TRAINING COURSE

ON

SOFTWARE FOR GROUNDWATER DATA MANAGEMENT

UNDER

WORLD BANK FUNDED HYDROLOGY PROJECT

LECTURE NOTES
ON

GROUNDWATER MODELLING SOFTWARES
(UNIT-5)

BY

P K MAJUMDAR

ORGANISED BY

NATIONAL INSTITUTE OF HYDROLOGY
ROORKEE - 247 667
INDIA

GROUNDWATER MODELLING SOFTWARE FOR HARD ROCK REGION

1.0 INTRODUCTION

Groundwater modelling may be used for a variety of purposes, some of which are; estimation of aquifer parameters, regional simulation of groundwater levels, conjunctive use of surface and groundwaters, irrigation planing and /or aquifer management. Use of classical porous media models in hard rock region may not give always an approximate solution to certain degree acceptable limit. Flow phenomena through fractured media is quite different to that of granular porous media. Secondary porosity is more important in rocks as compared to grain size porosity. Fracture dimensions and configurations play vital role in the value of the properties like permeability, hydraulic conductivity and storativity of the rock masses.

The analysis of flow, and displacement processes in rock has a long history in connection with the production of oil from underground reservoirs. However, it is only in the past fifteen years that this analysis has been extended to include detailed structural properties of the media. These studies are quite diverse in the physical phenomena that they consider.There are two types of non-classical hard rock aquifer models-the discrete and continuum models. Continuum models represent the classical engineering approach to describing materials of complex and irregular geometry, characterized by several length scales. The physical laws that govern fluid transport at the microscopic level are well understood, with the exception of ultramicroporous structures. Leaving aside that case, one could in principle write down differential equations for momentum, energy, and mass and the associated initial and boundary conditions at the fluid-soil interface.

However, as the interface in typical rocks is very irregular, practical and economical techniques are not available for solving such boundary-value problems-even in the unlikely event that one knows the detailed morphology of the medium. Determination of the precise solid-fluid boundary in anything but the simplest rocks is, and will probably remain, a very difficult (if not impossible) task; the boundary (even if known) within which one would have to solve the equations of change would be so tortuous as to render the problem mathematically intractable. Moreover, even if the solution of the problem could be obtained in such great detail, it would contain much more information than would be useful in any practical sense. Thus it becomes essential to adopt a macroscopic description at a length scale much larger than the dimension of individual pores or fractures.

Macroscopic properties such as effective transport coefficients are defined as averages of the corresponding microscopic quantities (see, for example, slattery,1967,1969; Whitaker,1967). The averages must be taken over volume V that is small enough compared to the volume of the system, but large enough for the equation of change to hold when applied to that volume. At every point in the medium one uses the smallest such volume and , thereby, generates macroscopic field variables obeying equations such as Darcy's law of flow or Fick's law of diffusion. The reasons for choosing the smallest suitable volume for averaging are to allow in the theory suprapore variations of the porous medium and to

generate a theory capable of treating the usual macroscopic variations of effective properties. There are several situations in which the conditions for the validity of such an averaging are not satisfied. Even when the averaging is theoretically sound, the prediction of macroscopic properties is often difficult because of the complex structure of rock. In any case, with empirical, approximate, or exact formulae for the transport coefficients and other effective properties, the results of a given phenomenon in a porous medium can be analyzed with the macroscopic theory.

Past theoretical attempts to derive macroscopic transport coefficients from the microstructure of the rock entailed a simplified representation of the pore space, often as a bundle of capillary tubes(Scheidegger, 1974). In this model, the capillaries were initially treated as parallel and then, later, as randomly oriented. These model are relatively simple, easy to use, and sufficiently accurate, provided that the relevant parameters are determined experimentally and the interconnectivity of the pore space does not play a major role.

Having derived macroscopic equations and suitable effective transport properties, one has the classical description of the system as a continuum. We shall therefore refer to various models associated with this classical description as continuum models. These models have been widely applied because of their convenience and familiarity to the engineer. They do have some limitations, one of which was noted above in the discussion concerning scales and averaging. They are also not well suited for describing those phenomena in rock in which the connectivity of the pore space or a fluid phase plays a major role. Such models also break down if there are long-range correlations in the system.

