
A 3-Dimensional Computer Model to Simulate Fluid Flow and Contaminant Transport Through a Rock Fracture System

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A 3-Dimensional Computer Model to Simulate Fluid Flow and Contaminant Transport Through a Rock Fracture System

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ABSTRACT

A 3-dimensional fracture generating scheme is presented which can be used to simulate water flow and contaminant (solute) transport through fracture system of a rock. It is presently limited to water saturated conditions, zero permeability for the rock matrix, and steady state water flow, but allows for transient solute transport. The scheme creates finite planar plates of uniform thickness which represent fractures in 3-dimensional space. A given fracture (plate) has the following descriptors: center location, orientation, shape, areal extent and aperture. Each parameter can be described by an appropriate probability distribution. Individual fractures are generated to form an assemblage of a certain fracture density. All fracture intersections and boundary/fracture intersections are determined and deadend fractures are eliminated. Flow through the fracture assemblage is considered laminar and described by Poiseuille's law. The principle of mass conservation at each intersection is used to develop the global matrix equation, which is solved subject to specified boundary conditions to yield the head and flow distribution at each intersection. Solute transport is considered to be advective between intersections with complete mixing at each intersection. Solutes added to the flow system can be explicitly followed and concentration vs. time relationships can be determined anywhere in the system. Some examples are included.

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A 3-DIMENSIONAL COMPUTER MODEL TO SIMULATE FLUID FLOW
AND CONTAMINANT TRANSPORT THROUGH A ROCK FRACTURE SYSTEM

EXECUTIVE SUMMARY

A 3-dimensional fracture generating scheme has been developed to simulate fracture systems in a rock mass. Numerical experiments can be performed on the generated fracture system to examine its hydraulic and contaminant transport characteristics. The computer code is now limited to a fracture system filled with a single fluid, to an impermeable medium between fractures, and to steady state flow conditions. The code is being extended to simulate unsaturated fractured rock and where the rock matrix has a finite permeability.

The major purpose of performing numerical experiments on artificially generated fracture networks is to improve the understanding of flow and contaminant movement through a fractured medium, such as that surrounding a waste repository. Because the geometry of the fracture network determines flow paths and relative travel times for contaminants, recreating these networks with a computer allows the analysis of the isolation capabilities of a specified geologic environment. These types of analyses can also provide assessment of various measurement techniques in relation to effective sample size of measurement. When used in conjunction with a field testing program, the model is useful for planning, performance and analysis of experimental results.

Discrete fracture generators described in the literature are limited to 2-dimensional systems. In such a network, a fracture is represented by a straight line of infinite extent in the third dimension. A major criticism of these 2-dimensional models is the constraint of flow in only two dimensions. The problems associated with using a 2-dimensional model are even more severe when simulating contaminant transport. In some cases, the regional flow system can be viewed as 1-dimensional or 2-dimensional, but the movement of contaminants through a porous medium is always 3-dimensional. This is demonstrated by the advection-dispersion phenomena. Any study of dispersion in a 3-dimensional fracture system using a 2-dimensional model will lead to moot results. Thus the development of a 3-dimensional fracture network generator is motivated by the need to more accurately model contaminant flow.

The formulated fracture generator scheme creates finite planar fractures in 3-dimensional space. In this model, a fracture is simulated by a plate of uniform thickness. Thus the thickness of the plate represents the apparent hydraulic aperture of a fracture. To define a finite plate (or fracture) in 3-dimensional space, the following geometric input parameters are required: location, orientation, shape, areal extent and thickness. In addition, the density of the fractures (the number of fractures per unit volume) is required to complete the network. Each of these parameters can be described by an appropriate probability distribution. These

probability distributions can be independent of each other or correlated. Thus one realization of a network is the assemblage of a certain number of randomly generated finite plates of which the geometric parameters describing each individual plate are sampled from its respective probability distribution.

To generate a discrete network, a global coordinate system is first defined. The location parameters specify the center of the plate in global coordinates. Two angles are required to specify the orientation of a surface in the global, 3-dimensional space. The shape of each fracture can be circular, rectangular, elliptical, or any other computable shape provided that the boundaries can be expressed by analytic functions. Areal extent is given by the length scale associated with the specific shape, e.g., a radius defines a circular disk. Within each plate, a local 2-dimensional coordinate system is established. One additional angle is required to denote the rotation of the local 2-dimensional coordinate system when a non-circular shaped fracture is used in the network.

Once the desired number of plates have been generated, the program will define all intersections and delete isolated fractures (those that do not connect to any boundary or other fractures). The intersection of two finite surfaces is a finite line. Because the flow takes place from fracture to fracture through the intersections, a fracture must be intersected by at least two others to become conductive. Thus dead-end fractures (those only intersecting one other fracture) also need to be identified.

This program can also be used to isolate an arbitrarily oriented sub-volume of sample at any location within the global network. For this isolated sample, all information regarding boundary and interior intersections is explicitly defined. This procedure simulates the sampling process in actual field conditions.

Once a realization of the fracture network has been formed and a sub-volume of sample has been isolated and defined, experiments can be performed on the sample to study flow and transport characteristics.

Although the simulated fracture network is in 3-dimensional space, flow within each fracture is considered 2-dimensional in the local coordinate system defined for each individual fracture. The actual flow behavior between intersections within each fracture is an area of research in itself. For now a simplified flow condition is used. This restriction can be relaxed to incorporate a more complicated flow analysis within each fracture when a procedure becomes available.

The fractures are idealized as smooth parallel plates, and fluid flow in the fracture is assumed laminar and described by Poiseuille's law. Thus, the hydraulic conductivity and the flow region between all intersections for each fracture can be determined. This simplified treatment allows the representation of a line intersection by a nodal point at its center. The principle of mass conservation, which ensures the net flux through each internal intersection (or nodal point) is zero, is used to assemble the global matrix equation. When proper boundary conditions are imposed on the external surfaces, the

global matrix equation is solved and the pressure (or head) distribution within the sample is defined.

Once the flow domain is defined, the analysis is carried one step further to study mass transport characteristics. Mass transport is assumed advective between intersections with complete mixing at each intersection. The flow analysis provides a complete set of information in terms of velocity, travel time and flux between every two intersections. Thus, at any nodal point, the tree-type network structure of the inflow is defined. This enables the examination of all possible flow routes in the network.

A slug (either continuous or finite in time) of tracer introduced into the system can be explicitly followed. This technique, which is different from conventional particle-tracking techniques, provides an explicit concentration vs. time relationship anywhere in the system without any probabilistic influence or limitation due to space/time discretization.

Several experiments have been designed to study the scale effects and flow/transport properties of a fracture network. The results of these experiments are not included in this report but will be presented in technical papers. The purpose of this report is to present the details of the computer code for the fracture generator scheme and for some examples of numerical experiments using generated fracture systems.

1. INTRODUCTION

A 3-dimensional fracture generator scheme has been formulated and used to study fluid flow and contaminant transport characteristics of rock fracture systems. In this paper, the detailed development of the computer code and examples of flow and mass transport numerical experiments are presented.

Examination of flow and contaminant transport through the use of artificially-generated fracture systems provides insight and improved understanding of these processes in real fracture systems. Also, such examinations can provide useful information on sample size and measurement techniques for field assessments. With sufficient and reliable fracture data on a real rock system, the real system may be adequately simulated to yield useful estimates of contaminant travel times and release rates to a location at some distance from a given source.

Discrete fracture generators described in the literature are limited to 2-dimensions and use oversimplifying assumptions. For a 2-dimensional fracture network generator, a fracture is represented by a straight line which is of infinite extent in the third dimension. This assumption results in a no flow condition in the third direction which is unrealistic for real fracture systems. For problems involving the simulation of mass transport, a 2-dimensional network

model creates even more severe departures from expected values. While pressure heads might be adequately modelled using a 1- or 2-dimensional network, the dimensionality of contaminant transport models can not be so reduced. It is a moot point whether a 2-dimensional representation of dispersion in a discrete fracture system will yield accurate results. To understand transport mechanisms, there exists an obvious need for the ability to model solute transport in 3-dimensional space.

In general, the code presented here generates planar fractures located in a 3-dimensional region. The generated fracture system is referred to as a global fracture network. A subvolume sample can be isolated from the global network and subjected to pre-designed fluid flow and mass transport experiments. Results of these experiments can then be used in the interpretation of the hydraulic and mass transport characteristics of the fracture network.

The main logic of program development can be divided into four categories: 1) generation of the fracture network; 2) isolation of the study sample; 3) design and performance of flow experiments; and 4) design and performance of transport experiments.

The code is written in standard ANSI FORTRAN-77 and has been used on the CDC Cyber-175 and 6600/7600 series computer systems. A program listing is presented in Appendix A.

2. CODE DEVELOPMENT

The 3-D fracture generator and test codes consist of an assembly of several major driving subprograms to perform different tasks. The major functions of these driving subprograms are listed in Figure 1.

To minimize storage requirements, subroutines 1 - 8 are called under one main program to set up the fracture network and perform the hydraulic tests, while subroutines 9-10 are called under a second main program to perform the mass transport experiments. A temporary data file is used to transfer information from the first to the second program.

