereof (Nelson, 1985). Open fractures may provide conduits for the movement of ground water and contaminants through an otherwise relatively impermeable rock mass. Mineral-filled fractures are filled either partially or completely by secondary cementing materials such as quartz or carbonate minerals, thereby reducing or eliminating fracture porosity and permeability. Deformed fractures may be infilled with permeability-reducing gouge, a finely abraded material produced by the cataclasis of grains in contact across a fault plane during displacement of the rock masses. Other deformed-fracture features include slickensides, which are striated surfaces formed by frictional sliding along a fault plane. Slickensides reduce permeability perpendicular to the fracture plane, but the mismatch of fracture surfaces may increase permeability along the fracture plane. Very little displacement is necessary to produce gouge or slickensides. The deposition of a thin layer of low permeability material, fracture skin, may prevent the free exchange of fluids between the rock matrix and fracture (Moench, 1984).

Major factors affecting ground-water flow through fractured rock include fracture density, orientation, effective aperture width, and the nature of the rock matrix. Fracture density (number of fractures per unit volume of rock) and orientation are important determinants of the degree of interconnection of fracture sets, which is a critical feature contributing to the hydraulic conductivity of a fractured rock system (Witherspoon, et al., 1987). Only interconnected fractures provide pathways for ground-water flow and contaminant transport. Fractures oriented parallel to the hydraulic gradient are more likely to provide effective pathways than fractures oriented perpendicular to the hydraulic gradient. Fractured rock systems simulate equivalent porous media when the fracture apertures are constant, the fracture orientations are randomly distributed and the fracture spacing is small relative to the scale of the system (Long, et al., 1982).

The cross-sectional area of a fracture will have an important effect on flow through the fracture. Fracture-flux is proportional to the cube of the fracture aperture (distance between rock blocks). The relationship between flux and aperture appears to be true for fractures with apertures greater than 10 microns (Witherspoon, et al., 1987). Fracture apertures, and therefore flow through fractures, are highly stress-dependant, and generally decrease with depth (Gale, 1982).

The nature of the rock matrix plays an important role in the movement of water and contaminants through fractured rock systems. Metamorphic and igneous rocks generally have very low primary porosity and permeability. Fractures may account for most of the permeability in such systems and the movement of water and contaminants into and out of the rock matrix may be minimal. Sedimentary rocks generally have higher primary porosity and varying permeability. Coarse-grained materials such as sandstone have relatively high primary porosity and significant matrix permeability. Fine-grained materials such as shale have high primary porosity and low permeability. Fractures may enhance the permeability of all types of materials. High porosity allows significant storage of water and contaminants in the rock matrix. Authigenic clays formed during the weathering of certain rock-forming minerals may significantly reduce the porosity and permeability of the fractures and rock matrix. Rates of contaminant migration into and out of the rock matrix will depend on the permeability of the matrix, the presence of low-permeability fracture skins, and the matrix diffusion coefficient of the contaminant.

A complete description of a contaminated fractured rock system would include data on the dimensions of the system, the length, aperture width, location, and orientation of each fracture, the hydraulic head throughout the system, the porosity and permeability of the rock matrix, the sources of water and contaminants, the nature and concentrations of the contaminants throughout the system, and the chemical interactions between the contaminants and rock matrix. Presently, collection of such detailed information is neither technically possible, nor economically feasible on the scale of most contaminated sites. However, most ground-water models, especially those describing contaminant transport, require this type of information as input. In general, the more detailed the site characterization, the greater the probability of success in modeling the site. The accuracy of flow and transport modeling in fractured rock systems is highly dependent on the accuracy and extent of site characterization data.

Hydrogeologic Characterization Methods

Hydrogeologic characterization methods are usually most successful when used in conjunction with one another. These methods may include coring, aquifer tests, tracer tests, surface and borehole geophysical techniques, borehole flowmeters, and other tools. Important information may be gathered before, during, and after drilling operations.

Coring

Core material obtained during drilling operations can yield information on the density, location, and orientation of fractures, and provide samples for physical and chemical testing. Information concerning fracture roughness and mineral precipitation on fracture surfaces can also be obtained from core samples. Information collected during air hammer drilling operations with open hole completions includes the location of major water bearing fractures, changes in hydraulic head with depth, and changes in the ground-water geochemistry. In certain instances, cores may be taken diagonally to intercept near vertical fractures and determine fracture azimuth. A major drawback of coring is the relatively high cost. However, the information obtained from coring operations often makes this characterization technique cost-effective.