The second class of models, the discrete models, are free of these limitations. These models have been advanced to describe phenomena at the microscopic level and have been extended in the last few years to describe various phenomena at he macroscopic level. Their main shortcoming, from a practical point of view, is the large computational effort required for a realistic discrete treatment of the system. They are particularly useful when the effect of the pore-space interconnectivity or long-range correlations is strong. The discrete models are mostly based on a network representations of the rock. The original idea of network representation of a pore space is rather old(Owen, 1952; Fatt, 1956), but it was only in the early eighties that systematic and rigorous procedures were developed (Mohanty, 1981; Lin and Cohen, 1982) to map, in principle, any disordered rock onto an equivalent random network of bonds and sites. Once this mapping is complete, one can study a given phenomenon in porous media in great detail.

However, only in the past fifteen years have ideas from the statistical physics of disordered media been applied to flow, dispersion, and displacement processes in porous rocks. These concepts include percolation theory (Stauffer and Aharony, 1992; Sahimi, 1993b), the natural language for describing connectivity effects, diffusion limited growth processes(Meakin, 1988), which describe fundamentally nonequilibrium growth processes, fractal concepts(Mandelbrot, 1982; Bunde and Havlin, 1991), which are the main tool for describing the self-similarity and self-affinity of the morphology of a system and the effect of long-range correlations, and universal scaling laws, which describe how and under what conditions the effective macroscopic properties of a system may be independent of its

microscopic details. It is most important to define relevant ideas and techniques from the statistical physics of disordered media and their applications to the processes of interest , and review the progress that has been made as a result of such applications, in particular, the important effect of the connectivity of the pores or fractures of the system on the phenomena of interest and point out how scaling and fractal concepts provide powerful tools for describing flow, dispersion, and displacement process in reservoir rocks.

In recent years, quit a number of discrete fracture network models have been developed to represent fracture flow. In general, the dimension, orientation and flow properties of each fracture is treated randomly and, by monte carlo simulations, realizations of a possible portion of the fractured medium with the same statistical properties as the observed ones are generated and analyzed.

To have any representativeness, such models must be three dimensional representation. But then, the size of the domain which can be represented in 3-D is very limited, because of computational constraints since the number of unknowns very rapidly becomes immense, as the size of the area is increased. One must therefore conceptually define the use that can be made of such calculations in predicting the flow in a large fractured rock mass. Three stochastic concepts which must be understood to arrive at the prediction of this large scale flow (in other words, to address the problem of the scale effect in fractured media) are as follows:

1. Connectivity of the fracture system. Simple criteria suggesting the existence of a large scale behaviour would be discussed on the percolation theory.

2. Stationarity of the fracture properties. Constraints imposed on modeling by the hypothesis of stationarity would be discussed as well as possible treatment of non stationary systems.

3. Ergodicity. This is a key issue, enabling us to pass from the spatial domain to the stochastic essemble of realization domain, and vice versa. Based on this issue, methods of calculating an equivalent continuous system as well as the variability within this continuum are discussed.

In this lecture, assessment of flow properties of fractured media would be discussed where the blocks(or matrix) between fractures are so low a permeability, compared to that of the fractured network, that they can be considered impervious. For a long time, hydrogeologists have studied semi-empirically the flow of fluids in single fractures and expressions linking hydraulic gradient and velocity in the fracture plane have been developed. How to move from a single fracture to a set of fractures is a major problem which has not yet received a complete answer.

One of the first points to consider is that of the existence of an "equivalent porous medium" (EPM) which behaves macroscopically as the fractured medium. This problem is generally tackled by using the concept of the representative elementary volume (REV) (Bear, 1972): it is generally assumed that if a large enough volume of fractured rock is considered,

which has enough intersecting fractures to "average" the directional flow along each fracture, an "EPM" can be defined at this scale i.e. the flow through the rock mass can be described by Darcy's law using a second order symmetric permeability tensor. Such a concept (i) only applies to the flow conditions where, for each individual fractures, the velocity head gradient relation is linear (which is not always the case; it depends on Reynold's number and the roughness in the fracture), and (ii) is by definition, approximate, i.e., for a given size of the REV, the anisotropic Darcy's law applies only within a predefined tolerance band. This concept is not sufficient to understand fracture flow; connectivity concepts must be introduced.