2.1 Generation of Fracture Network

In the fracture generator, a fracture is represented by a 2-dimensional finite plate of a fixed thickness. A simulated fracture network is a collection of a selected number of individual finite plates in a 3-dimensional volume. The spaces bounded by these fracture planes are considered to be an impermeable rock mass.

To define each finite planar fracture in the 3-dimensional volume, the following geometric parameters are required: 1) center location, 2) orientation, 3) shape and areal extent, and 4) aperture. Figure 2 illustrates how a fracture is defined in the global region. In Figure 2, the center of the fracture is designated by point R_0 having a

<u>Major Subroutine</u>	<u>Function</u>
1. INPFRCT	Generate geometric parameters for each fracture plane.
2. SUBFRCT	Find line intersections between fractures.
3. INPCUT	Generate geometric parameters for boundary surfaces of rectangular block of samples.
4. SUBCUT	Find line intersections between fracture and boundary surface.
5. SUBDEAD	Delete dead end fractures from the network.
6. SUBBOND	Assign pressure boundary conditions on boundary surfaces.
7. SUBMTRX	Assemble the global matrix equation and find the head distribution.
8. SUBMSBL	Calculate fluxes across boundary surfaces.
9. FLOWNET	Create flow network to be used in TRACER subroutine.
10. TRACER	Generate breakthrough curves for mass transport.

Figure 1. Code subroutines and designated functions.

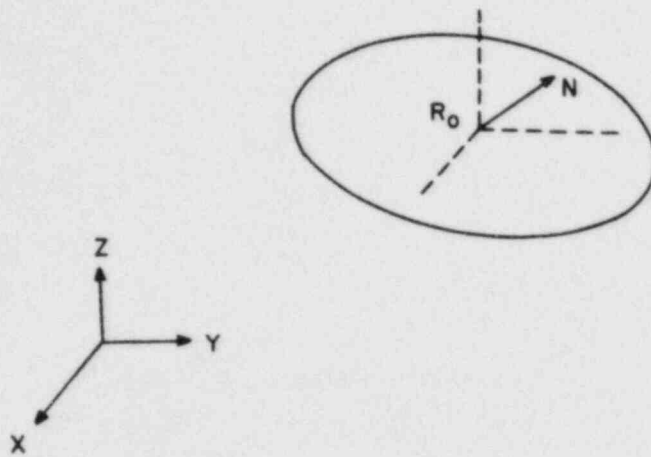


Figure 2. A finite fracture in 3-dimensional space where R_0 is the center of the fracture and R_0N is the normal vector.

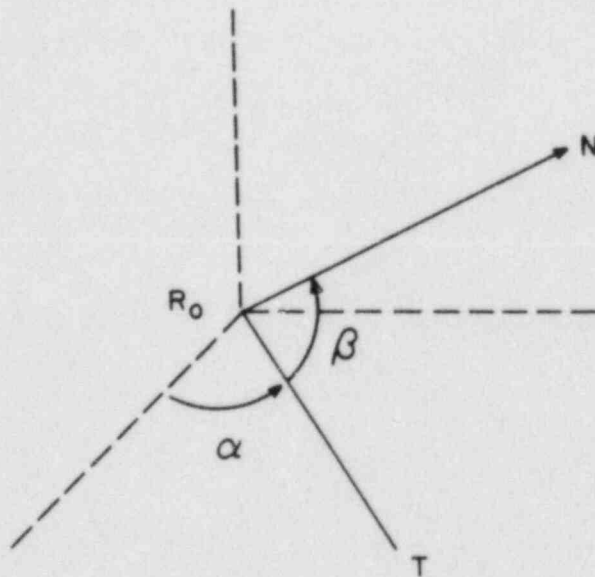


Figure 3. The definition of two angles of rotation, α and β , used in specifying the orientation of the normal vector.

global coordinate of (X_0, Y_0, Z_0) . The orientation of the plane is defined by two angles of rotation, α and β (Figure 3). In fact, α and β are used in specifying the orientation of a vector located at point R_0 and normal to the fracture plane. α is the horizontal angle measured counterclockwise from the +X axis. β is the elevation angle in the plane with R_0T and measured from the XY plane. The equation of an infinite plane encompassing the finite fracture is:

$$aX + bY + cZ = aX_0 + bY_0 + cZ_0 \quad (1)$$

where

$$a = \cos \beta \cos \alpha$$

$$b = \cos \beta \sin \alpha$$

$$c = \sin \beta.$$

To define a fixed shaped finite region in an infinite plane, a local coordinate system is needed (Figure 4). This local coordinate system is 2-dimensional with the origin at the center of the fracture. The local coordinate system (x', y') is selected such that its axes coincide with the characteristic axes of a particular shaped fracture. The local coordinate system is specific to each fracture plane, and has to be defined for every fracture. One additional angle, γ , is required to define the orientation of the local (x', y') coordinates. This additional angle is not necessary when a circular shaped fracture is generated due to its axisymmetrical nature.

In Figure 4, since R_0N is a normal vector of the fracture plane, a vector origin at R_0 having a horizontal angle of α and vertical angle of $\beta - 90^\circ$ must lie on the fracture plane. Let this vector be denoted as R_0X . This temporary vector R_0X is used as a reference to define the orientation of a local (x', y') system. The +x' axis of the local x', y' coordinate system is rotated by γ angle measured counterclockwise from the R_0X temporary axis. The transformation between the global network generating coordinate system (X, Y, Z) and the local fracture based coordinate system (x', y') is given below:

$$\begin{Bmatrix} X \\ Y \\ Z \end{Bmatrix} = \begin{Bmatrix} X_0 \\ Y_0 \\ Z_0 \end{Bmatrix} + [A] [B] \begin{Bmatrix} x' \\ y' \end{Bmatrix} \quad (2)$$

where

$$[A] = \begin{bmatrix} \sin \beta \cos \alpha & -\sin \alpha \\ \sin \beta \sin \alpha & \cos \alpha \\ -\cos \beta & 0 \end{bmatrix} \quad (2a)$$

and

$$[B] = \begin{bmatrix} \cos \gamma & -\sin \gamma \\ \sin \gamma & \cos \gamma \end{bmatrix} \quad (2b)$$

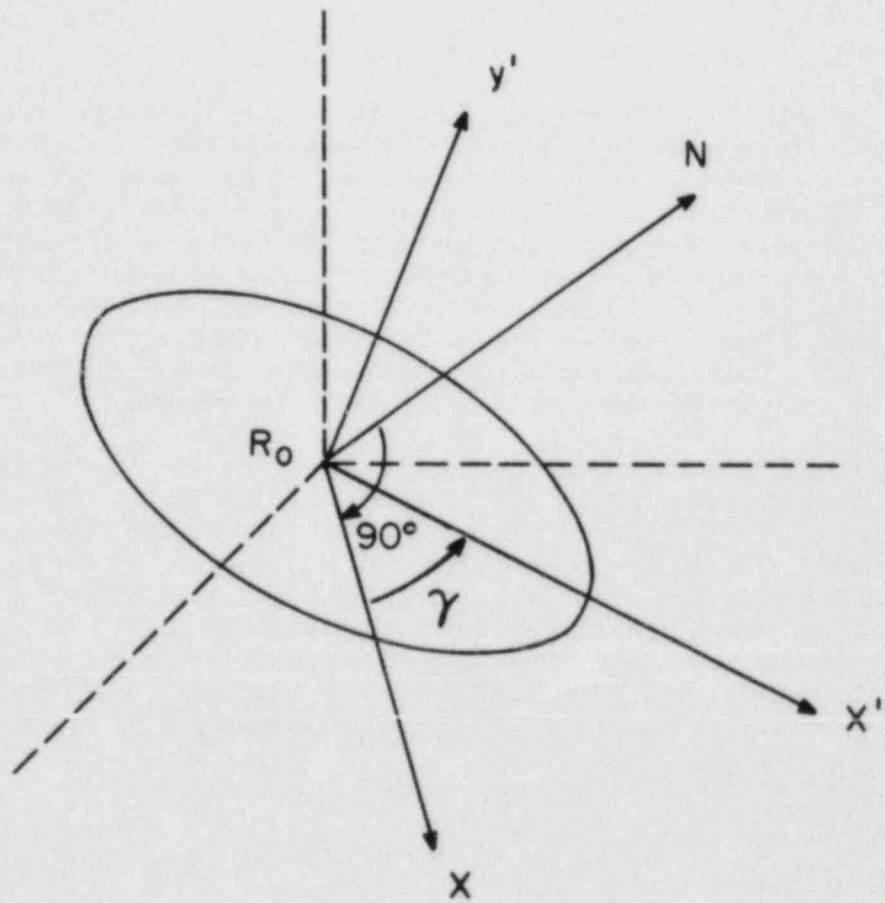


Figure 4. The definition on an in-plane rotational angle, γ , used in specifying the orientation of a local coordination system (x' , y')

Once the local coordinate system is established, the bounded regions of some regular shapes can be defined easily. For example, equation 3 defines the region of an ellipse and equation 4 defines the region of a rectangle.

$$\frac{(x')^2}{r_1^2} + \frac{(y')^2}{r_2^2} \leq 1 \quad (3)$$

$$x' \leq r_1 \text{ and } y' \leq r_2. \quad (4)$$

Note that a circle and a square are special cases of an ellipse and a rectangle.