Aquifer Tests

Aquifer tests, including constant rate pumping tests and slug tests, can provide hydraulic conductivity and anisotropy information for fractured formations. These tests also allow the estimation of average fracture apertures of a medium. The same tests that are commonly used for unconsolidated porous media can be used for fractured media. The test results, however, will generally be more difficult to interpret. Barker and Black (1983) note that transmissivity values will always be overestimated by applying standard type curve analysis to fissured aquifers. Other more complex tests, such as cross-hole packer tests, are particularly applicable to fractured media.

Hsieh, et al. (1985a,b) describe a method of determining the three-dimensional hydraulic conductivity tensor. The method consists of injecting fluid into, or withdrawing fluid out of, selected intervals isolated by inflatable packers and monitoring the transient response in isolated intervals of neighboring wells. This method is applicable to situations where the principal directions of the hydraulic conductivity tensor are not necessarily vertical and horizontal. A minimum of six cross-hole tests is required to determine the six independent components of the hydraulic conductivity tensor. In practice, scatter in the data is likely to be such that more than six cross-hole tests will be required. Hsieh, et al. conclude that failure to fit data to an ellipsoidal representation indicates that the rock cannot be represented by an equivalent, continuous, uniform, anisotropic medium on the scale of the test. Depending on the application to be made, the test may be repeated on a larger scale, or the data may be interpreted in terms of discrete fractures of the system.

Aquifer tests can provide information on aquifer anisotropy, heterogeneity and boundary conditions, but do not provide information on the range of fracture apertures or surface roughness. One of the major drawbacks associated with long-term aquifer testing is storage and treatment of the large volume of water discharged during the test.

Tracer Tests

Tracer tests can provide information on effective porosity, dispersion and matrix diffusion, generally unobtainable from other hydrogeologic methods. Tracer tests can either be conducted under natural gradient or forced gradient conditions. The primary disadvantages of tracer tests include the time, expense, number of necessary sampling points, and difficulties associated with data interpretation. However, the important information provided by tracer tests is difficult to obtain by any other means. Davis, et al. (1985) provide a good introduction to the use of tracers in ground-water investigations.

Geophysical Tools

Both surface and borehole geophysical methods can be used to characterize fractured rock systems. Application of surface geophysical methods such as ground-penetrating radar, magnetometer surveys, and seismic and remote sensing techniques should be evaluated before a drilling program is initiated. These techniques may provide insight to potential monitoring well locations by revealing the orientation of major fracture systems. However, the correlation of major surface geophysical features with contaminant transport processes in fractured media has yet to be thoroughly characterized.

Borehole walls are usually less susceptible to fractures induced during drilling operations than cores. Borehole geophysical techniques can usually provide a more reliable estimate of fracture density than cores. However, as indicated by Nelson (1985) in a review of down-hole techniques, responses used to detect fractures on well logs are non-unique and require detailed knowledge of the tool and the various rock property effects, which could cause fracture-like responses. Borehole geophysical methods include acoustic, electrical resistivity, caliper, gamma and other high energy borehole logging techniques. The acoustic televiewer presents a continuous image of the acoustic response of the borehole face, and can detect fracture apertures as small as one millimeter. This oriented tool also allows the determination of fracture orientations. Caliper logs are best suited for determining relative fracture intensity in continuous, competent rock. Advances in electronic

and desorption assumes that the processes are described by linear isotherms and ignores sorption kinetics. Some models account separately for sorption processes in the fractures and within the rock matrix. In porous rocks, the available surface area within the matrix is likely to be so much greater than that in the fractures that sorption within the matrix will probably be more important than sorption in the fractures, assuming that the contaminants have time to diffuse into the matrix.

None of the available models appear to explicitly account for ion-exchange processes. While many of the organic chemicals of concern are not ionized in solution, other contaminants such as heavy metals could be, depending on the pH of the system. Little experimental or theoretical work has been done in this area; more work is needed.