The second issue is that of determining the equivalent hydraulic conductivity of the EMP. There are two possible approaches that are used traditionally; one is based on geometry, the other on hydraulic test. In the geometrical approach each fracture of the medium is assumed of infinite extension, thus ensuring a perfect connectivity of the fracture network. The fractures are mapped (e.g. on an outcrop) to determine their aperture, direction, dip and density; it is usual, but not obligatory, to group the fractures into a finite number of classes of direction (e.g. 3 or 4). Assuming that the properties and density of the fractures remain the same everywhere, the hydraulic conductivity tensor of the EPM is calculated by geometrically adding up the directional hydraulic conductivity of each fracture (or family of fractures). It is generally agreed that the assumption of infinite extent for the fractures is a severe limitation and that the determination of the fracture aperture from outcrops is very unreliable.

In the hydraulic test approach one can try to determine the equivalent hydraulic aperture of each fracture (or average fracture aperture for a family of fractures) by performing an injection test (in a borehole with double packers) isolating one fracture. These equivalent hydraulic apertures are used in the "geometric' approach above. It is, however, very difficult to locate and isolate single fractures in order to conduct such test. Moreover a very large number of tests are required.

Another approach is to make injection test over long borehole sections and to determine directly either the local hydraulic conductivity (e.g. the classical lugeon test) or the global conductivity tensor from pressure measurements in adjacent packed sections of other wells (using an inverse technique). Both approach assume that the necessary size of the EPM is already reached at the scale of the test (length of section, or distance between boreholes). This assumption again is very strong. A third approach is to identify the hydraulic properties of a given fracture from the response of a pumping test. Assuming a given geometry of the fracture intersecting the well (e.g. horizontal, vertical..). ,), Gringarten (1982) has published type curves to determine its hydraulic property from drawdown measurements. This approach, used in the petroleum industry, only gives the local properties of a major fracture and does not assume that an EPM exists.

2.0 SANDIA WASTE-ISOLATION FLOW AND TRANSPORT MODEL FOR FRACTURED MEDIA(SWIFT III).

This Flow and Transport Model is a fully transient, three-dimensional model which solves the coupled equations for transport in geologic media. The processes included are : Fluid Flow, Heat transport, Dominant-species miscible displacement, Trace-species miscible displacement. The first three processes are coupled via fluid density and viscosity. Together they provide the velocity field on which the fourth process depends. The computer model described herein extends the capabilities of SWIFT(Reeves and Cranwell, 1981) to include fractured media.

2.1 APPLICATIONS OF SWIFT

Because the SWIFT model is general, it has many possible applications. They include, but are not limited to, the following:

1. Nuclear waste isolation in both fractured and unfractured formations
2. Injection of industrial wastes into saline aquifers
3. Heat storage in aquifers
4. In-situ solution mining
5. Migration of contaminants from landfills
6. Disposal of municipal wastes
7. Salt-water intrusion in coastal regions
8. Brine disposal from petroleum-storage facilities
9. Brine disposal as a byproduct of methane production from geo-pressured aquifers
10. Determination of aquifer transport parameters from well-test data

2.2 MATHEMATICAL IMPLEMENTATION

The SWIFT II model is designed to simulate flow and transport processes in both singly and doubly porous media. The analyst designates the fractured regions of the system to which dual porosity is to be applied. In those particular regions two sets of equations are solved, one for the fracture processes and the other for the matrix processes. The fracture-porosity equations describing flow and transport for the fractured regions are identical to the singly-porosity equations for the nonfractured zone, except for sink terms giving the losses to the matrix. Consequently, one general set of equations which applies to both zones is presented, which will be called the global set of equations. The matrix-porosity equations for the fractured zone differ somewhat from their global counterparts. Therefore, a separate set of equations is presented which will be called the local set of equations. As was mentioned in the introduction, a variable-density formulation is used throughout. Density (and viscosity, porosity and enthalpy) is taken to depend relatively heavily on pressure, temperature and brine concentration, but not on radionuclide concentrations. For this reason, the flow, heat, and brine equations are termed the primary equations.

A steady-state solution option is provided for the global primary equations with two qualifications. First, it is assumed that heat-transport is basically a transient process.

Certainly, this is true for high-level nuclear waste repositories, a dominant application for the code. Thus, heat transport, like radionuclide transport, is not included in the steady-state option. Secondly, it is assumed that matrix processes are negligible at steady-state. Consequently, the state equations for the matrix porosity are not solved for the steady-state option. Of course, the code will permit transient solution of radionuclide transport (with or without dual porosity) in conjunction with steady-state solution of the primary equations since this is perceived as a very desirable simulation procedure.