The areal extent of a particular shaped fracture is defined by characteristic lengths associated with that shape. The r_1 and r_2 are the characteristic lengths for an ellipse and a rectangle but they bear different meanings for different shapes. The present computer program can handle elliptical and rectangular shaped fractures. Extension to other shapes are straightforward as long as the boundaries can be expressed by analytical functions.

A single value is assigned to each fracture to represent the aperture. Although the aperture is variable in a natural setting, this single value represents an averaged equivalent hydraulic aperture.

Field observations have suggested that some geometric parameters may follow certain statistical distributions. Subroutine INPFRACT uses random number generators of different distributions to create a fracture network. It has four random number generating subroutines to create normal, log-normal, uniform, and exponential distributions.

Once a set of individual fractures is generated, subroutine SUPFRACT is called to find the line intersects among the fractures. The procedure of finding the intersecting finite line segments between two finite planes consists of two steps: 1) find the intersecting line between two infinite planes containing these two finite fractures, and 2) truncate the infinite line to a finite segment such that it is common to both finite fractures.

Let equation 5 be the equation of an infinite plane containing finite fracture 1:

$$a_1X + b_1Y + c_1Z = d_1 \quad (5)$$

Similarly, equation 6 describes a second plane containing fracture 2:

$$a_2X + b_2Y + c_2Z = d_2 \quad (6)$$

The equation of a line, L_{12} , common to both planes is given as:

$$\bar{R} = \bar{R}_1 t + \bar{R}_2 \quad (7)$$

or

$$\begin{pmatrix} X \\ Y \\ Z \end{pmatrix} = \begin{pmatrix} X_1 \\ Y_1 \\ Z_1 \end{pmatrix} t + \begin{pmatrix} X_2 \\ Y_2 \\ Z_2 \end{pmatrix} \quad (7a)$$

where t is a scalar.

If $e = c_2 b_1 - c_1 b_2 \neq 0$, then

$$\bar{R}_1 = \begin{pmatrix} X_1 \\ Y_1 \\ Z_1 \end{pmatrix} = \begin{pmatrix} 1 \\ (a_2 c_1 - a_1 c_2)/e \\ (b_2 a_1 - b_1 a_2)/e \end{pmatrix} \quad (8a)$$

and

$$\bar{R}_2 = \begin{pmatrix} X_2 \\ Y_2 \\ Z_2 \end{pmatrix} = \begin{pmatrix} 0 \\ (c_2 d_1 - c_1 d_2)/e \\ (d_2 b_1 - d_1 b_2)/e \end{pmatrix} \quad (8b)$$

or if $e = b_2 a_1 - a_2 b_1 \neq 0$.

$$\bar{R} = \begin{pmatrix} X_1 \\ Y_1 \\ Z_1 \end{pmatrix} = \begin{pmatrix} (c_2 b_1 - c_1 b_2)/e \\ (a_2 c_1 - a_1 c_2)/e \\ 1 \end{pmatrix} \quad (9a)$$

$$\bar{R} = \begin{pmatrix} X_2 \\ Y_3 \\ Z_2 \end{pmatrix} = \begin{pmatrix} (b_2 d_1 - d_2 b_1)/e \\ (d_2 a_1 - d_1 a_2)/e \\ 0 \end{pmatrix} \quad (9b)$$

or if $e = a_2 c_1 - a_1 c_2 \neq 0$

$$\bar{R}_1 = \begin{pmatrix} X_1 \\ Y_1 \\ Z_1 \end{pmatrix} = \begin{pmatrix} (b_2 a_1 - b_1 a_2)/e \\ 1 \\ (c_2 b_1 - c_1 b_2)/e \end{pmatrix} \quad (10a)$$

$$\bar{R}_2 = \begin{Bmatrix} X_2 \\ Y_2 \\ Z_2 \end{Bmatrix} = \begin{Bmatrix} (a_2d_1 - a_1d_2)/e \\ 0 \\ (d_2c_1 - d_1c_2)/e \end{Bmatrix} \quad (10b)$$

Once R_1 and R_2 are found, the intersecting line L_{12} can be represented by two distinct points on the line by choosing two different values of t . Procedures to truncate this line to a finite line segment common to both fractures are:

- 1) Transform T_1 and T_2 [Assume that points T_1 and T_2 are two distinct points on L_{12}], to local coordinates defined on fracture 1 and find the two boundary point intersects, P_{11} and P_{12} , between the line L_{12} and the boundary of fracture 1, if they exist.
- 2) Similar to step 1, find the two boundary points, P_{21} and P_{22} , representing the intersection between line L_{12} and fracture 2. If line P_{12} does not intersect either one of the two fracture boundaries, then the two fractures do not share a common line (Figures 5a and 5b).
- 3) If line L_{12} intersects both fractures, then points P_{11} and P_{12} are checked to see if they are contained within the boundary of fracture 2. Similarly, points P_{12} and P_{22} are checked on fracture 1. If the two fractures share a common line segment, then two of the four points should be common to both fracture regions (Figures 6a and 6b). These two points are two end points of the finite line segment.

A complete fracture network is defined after all fracture intersections are determined.

2.2 Isolation of Samples

After the creation of a global fracture network, a subvolume contained inside the global region can be isolated.

Subroutines INPCUT and SUPCUT are designed to perform the task of sample isolation. A rectangular block of sample is defined by its center location (COR0), the rotation angles (COAL) and its size (COSZ). A sample coordinate system is defined at the center of the sample with an orientation that each sample boundary is perpendicular to one of the new coordinate axes. The rotation angles (COAL) are horizontal and vertical angles of rotation between the new X_s -axis of the sample coordinate system and the global X_g -axis (Figure 7).

Within an isolated sample, the finite line segments between fractures are further truncated to the boundary of the sample, these are called internal intersects. The line intersections between rectangular boundary surfaces and fracture planes are called external intersects. These internal and external intersects are expressed in sample

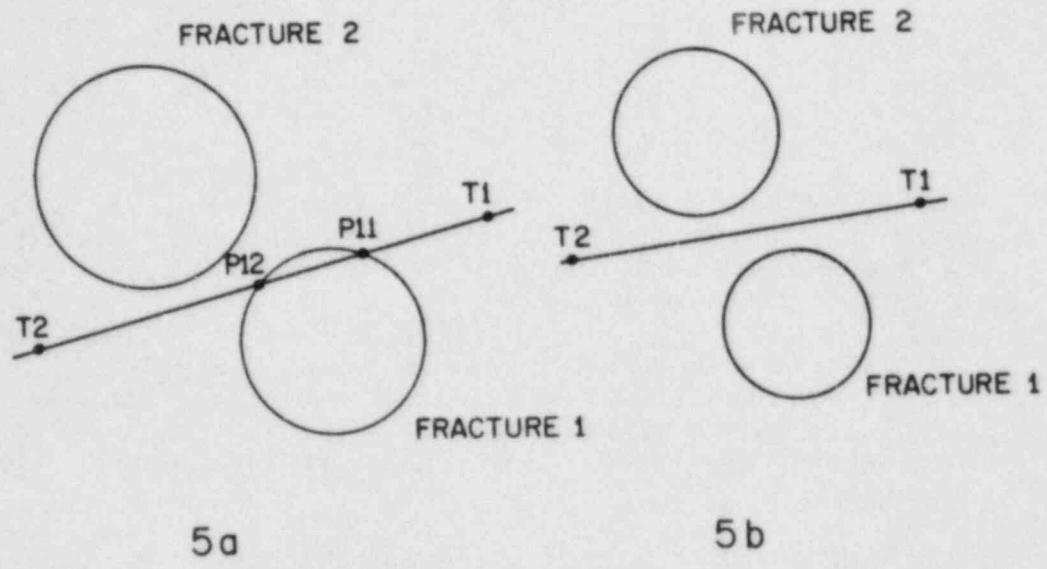


Figure 5. The intersecting line L_{12} (represented by two distinct points T_1 and T_2) between two infinite planes encompassing Fractures 1 and 2 intersects: (a) only one fracture; and (b) neither fracture.