Radioactive Decay

Much of the work on modeling flow and transport in fractured systems has been motivated by concerns about the disposal of radioactive waste. Consequently, there are a number of models that account for the radioactive decay of single radionuclides and radionuclide chains.

Chemical Reactions and Biological Processes

Very little work has been done that deals specifically with chemical reactions and biological processes in fractures. None of the models account for these processes. This is an important topic, and more work needs to be done on it.

Multiphase Flow

Models for flow and transport in fractured systems appear to be limited to single-phase flow. That is, they can simulate the flow of water alone, or the transport of contaminants that are dissolved in water. The models cannot simulate the flow of a system of water and an immiscible phase such as an oily waste, nor the transport of a contaminant dissolved in an immiscible phase. At the present time neither the capability of modeling multiphase flow in homogeneous media, nor the capability of modeling solute transport in fractured systems is advanced enough to implement a practical code for modeling multiphase flow in fractured systems (Streile and Simmons, 1986). Schwille (1988) has studied the qualitative behavior of dense non-aqueous liquids in laboratory models. His book contains a number of interesting photographs. This is another area where more research is needed.

Available Models

This section describes types of models that are available to describe flow and transport in fractured rock systems. Specific models will not be mentioned by name because the information is likely to become outdated in a short period of time. A good starting place for obtaining information on publicly available models is the International Ground Water Modeling Center, located at Butler University in Indianapolis, Indiana. They can provide a list of available models and information on specific models on the list.

Freeze and Cherry (1979) describe the development and use of a mathematical ground-water model as "a four-step process, involving (1) examination of the physical problem, (2) replacement of the physical problem by an equivalent mathematical problem, (3) solution of the mathematical problem with accepted techniques of mathematics, and (4) interpretation of the mathematical results in terms of the physical problem." Successful modeling of a ground-water contamination problem, whether in fractured rock or not, requires that all four of these steps be carried out correctly. While step (3), solution of the mathematical problem, could conceivably be carried out by a person who knew almost nothing about ground water, successful completion of the other three steps requires a thorough knowledge of hydrogeology in general, along with specific knowledge of the hydrogeology of the site to which the model is to be applied.

Fractured systems present several difficulties which hinder the replacement of the physical problem by an equivalent mathematical problem -- step (2). One difficulty is that the spatial distribution of the fractures and the way in which they control the flow is usually not known, nor is it even knowable in a practical sense. A second difficulty is that even if this information were available, including it in the mathematical problem would make the mathematical problem so complex that a solution could not be found. As a result, all mathematical models include certain assumptions about, and simplifications of, the actual physical problem. For example, the model may assume that the fractures are of uniform width with parallel sides, and/or that they form a regular geometric pattern. Comparable assumptions are also made about other physical, chemical, and biological processes. Consequently, the mathematical model provides only an approximate description of the physical system under study. The model can still be very useful, but anyone using a mathematical model should be fully aware of these assumptions and simplifications and their effect on the appropriateness of the model for the problem of interest.

Mathematical models that describe ground-water systems are usually written in terms of partial differential equations. If the equations are simple enough, the solution to the equations can be expressed in a closed mathematical form (e.g., a formula). This type of solution is called an analytical solution. More generally, the equations in the model are too complex to find an analytical solution, and a numerical method must be used to solve the problem. Models for fractured systems include those with analytical solutions as well as those with numerical solutions.

For either type of solution, the product available to the model user is a computer code in a high level language such as FORTRAN. The hardware requirements to run the code will vary from a personal computer (PC) to a main-frame type of computer. As expected, the more complex models usually have greater hardware requirements.

Models with Analytical Solutions

Models for which analytical solutions have been obtained are basically one dimensional. An example of this type of solution is a model describing solute transport in a single fracture or a set of parallel fractures. Processes that are included in the model include diffusion in and out of the rock matrix along a direction perpendicular to the plane of the fracture, adsorption on the fracture face and in the rock matrix, and radioactive decay. The solution to this problem has been published in the open literature (Sudicky and Frind, 1982) and is simple enough that the computer code can run on a personal computer.