2.2.1 The Global Transient-state Equations for Flow

The transport equations are obtained by combining the appropriate continuity and constitutive relations and have been presented by several authors, including Cooper(1966), Reddell and Sunada (1970), Bear(1979), and Aziz and Settari(2979). Sink terms are included for fractured zones in which losses to the rock matrix are significant. The resulting relation for flow may be stated as follows:

$-\nabla.(\rho u)$	$-\quad q$	$-\quad q_w$
convection	production	sink/source

$+\ R_C$	$-\quad \Gamma_w$	$= \frac{\partial}{\partial t}(\varnothing\rho)$
salt dissolution	loss to matrix	

Several quantities in Equation require further definition in terms of the basic parameters.

Darcy flux :

$$u = -(k/\mu).(\nabla p - \frac{\rho g}{g_c}\nabla z)$$

Porosity :

$$\varnothing = \varnothing_o\,[1+C_R\,(p-p_o)]$$

Fluid density:

$$\rho = \rho_o[1+C_w(p-p_o)- C_T(T-T_o)+ C_C C^{\wedge}]$$

Fluid viscosity:

$$\mu = \mu_R\,(C^{\wedge})\exp[B(C^{\wedge})(T^{-1}- T_R^{-1})]$$

Where parameter C_C is defined in terms of an input density range(ρ_1 - ρ_N) and the reference density ρ_o:

$$C_C = (\rho_1 - \rho_N)/\rho_o$$

2.2.2 The Global Steady-state Equations for Flow

In safety evaluations for nuclear-waste repositories, quite often the time frame of interest may extend over many thousands of years. Typically, the assumption of time-invariant flow and brine conditions is justified in such cases due to the lack of specific data for such a long period of time. For the fluid flow, the overall effect of transient rainfall boundary conditions may have a minor effect on radionuclide transport. Duguid and Reeves [1976] have shown this for a combined saturated-unsaturated simulation of tritium transport averaged over a period of only one month. Two steady-state options have been included. The first option permits solution of the time-independent flow equation:

Fluid (stead-state):

$$\underset{\text{convection}}{-\nabla.(\rho u)} \; \underset{\text{production}}{-\; q} \; \underset{\text{sink/source}}{-\; q_w} \; \underset{\text{salt dissolution}}{+\; RC'} = 0$$

In both options the accumulation and the matrix-loss term are set to zero. For the steady-state fluid-flow option, however, the salt dissolution term is also set to zero. The second option permits a coupled time-independent solution for fluid flow.

2.2.3 Local Transient-state Equations for Flow Within the Rock Matrix

The flow and transport processes occurring within the rock matrix are conceptualized as being one-dimensional in a lateral direction relative to the movement in the fractures. Thus, it is assumed that the fractures provide the only means for large-scale movements through the entire system while the matrix provides most of the storage of the system. The approach used here to treat the fracture matrix system is similar to that used by Bear and Braester[1972],Huyakorn et al.[1983], Pruess and Narasimhan [1982], Tank et al. [1981], Grisak and Pickens[1980], Streltsova-Adams[1978], and rasmuson et al.[1982].

Conservation equations used here for the matrix are very similar to those presented in Section for global transient equation. They are as follows

$$\underset{\text{conduction}}{-\nabla.(\rho' \underline{u}')} \; \underset{\text{gain from fracture}}{+\; r'_w} = \underset{\text{accumulation}}{\frac{\partial}{\partial t}(\varnothing' \rho')}$$

It is anticipated that either parallel fractures or intersecting sets of parallel fractures will be treated. A Prismatic block is invoked in the numerical solution, and for the latter, either prismatic or spherical blocks may be used to approximate the actual matrix geometry. Thus, either one-dimensional Cartesian or spherical geometry may be used for the local matrix equations. In either case, he interior boundary is assumed to be a reflective no flow

boundary. The fracture/matrix interface provides a source r' which is identical to the fracture loss r to within a geometrical scaling factor. The flow equation is coupled by following relations for

Darcy flux :

$$u' = -(k'/\mu')vp'$$

Porosity :

$$\varnothing' = \varnothing_o' [1+C_R'(p'-p_o)]$$

Fluid density:

$$\rho' = \rho_o[1+C_W'(p'-p_o)- C_T(T'-T_o)+C_CC']$$

Fluid viscosity:

$$\mu = \mu_R (C^{\hat{}})\exp[B(C^{\hat{}})((T')^{-1}- T_R^{-1})]$$

Parameter C_c is assumed to have negligible importance in determining Darcy velocities within the matrix.