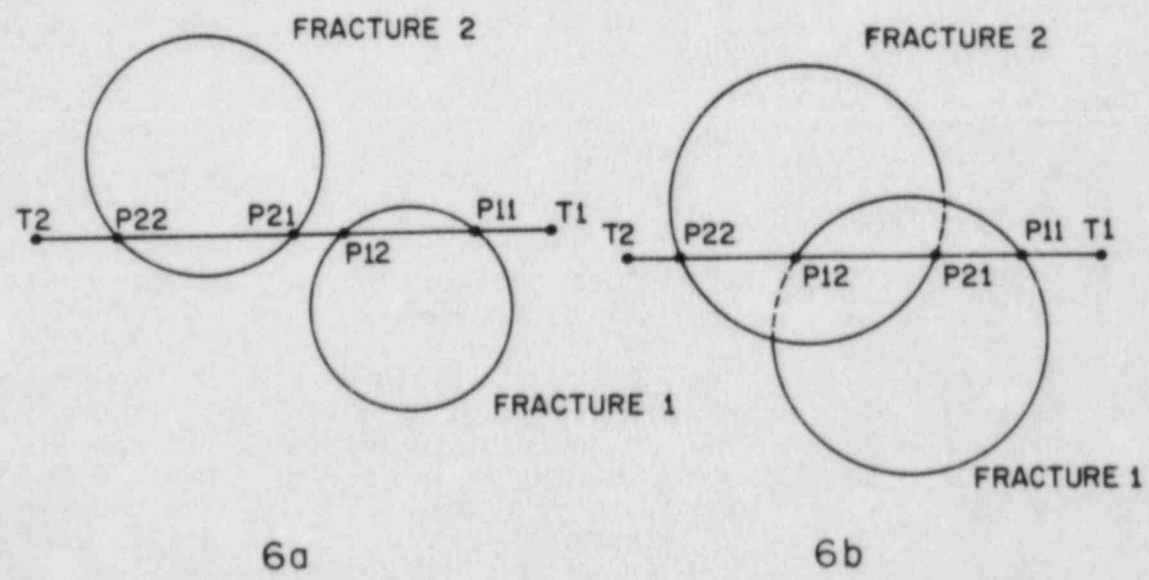


Figure 6. The intersecting line L_{12} (represented by two distinct points T_1 and T_2) between two infinite planes encompassing Fractures 1 and 2, intersecting both fractures, but (a) does not have a finite section common to both fractures; and (b) has a common segment.

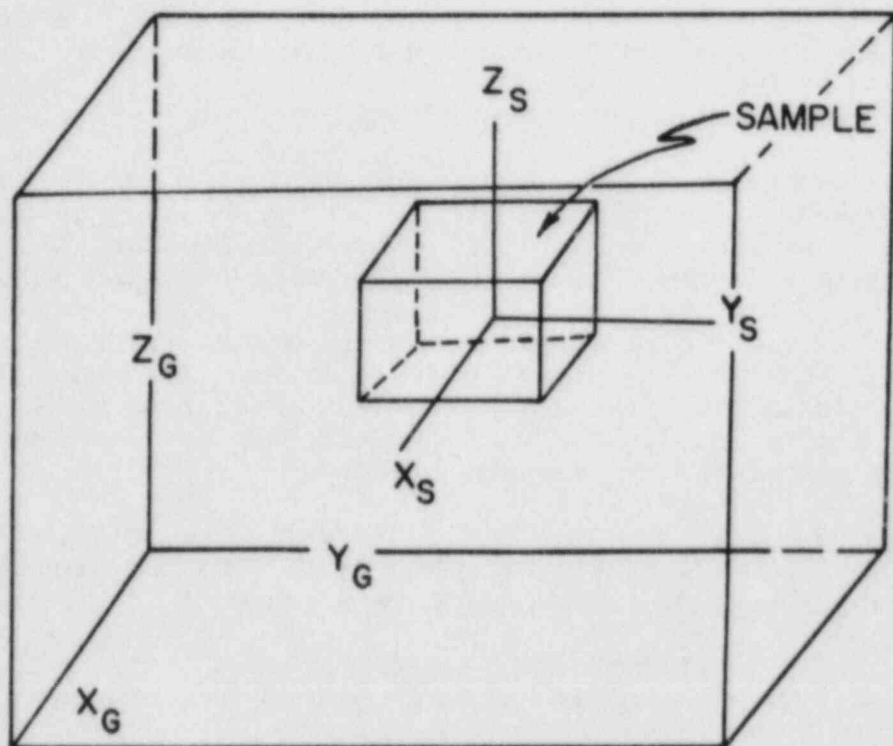


Figure 7. The global fracture network generating coordinate system (X_G, Y_G, Z_G) and the sample coordinate system (X_S, Y_S, Z_S) .

coordinates and the transformation from the global coordinate system to the sample coordinate system is given below:

$$\begin{pmatrix} X_s \\ Y_s \\ Z_s \end{pmatrix} = \begin{bmatrix} \cos \alpha \cos \beta & \sin \alpha \cos \beta & \sin \beta \\ -\sin \alpha & \cos \alpha & 0 \\ -\cos \alpha \sin \beta & -\sin \alpha \sin \beta & \cos \beta \end{bmatrix} \begin{pmatrix} X_g - X_o \\ Y_g - Y_o \\ Z_g - Z_o \end{pmatrix} \quad (11)$$

where subscripts s and g, denote sample, and global coordinate systems, α and β are horizontal and vertical angles of rotation for the $+X_s$ axis of the sample coordinate system measured from the $+X_g$ axis of the global coordinate system. X_o , Y_o and Z_o are the center of the sample expressed in the global coordinate system.

2.3 Design of Flow Experiment

The formulation of flow experiments consists of the following steps: 1) assemble the flow network; 2) assign boundary conditions; 3) solve the matrix equation to obtain the pressure/hydraulic head distribution; and 4) calculate fluxes across boundary surfaces.

The flow network is assembled from individual fractures where flow takes place from one intersection to another. The actual flow pattern in an individual fracture is not well understood and is an area of research in itself. The simplification made in the present code can be relaxed when more knowledge is gained.

Figure 8 shows a fracture being intersected by two other fractures, having intersections A and B. To calculate the flow between A and B, the following simplified assumptions are used:

- 1) flow between A and B is laminar and uniform;
- 2) the pressure head along A and B is constant.

These assumptions allow us to simplify the representation of a finite line segment to a point at the center of the line and its length. The steady state flux from A to B, $F_{A,B}$, can then be calculated by:

$$F_{A,B} = \frac{gb^3}{12} \frac{L_A + L_B}{2} \frac{P_A + Z_A - P_B - Z_B}{D_{A,B}} \quad (12)$$

where ρ is fluid density, g is the gravitational constant, μ is dynamic viscosity, b is aperture, L_A and L_B are length of line segment A and B, P_A and P_B are pressure heads along A and B, Z_A and Z_B are elevation heads at the midpoints of A and B, $D_{A,B}$ is the distance between midpoints at A and B. Equation 12 can be simplified to:

$$\begin{aligned} F_{A,B} &= C_{A,B} (H_A - H_B) \\ &= C_{A,B} (P_A - P_B) + C_{A,B} (Z_A - Z_B) \\ &= C_{A,B} (P_A - P_B + C_{A,B,Z}) \end{aligned} \quad (13)$$

where $H_A = P_A + Z_A$, $H_B = P_B + Z_B$; and $C_{A,B,Z} = C_{A,B} (Z_A - Z_B)$.

The principle of mass conservation is used to assemble the global flow network from formulations between individual intersections. Figure 9 is used to illustrate a simple flow network and is used as an example to demonstrate the formation of the global network flow equations. In Figure 9, there are 4 fractures, forming a network of 3 internal intersections and 3 external intersections. The principle of mass conservation implies that: 1) the sum of all fluxes across all boundary surfaces must be zero; and 2) the sum of all fluxes through any internal intersection must be zero.

If F_j equals the total flux across the j th intersection, and $F_{i,j}$ is a component flux of F_j representing the flux from the i th intersection to the j th intersection. The following mass balance equations are obtained:

$$F_1 = F_{2,1} + F_{3,1} + F_{4,1} = 0 \quad (14a)$$

$$F_2 = F_{1,2} + F_{3,2} + F_{5,2} = 0 \quad (14b)$$

$$F_3 = F_{1,3} + F_{2,3} + F_{6,3} = 0 \quad (14c)$$

$$F_4 = F_{1,4} \quad (14d)$$

$$F_5 = F_{2,5} \quad (14e)$$

$$F_6 = F_{3,6} \quad (14f)$$

$$F_4 + F_5 + F_6 = 0 \quad (14g)$$

Expanding equation 14a, using the relationship given in equation 13, we obtain:

$$\begin{aligned} F_1 = & C_{2,1}(P_2 - P_1) + C_{2,1,Z} + C_{3,1}(P_3 - P_1) + C_{3,1,Z} \\ & + C_{4,1}(P_4 - P_1) + C_{4,1,Z} = 0 \end{aligned} \quad (15)$$

If the boundary pressure, (P_4), is known, the equation can be rearranged to contain all the known values on the right hand side:

$$\begin{aligned} & [-C_{2,1} - C_{3,1} - C_{4,1}]P_1 + C_{2,1}P_2 + C_{3,1}P_3 \\ & = -C_{2,1,Z} - C_{3,1,Z} - C_{4,1}P_4 - C_{4,1,Z} \end{aligned} \quad (16)$$

Equations 14b and 14c can be rewritten in the same fashion to obtain:

$$\begin{aligned} & C_{1,2}P_1 + (-C_{1,2} - C_{3,2} - C_{5,2})P_2 + C_{3,2}P_3 \\ & = -C_{1,2,Z} - C_{3,2,Z} - C_{5,2}P_5 - C_{5,2,Z} \end{aligned} \quad (17)$$

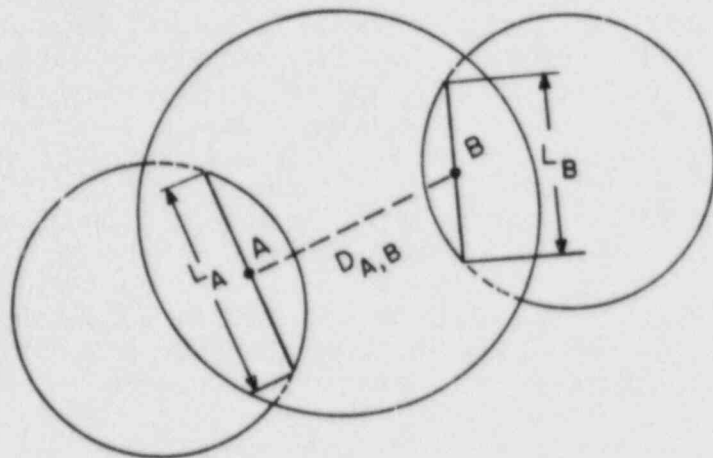


Figure 8. Diagram of one fracture intersected by two other fractures to illustrate the basic flow equation between fracture intersects.