To arrive at an analytical solution for this problem, the parallel fracture model assumes that the fracture or set of fractures has a uniform aperture and is in a homogeneous rock matrix, and that the fractures in a set of parallel fractures are uniformly spaced. To use this model, one must have an estimate or measurement of the following parameters: the flow velocity in the fracture, the longitudinal dispersivity in the fracture, the fracture aperture or width, the fracture spacing for a set of fractures, the matrix porosity, the matrix tortuosity, the diffusion coefficient of the solute in water, the fracture retardation factor or partition coefficient, the matrix retardation factor or partition coefficient, and the half-life if the solute is a radioactive species.

This model obviously describes a highly idealized situation and would not be a suitable predictive tool for dealing with a real contamination problem. However, it could have some use in building an understanding of the system and the interactions of the pollutants within the system. It is easy to vary the effect of the fracture apertures, fracture spacing, matrix porosity, and so forth, and see the effect that each of these parameters has on the rate at which pollutants move through the system. Used with the proper degree of professional judgement, the results of the model could provide guidance in making a decision. One possible application would be in comparing solute transport in two fractured systems from which cores had been collected to provide information on the parameters that are included in the model.

Analytical solutions have also been published in the open literature for dual-porosity, or "two-region" models of one-dimensional flow through systems composed of porous blocks with well-defined geometry (van Genuchten and Dalton, 1986). Those geometries for which solutions are available include close-packed spheres, hollow cylindrical macropores, close-packed solid cylinders, and rectangular blocks. Data and hardware requirements for running these codes are similar to those for the parallel crack model.

Models with Numerical Solutions

Models for which only numerical solutions are available are often referred to as numerical models. Codes for these models are likely to require more input data and greater computer power than those for analytical models. The reward for this extra work is that one can investigate more complicated problems using numerical models than one can using only analytical models.

One example of a numerical model for fractured rock systems is a two-dimensional model that can simulate both ground-water flow and contaminant transport in a fractured aquifer. The step up from a one-dimensional system to a two-dimensional system allows one to model a more complex situation, but it also requires a more complex set of differential equations and a more complex code. The model uses a dual porosity approach and allows for some specific fracture geometries. Processes that are included in the model include advective-dispersive transport in the fractures, diffusion in the matrix blocks, sorption in the fractures and in the matrix, and radionuclide decay chains.

This two-dimensional code requires data on the system dimensions, the transmissivity, the storage coefficient, and the fracture aperture and spacing if it is to be used to predict ground-water flow. The input data requirements for predicting solute transport include all of those listed for the one-dimensional analytical model described above plus values for the solute concentrations at the system boundaries.

While codes like this have utility for understanding system behavior, they should not be used as predictive tools. Like all ground-water models, they will be most useful when applied by a person with the necessary training and experience--typically, a professional hydrogeologist. To quote a recent report (van der Heijde, et al., 1988), "The application of computer simulation models to field problems is a qualitative procedure, a combination of science and art."

There are a number of numerical models that have been written to model flow and transport through systems of randomly oriented fractures and compare the results with experimental data. The results of this work have been of use in understanding the nature of flow and transport in fractured media, but this type of modeling is a research effort at this time.

Summary Remarks

The development of models to enhance understanding of and to predict contaminant transport in fractured rock systems continues to be an active area of research. Reliable, field-validated models that can be used to predict the results of clean-up scenarios at contaminated sites are not yet available. The models that are available help in developing an understanding of the behavior of the fractured rock system.

The application of mathematical models to contamination in fractured rock systems is hampered by difficulties in at least two major areas. The first problem is site characterization -- the collection of the necessary data to adequately describe the geologic and hydrologic properties of the system. Mathematical modeling is not a substitute for collecting data. In fact, data collection is an essential part of modeling the behavior of a site. Collecting the data required by existing models is difficult and expensive, and in many cases not possible with present techniques. More research is needed to find better ways to measure the properties of fractured rock systems. Conversely, there may be value in developing models that require data that can be collected.

The second problem is model validation--comparing the results of modeling to results obtained in the field. Validation of models is necessary if decision makers are to have confidence in them and be able to use them in planning and carrying out remedial work. Research is being done to validate models of contaminant transport in fractured rock systems, but more work is needed. One problem with model validation studies is the shortage of data sets for sites with a variety of geological and hydrogeological characteristics. This is where cooperation and coordination between those in the research community and those charged with remediating contaminated sites could prove mutually beneficial.

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