3.0 NUMERICAL SIMULATION OF FLUID FLOW IN A TWO-DIMENSIONAL DISCRETE FRACTURE NETWORK:Program NETFLOW.

The two-dimensional fracture flow theory used here is very similar to the theory of fluid flow in pipe networks. Typically a pipe network problem has a predetermined general structure and numerical methods are used for sensitivity analysis and design optimization. Since the same problem structure is repeated many times during a study, it is profitable to optimize right at the beginning the structure of the matrices to be solved numerically. Linear theory and graph theory methods are commonly used for these types of pipe network analysis (Kesavan and Chandrashekar, 1972; Isaacs and Mills, 1980).

The numerical model presented here is two-dimensional, and the rock matrix is assumed impermeable. A node conductance matrix is first set up by applying the mass balance constraint to each node in the network (i.e., the sum of flow rates at any free node must equal zero). Since this computer code is intended to be applied to actual field problems, it must simulate the fractures in a slice of rock large enough to be considered statistically homogeneous with respect to the fracture system. Moreover, the random fracture generation process produces a numerical matrix that is very dispersed in structure. By renumbering systematically all the nodes and by using a variable-bandwidth storage scheme, the code presented here reduces considerably the computer storage requirement for a large sparse matrix. A direct method of solution based on the Choleski algorithm is then used to solve the set of equations in a manner that is efficient in computing time.

3.1 MODEL FORMULATION

For steady-state laminar flow of an incompressible, viscous fluid between two smooth parallel plates, the analytical solution of the Navier-Stokes equation yields the following relationship for volume flow rate per unit width (e.g., Huitt, 1956):

$$q = - \frac{W^3 \gamma}{12\mu} \times \frac{\Delta\psi}{\Delta X}$$

Where W is the plate separation [L], γ is the weight density of the fluid [F/L3], μ is the dynamic viscosity [FT/L2]. x is the distance along the plates [L], and ψ is the hydraulic head [L]. In the solution of network flow problems, it is often convenient to define the conductance of the fluid conduit of length l as:

$$e = \frac{W^3 \gamma}{12 \mu l} \qquad [L^2T^{-1}]$$

i.e., the hydraulic conductivity multiplied by the cross-section and divided by the length.

Using Figure (to be supplied in the class) as an example, the flow rate at node 1 is expressed by:

$$e_a(\psi_2 - \psi_1) = -q_a$$

In this convention, flow into the system is positive and flow out is negative. For the internal node 2, the mass balance constraint requires that sum of flow rates into and out of that node equals.

$$e_a(\psi_1 - \psi_2) + e_b(\psi_3 - \psi_2) + e_d(\psi_4 - \psi_2) = 0$$

The numerous methods of simultaneously solving systems of equations like above can be divided in direct methods and iterative methods. Direct methods are generally faster but require larger computer computer memory than iterative methods. In the code NETFLO, the matrix and vectors of above Equation are rearranged and partitioned according to the degree of freedom of the nodes:

The matrix equation can be summarized by

$$\begin{matrix} E_{ff} & E_{fc} \\ E_{cf} & E_{cc} \end{matrix} \times \begin{matrix} \phi_f \\ \phi_c \end{matrix} = \begin{matrix} Q_f \\ Q_c \end{matrix}$$

This corresponds to two matrix equations:

$$E_{ff\phi f} + E_{fc}\phi_c = Q_f$$

and

$$E_{cf\phi f} + E_{cc\phi c} = Q_c$$

These equations can be used to compute the unknown head values (ϕ_f) and can give the flow rate at the boundary nodes (Q_c). The approach taken in program NETFLO is to compute the head at all the free nodes then to compute the flow rate in all the segments individually . Rearranging gives:

$$E_{ff\phi f} = Q_f - E_{fc\phi c} = Q_f^1$$

After setup of the augmented flux vector Q_f^1 , program NETFLO solves for ϕ_f using the Choleski algorithm .