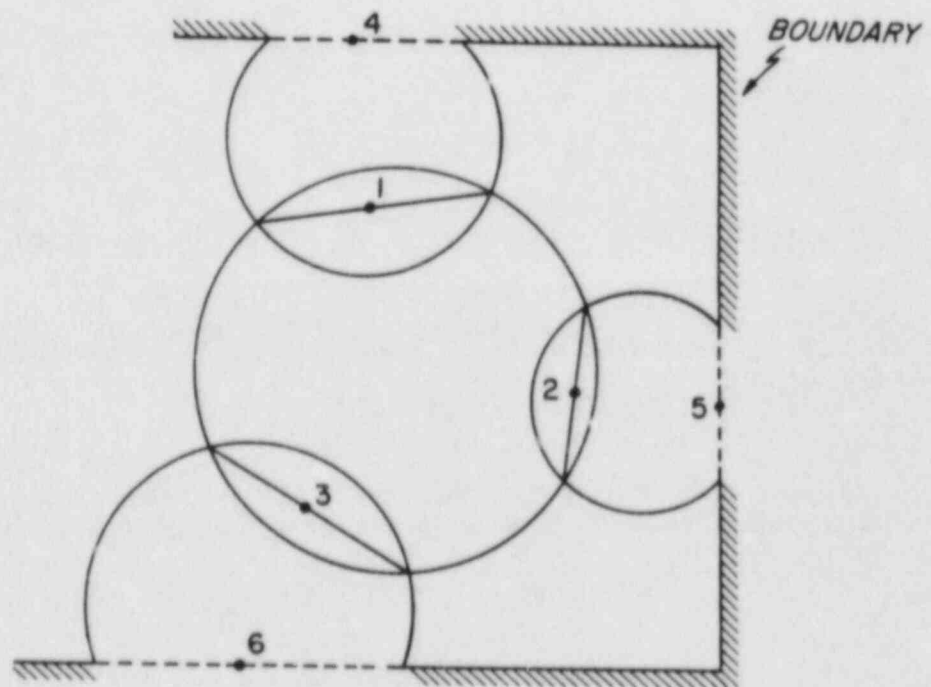


Figure 9. A sample fracture network to illustrate the derivation of the global mass balance equation.

and

$$\begin{aligned}
 & C_{1,3}P_1 + C_{2,3}P_2 + (-C_{1,3} - C_{2,3} - C_{6,3})P_3 \\
 & = -C_{1,3,2} - C_{2,3,2} - C_{6,3}P_3 - C_{6,3,2}
 \end{aligned}
 \tag{18}$$

Combining equations 16, 17 and 18, a matrix equation of order 3 is obtained:

$$[A] \{P\} = \{B\} \tag{19}$$

Matrix [A] is symmetric, positive, and definite. The Choleski's square root method can be used to decompose [A] to a product of two triangular matrices, [L] and [U],

$$[A] = [L] [U] \tag{20}$$

where [L] is a lower triangular matrix, and [U] is an upper triangular matrix, and [U] = [L] - transpose.

The entry of matrix [L], M_{kj} , is given by:

$$M_{kj} = \frac{a_{kj} - \sum_{p=1}^{j-1} M_{kp}M_{jp}}{M_{jj}}, \quad j=1, 2, K-1$$
(21a)

$$M_{kk} = (a_{kk} - \sum_{p=1}^{k-1} M_{kp}^2)^{1/2}$$
(21b)

Once [L] and [U] are determined, equation 20 can be rewritten as:

$$[L] [U] \{P\} = \{B\} \tag{22a}$$

Let $[U] \{P\} = \{R\}$ (22b)

then $[L] \{R\} = \{B\}$ (22c)

To solve for {P}, a temporary vector {R} of equation 22c is solved first by forward substitution. {P} is then determined by back substitution using equation 22b. Once the pressure heads of internal nodes are determined, the fluxes across the boundary surfaces can be calculated.

Subroutines SUBBOND, SUBMTRX and SUBMSBL are designed to perform the tasks described in this section, namely assign boundary conditions, assemble the network matrix equation and solve for the pressure head

along internal intersections and calculate fluxes across the boundary surfaces.

Before the assemblage of the flow network, the dead-end fractures must be identified. Dead-end fractures are those that do not intersect any boundary surface, or only intersect one other fracture. Based on the physical formulation, these dead-end fractures do not contribute to flow, thus they should not be included in the flow network. Mathematically, they result in a singular matrix, which hampers the analysis. Subroutine SUBDEAD is designed to delete dead-end fractures from the network.

2.4 Design of Mass Transport Experiments

Hydraulic analysis provides the pressure head distribution in the fracture network. From information on head distribution and fracture network, it is possible to reconstruct the flow network. For every intersection, the flow network contains the details of fluxes from all directly connected intersections and their corresponding travel time. Once the flow network is defined, it is possible to perform mass transport experiments based on the two following assumptions:

- 1) a piston type convective transport between intersections in the fracture, and
- 2) a complete mixing at the intersection.

A tracer source of any time variant function introduced anywhere in the system can be tracked explicitly. This capability allows the study of hydrodynamic dispersion in a fracture network.

According to the imposed assumptions, mass attenuation occurs at the intersection only. Figure 10 is used as an example. In Figure 10, the intersecting line segment is represented by a node at its midpoint. Intersects A, B and C provide inflow to X, and D and E are outflow intersects from X. $F_{A,X}$ denotes the flux from A to X, and can be calculated from equation 12. Assume $M_{A,X}$ denotes the tracer concentration in the stream $F_{A,X}$, the principle of mass conservation implies that:

$$F_{A,X} + F_{B,X} + F_{C,X} = -(F_{D,X} + F_{E,X}) \quad (23a)$$

$$M_{A,X}F_{A,X} + M_{B,X}F_{B,X} + M_{C,X}F_{C,X} = -(M_{D,X}F_{D,X} + M_{E,X}F_{E,X}) \quad (23b)$$

The assumption of complete mixing at the intersection, X, gives the following relation:

$$M_{D,X} = M_{E,X} = \frac{M_{A,X}F_{A,X} + M_{B,X}F_{B,X} + M_{C,X}F_{C,X}}{F_{A,X} + F_{B,X} + F_{C,X}} \quad (24)$$

The portion of $M_{D,X}$ or $M_{E,X}$ which is contributed from the specific inflow path, A - X, is given as:

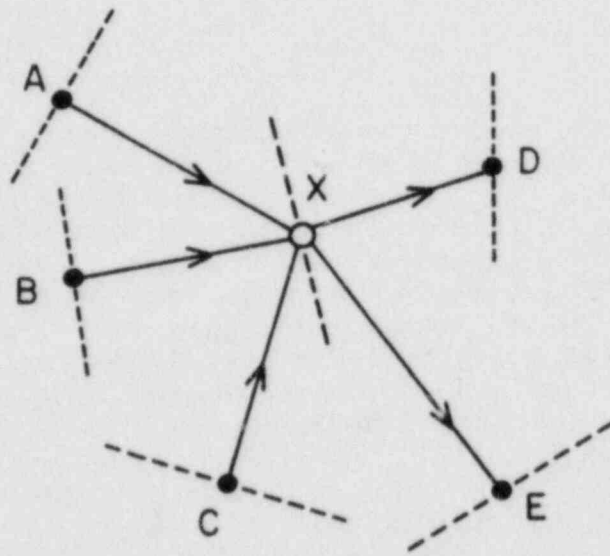


Figure 10. A sample flow network showing inflow and outflow components at intersection X.

$$L_{A,X} = \frac{M_{A,X} F_{A,X}}{F_{A,X} + F_{B,X} + F_{C,X}} = M_{A,X} R_{A,X} \quad (25a)$$

where

$$R_{A,X} = \frac{F_{A,X}}{F_{A,X} + F_{B,X} + F_{C,X}} \quad (25b)$$

and

$$\begin{aligned} M_{D,X} &= L_{A,X} + L_{B,X} + L_{C,X} \quad (26) \\ &= M_{A,X} R_{A,X} + M_{B,X} R_{B,X} + M_{C,X} R_{C,X} \end{aligned}$$

$R_{A,X}$ can be viewed as an attenuation coefficient. It represents the fraction of mass from a specific inflow route actually being reflected at an outflow route. Combining the concept of mass attenuation at the intersection and a piston type flow between intersections, the travel time and total mass attenuation can be calculated from the source point to the point of observation. Assume that between the tracer source and an observation point, there is a total of NR possible flow routes. For the jth flow route, it passes through K number of intersections, (or attenuation points). The total attenuation for this particular flow route is:

$$RT_j = \prod_{n=1}^K R_n \quad (27)$$

where R_n is the attenuation at the nth intersection. The travel time through route j is:

$$T_j = \sum_{n=1}^K t_n \quad (28)$$

where t_n is the travel time from intersection n-1 to intersection n. A mass change of DM at the source will be reflected through route j at a time lag of T_j units later at the point of observation with a change of dm_j , where

$$dm_j = DM * RT_j \quad (29)$$

An analysis including all possible flow routes will give a complete breakthrough history at the point of observation. Note that the point of observation can be anywhere in the network as long as it is downstream from the tracer source. The convective piston type transport assumption does not allow mass to be transported against the direction of flow.

Subroutines FLOWNET and TRACER are designed to perform the mass transport experiments. To minimize the core memory requirement, the fracture network structure and hydraulic head distribution are generated first and stored in a data file. FLOWNET and TRACER subroutines are then called from a second main program to carry out the determination of breakthrough curves.

3. EXAMPLE OF EXPERIMENTS

To demonstrate the usage of the code, two experiments are presented. The complete code listing and sample input/output are given in Appendix A.

In both experiments, the global fracture network consists of 200 circular fractures with their centers located inside a cubic volume of 200 X 200 X 200 length units. These 200 circular fractures are uniformly distributed inside the cubic volume. The uniform distribution is also used to generate the angles of rotation, radius, and aperture of each fracture. Thus the generated fracture network represents a homogeneous system.

In Experiment 1, a cubic sample of size $(L \times L \times L)$ is isolated from the fracture network (Figure 11). This sample is then placed in water such that the top surface is flush with the water surface, creating hydrostatic boundary conditions on all submerged boundary surfaces. The top surface is then pressurized to maintain a constant pressure of magnitude L length units (Figure 12). The pressure head distribution inside the sample is solved and the fluxes across all boundary surfaces are calculated. This experiment is used to examine the scale and boundary effects in the hydraulic conductivity structure.

Experiment 2 is a simulation of a hydraulic - tracer injection test (Figure 13). A cubic sample of size 180 length units, centered at the fracture generating region is isolated. At the center of the sample, a cubic volume of 20 length units on the side is identified as the injection zone. The sample is submerged in water to maintain a hydrostatic condition before injection starts. During the hydraulic injection test, the injection zone is pressurized to a constant head 100 units above its hydrostatic head. A steady state flow regime can be established. A continuous slug of tracer of concentration C_0 is introduced at the injection zone. The breakthrough curves are determined at every boundary (or outflow) intersects to study the mass transport characteristics of the simulated fracture sample.

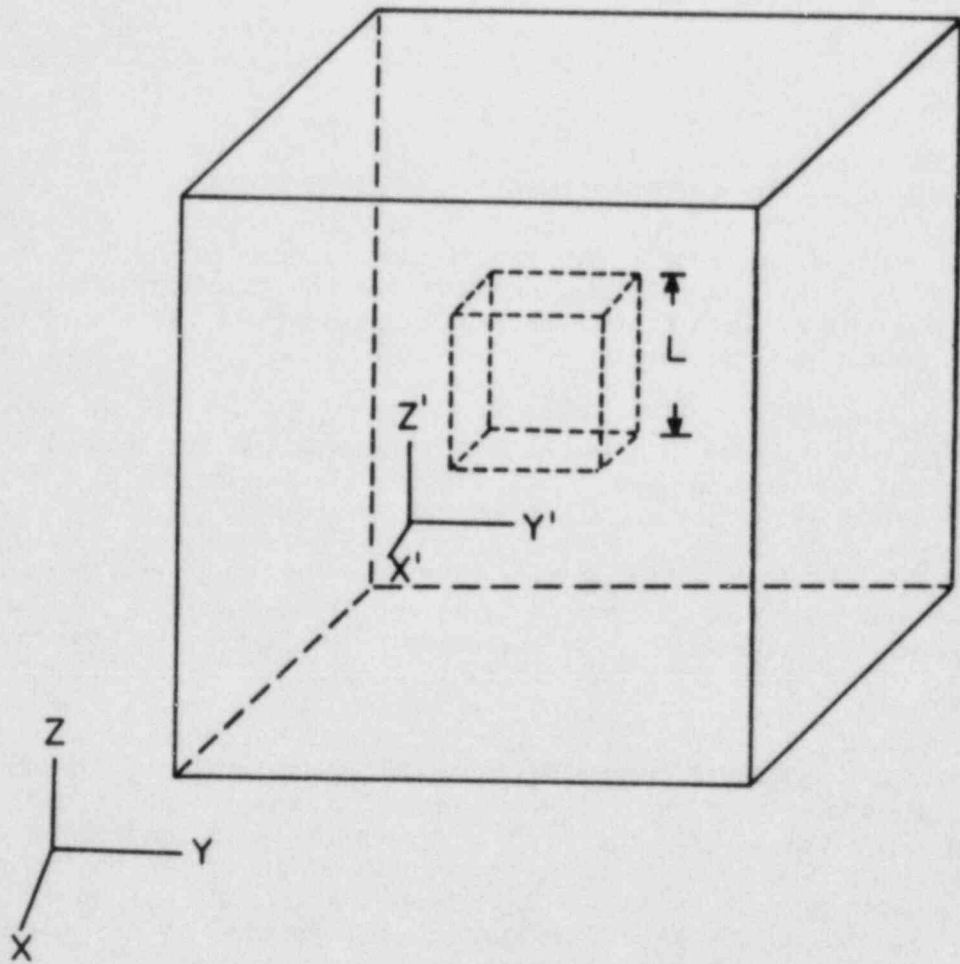


Figure 11. A cubic block sample of size L isolated from the global fracture region.

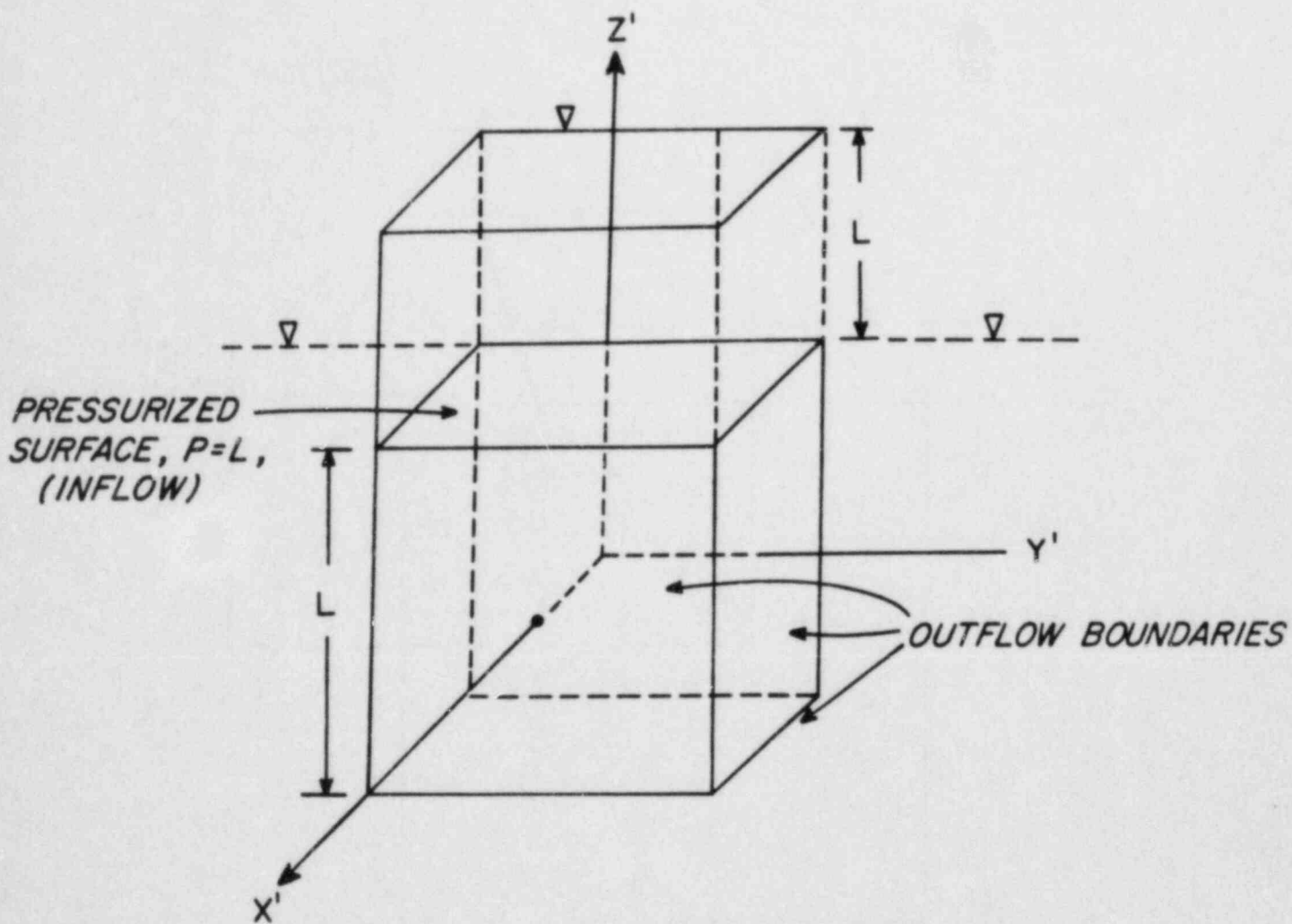


Figure 12. Schematic drawing of Experiment 1 showing a rock sample submerged in water with the top surface pressurized to a pressure head equal to the size of the block.

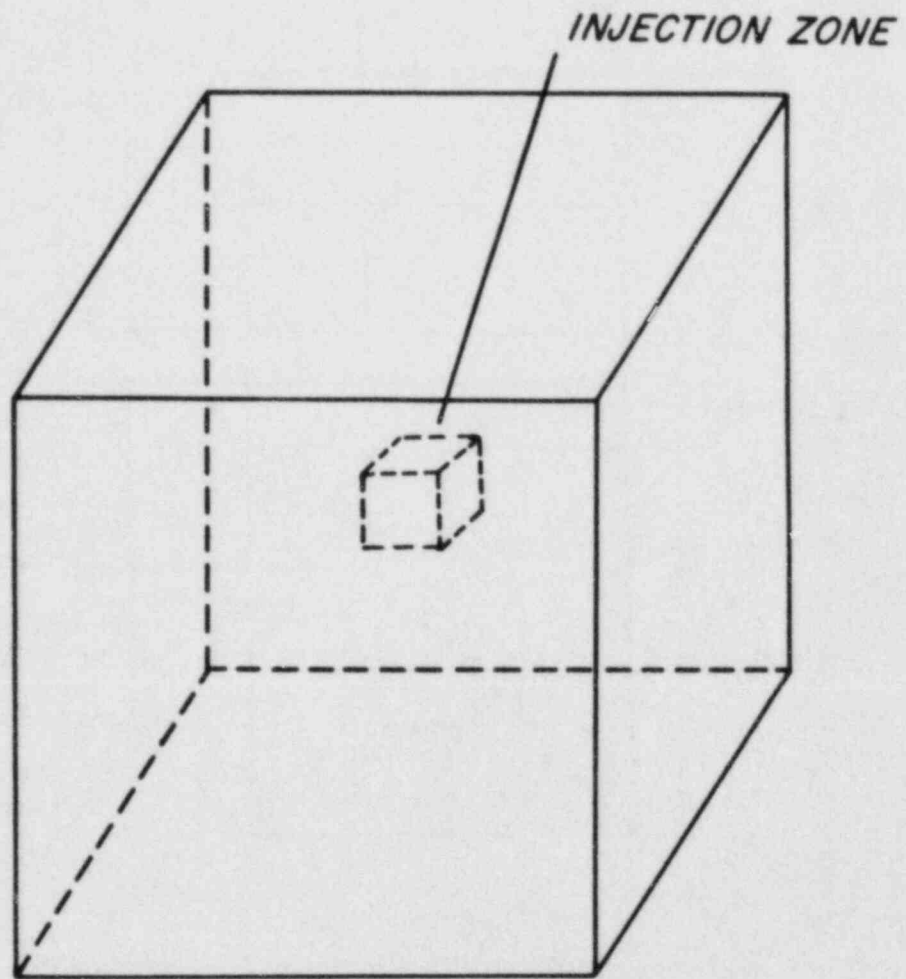


Figure 13. Schematic drawing of Experiment 2.

4. DISCUSSION

The fracture generating scheme presented is a useful tool for examining flow and transport through fractured systems. The present code is limited to steady state, saturated flow through a simulated fracture network where the rock matrix is impermeable. The code is being extended to simulate unsaturated fracture networks in rock of finite permeability.

Results of the two types of experiments are not included in this report. They are to be published in technical papers to follow. The purpose of this report is to present a detailed description of the computer code.

APPENDIX A: PROGRAM LISTING

A.1 Coordinate Systems Used in the Model

A.1.1 The Global Coordinate System:

The Global Coordinate System is a 3-D Cartesian coordinate system used in the creation of random fracture networks and in defining an isolated sample from the global network. The following arguments in the main program are expressed in the Global Coordinate System: XINP, XCUT, CORØ and COAL.

A.1.2 The Sample Coordinate System:

The Sample Coordinate System is a 3-D Cartesian coordinate system used to describe the intersections (or nodal points) contained inside a rectangular block of sample.

The coordinate system is defined at the center of the rectangular block, as specified by CORØ. The new +X axis is oriented COAL(1,1) degrees horizontally and COAL(2,1) degrees vertically from the +X axis of the Global Coordinate System (see Fig. X). The following arguments in the main program are expressed in the Sample Coordinate System: XYZI and XYZX.

A.1.3 The Fracture Local Coordinate System:

The Fracture Local Coordinate System is a 2-D Cartesian coordinate system defined at the center of each fracture or boundary surface, and is used to find the intersections (or nodal points) among fractures and boundary surfaces. For every surface, there is one such coordinate system defined.

For fracture K, the origin of the coordinate system is specified by XINP(J,K), J=1,3. XINP(4,K) and XINP(5,K) are the horizontal and vertical angles specifying the direction of the normal vector for the fracture plane. The +X axis of the Fracture Local Coordinate System is rotated XINP(6,K) degrees from a temporary axis having an orientation of XINP(4,K) degrees horizontally and XINP(5,K)-90 degrees vertically from the Global Coordinate Systems (see Fig. Y). This Coordinate System is used internally and should be transparent to the user.

A.2 Arguments Used in the Main Program:

NFRCT	Total number of fractures.
NSHP(I)	Vector of length NFRCT, containing the shape index of each individual fracture, I. Different shapes used in the program are: circle (NSHP=1), ellipse (NSHP=2), square (NSHP=3), rectangle (NSHP=4).
XINP(I,J)	Matrix of 9*NFRCT containing the geometric parameters describing each individual fracture, J. I=1,3 contain the global X-Y-Z coordinates specifying the center of the fracture. I=4,6 contain the angles (in degrees) used to specify the orientation of the fracture plane. I=7,8 are characteristic length scales specifying the areal extent of the finite fracture. I=9 contains the aperture of the fracture.
CORØ(I,J)	Matrix of 3*N, where N is the total number of rectangular blocks to be isolated simultaneously from the global fracture generating region, containing the center location (I=1,3) expressed in the Global Coordinates for the Jth sample block.
COAL(I,J)	Matrix of 2*N, where N is the total number of rectangular blocks to be isolated simultaneously from the global fracture generating region, containing the angles of rotation (I=1,2) for the Jth sample block.
COSZ(I,J)	Matrix of 3*N, where N is the total number of rectangular blocks to be isolated simultaneously from the global fracture generating region, containing the sizes (I=1,3) of the Jth sample block.
CORA(I,J,K)	Matrix of 3*3*N, where N is total number of rect-
CORB(I,J,K)	angular blocks existing simultaneously within the global fracture generating region, containing the Jacobian coefficients to be used for coordinate transformation between the Global and the Kth Sample Coordinate Systems. If XYZGLB(I), I=1,3 defines the location of a point in the Global Coordinates, and XYZSAM(I,K) is the same point expressed in the Jth Sample Coordinates, then:

$$\text{XYZSAM}(I,K) = \text{CORB}(I,J,K) * (\text{XYZGLB}(J,K) - \text{COR}\emptyset(J,K))$$

$$\text{XYZGLB}(I,K) = \text{COR}\emptyset(I,K) + \text{CORA}(I,J,K) * \text{XYZSAM}(J,K)$$

Note: these two expressions are matrix equations.

- NCUT Total number of rectangular boundary surfaces.
Each rectangular block of sample has 6 boundary surfaces.
- XCUT(I,J) Matrix of 8*NCUT containing the geometric parameters describing each rectangular boundary surface, J.
I=1,3 contain the global X-Y-Z coordinates specifying the center of the boundary surface.
I=4,6 contain the angles (in degrees) used to specify the orientation of the boundary surface.
I=7,8 are characteristic length scales specifying the areal extent of the boundary surface.
- NFR(I) Vector of length NFRCT containing information about the number of intersecting fractures for fracture I.
If INFR(J) denotes the total number of intersecting fractures for fracture J, then
- $$\text{INFR}(J) = \text{NFR}(J) - \text{NFR}(J-1) ,$$
- and
- $$\text{NFR}(J) = \text{INFR}(1) + \text{INFR}(2) + \dots + \text{INFR}(J) .$$
- NFRN(I) Vector of length NFR(NFRCT) (or 2*NNODE) containing the fractures intersected by a fracture.
If INFR(J) denotes the total number of intersecting fractures for fracture J, then NFRN(NFR(J-1)+1) contains the fracture number representing the intersected fracture; and NFRN(NFR(J-1)+INFR(J)) or NFRN(NFR(J)) contains the fracture number representing the intersection with fracture J.
- NCT(I) Vector of length NCUT containing information about the number of intersecting fractures for each rectangular boundary surface J.
If INCT(J) denotes the total number of intersecting fractures for boundary surface J, then
- $$\text{INCT}(J) = \text{NCT}(J) - \text{NCT}(J-1) ,$$
- and
- $$\text{NCT}(J) = \text{INCT}(1) + \text{INCT}(2) + \dots + \text{INCT}(J) .$$

NCTN(I) Vector of length NCT(NCUT) (or NBOND) containing the fracture numbers that intersect each individual rectangular boundary surface.
 If INCT(J) denotes the total number of intersecting fractures for boundary surface J, then NCTN(NCT(J-1)+1) contains the fracture number of the first intersecting fracture; and NCTN(NCT(J-1)+INCT(J)) or NCTN(NCT(J)) contains the fracture number of the INFR(J)th intersecting fracture.

NCF(I) Vector of length NFRCT containing information about the number of intersecting boundary surfaces for fracture I.
 If INCF(J) denotes the total number of intersecting fractures for fracture J, then

$$\text{INCF}(J) = \text{NCF}(J) - \text{NCF}(J-1) ,$$

and

$$\text{NCF}(J) = \text{INCF}(1) + \text{INCF}(2) + \dots + \text{INCF}(J) .$$

NCFN(I) Vector of length NCF(NFRCT) (or NBOND) containing the boundary surfaces numbers that intersect each individual fracture.
 If INCF(J) denotes the total number of intersecting boundary surfaces for fracture J, then NCFN(NCF(J-1)+1) contains the boundary surface number of the first intersecting boundary; and NCFN(NCF(J-1)+INCF(J)) or NCFN(NCF(J)) contains the boundary surface number of the INFR(J)th intersecting boundary.

NNODE Total number of fracture-fracture intersections contained inside the rectangular block of sample. Note that each each intersecting line segment is represented by a nodal point located at the center of the line segment. The fracture-fracture intersections are referred as internal nodes.

NDID(I,J) Matrix of length NNODE*2 containing the intersecting fracture numbers at internal node I. Thus, internal node I is the intersection of fracture NDID(I,1) and fracture NDID(I,2).

NDFR(I) Vector of length NFR(NFRCT) (or 2*NNODE) containing the internal nodal numbers of fracture intersects.
 If INFR(J) denotes the total number of intersecting fractures for fracture J, then NDFR(NFR(J-1)+1) contains the internal nodal number representing the intersection of fracture J and fracture

NFRN (NFR (J-1)+1) [and NDFR (NFR (J-1)+INFR (J)) or NDFR (NFR (J)) contains the nodal number representing the intersection between fracture number J and fracture number NFRN (NFR (J))].

NBOND Total number of fracture-boundary surface intersections. Note that each each intersecting line segment is represented by a nodal point located at the center of the line segment. The fracture-boundary surface intersections are referred as external nodes.

NDXD (I,J) Matrix of length NBOND*2 containing the intersecting fracture number (J=1) and boundary surface number (J=2) for external node I. Thus, external node I is the intersection of fracture NDXD (I,1) and boundary surface NDXD (I,2).

NDCF (I) Vector of length NCFR (NFRCT) (or NBOND) containing the external nodal numbers of fracture-boundary intersections.
If INCF (J) denotes the total number of intersecting boundary surfaces for fracture J, then NDCF (NCF (J-1)+1) contains the external nodal number representing the intersection of fracture J and boundary surface NCFN (NCF (J-1)+1); and NDCF (NFR (J-1)+INCF (J)) or NDCF (NFR (J)) contains the nodal number representing the intersection between fracture number J and boundary surface number NCFN (NCF (J)).

NDCT (I) Vector of length NCT (NCUT) (or NBOND) containing the external nodal numbers of fracture-boundary intersections.
If INCT (J) denotes the total number of intersecting fractures for boundary surface J, then NDCT (NCT (J-1)+1) contains the external nodal number representing the intersection of boundary surface J and fracture NCTN (NCT (J-1)+1); and NDCT (NCT (J-1)+INCT (J)) or NDCT (NCT (J)) contains the nodal number representing the intersection between boundary surface number J and fracture number NCTN (NCT (J)).

XYZI (I,J) Matrix of NNODE*4 containing the location (J=1,3) and length (J=4) of fracture-fracture intersections. the fracture-fracture intersection is represented by a nodal point located at the center of the line segment. The location is expressed in the 3-D Sample Coordinate System.

XYZX(I,J) Matrix of NBOND*4 containing the location (J=1,3) and length (J=4) of fracture-boundary surface intersections. The fracture-boundary surface intersection is represented by a nodal point located at the center of the line segment. The location is expressed in the 3-D Sample Coordinate System.

PO(I) Vector of length NBOND containing the pressure heads, expressed in length units, on the external (fracture-boundary surface intersection) nodes.

PX(I) Vector of length NNODE containing the pressure heads, expressed in length units, on the internal (fracture-fracture intersection) nodes.

C
C
C

```
COMMON /FRCT/ NFRCT, NSHP (200), XINP (9, 200), NFR (200), NFRN (1000)
COMMON /CUTT/ NCUT, XCUT (9, 12), NCT (12), NCTN (300)
COMMON /CFCE/ NCF (200), NCFN (300)
COMMON /NODE/ NNODE, NDID (400, 2), NDFR (1000)
COMMON /BOND/ NBOND, NDXD (400, 2), NDCF (300), NDCT (300)
COMMON /XYZZ/ XYZI (400, 4), XYZX (400, 4)
COMMON /MTRX/ PO (400), PX (400)
CALL INFRCT
READ (1, *) NSET
DO 10 J=1, NSET
CALL INPCUT
CALL SUPFRC
CALL SUPCUT
CALL SUPDEAD
CALL SUBMTRX
10 CONTINUE
STOP
END
```



```

C -----
C   GENERATE RANDOM FRACTURES --- CIRCULAR DISC
C -----
      DDS1=DBLE (DS1)
      DDS2=DBLE (DS2)
      DDS3=DBLE (DS3)
      DDS4=DBLE (DS4)
      CALL RANDUFM (DDS1,NFRCT+5,WORK1)
      CALL RANDUFM (DDS4,NFRCT+5,WORK2)
      CALL RANDUFM (DDS3,5*NFRCT+5,WORK)
      DO 10 J=1,NFRCT
      NSHP (J) = 1
      XINP (1,J)=REAL (INT (FRX*WORK (      J+2)))
      XINP (2,J)=REAL (INT (FRY*WORK ( NFRCT+J+2)))
      XINP (3,J)=REAL (INT (FRZ*WORK (2*NFRCT+J+2)))
      XINP (4,J)=REAL (INT (360.*WORK (3*NFRCT+J+2)))
      XINP (5,J)=REAL (INT (360.*WORK (4*NFRCT+J+2)))
      XINP (6,J)=0.0
      XINP (7,J)=REAL (INT (FRCTLTH*WORK1 (J+2)))
      XINP (8,J)=XINP (7,J)
      XINP (9,J)=(REAL (INT (FRCAPTR*WORK2 (J+2)))+1.0) * XFCT
10  CONTINUE
      RETURN
      END

```

C
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SUBROUTINE INPCUT

PURPOSE: THIS SUBROUTINE READS IN THE CENTER LOCATION (COR0),
ROTATION (COAL), AND SIZE (COSZ) OF A RECTANGULAR BOLCK
AND GENERATES THE GEOMETRIC PARAMETERS FOR EACH OF THE
RECTANGLE BOUNDARY SURFACES. THIS SUBPROGRAM CHANGES THE
CONTENTS OF THE FOLLOWING VARIABLES: NCUT, COR0, COAL, COSZ,
XCUT, CORA, CORB.

```
COMMON /FRCT/ NFRCT, NSHP(200), XINP(9,200), NFR(200), NFRN(1000)
COMMON /CUTT/ NCUT, XCUT(9,12), NCT(12), NCTN(300)
COMMON /CORD/ COR0(3,2), COSZ(3,2), COAL(2,2),
1          CORA(3,3,2), CORB(3,3,2)
REAL WKALP(12), WKBTA(12), WKX(3), WKYZ(18)
INTEGER NWAL(6), NWBT(6)
DATA PI, DG2RAD / 3.141592654, 0.0174532925199433/
DATA WKALP /1., 0., 1., 180., 1., 90., 1., 270., 1., 0., 1., 0./
DATA WKBTA /1., 0., -1., 0., 0., 0., 0., 0., 1., 90., 1., 270./
DATA NWAL / 3, 3, 3, 3, 1, 1 /
DATA NWBT / 2, 2, 1, 1, 2, 2 /
DATA WKYZ /1., 0., 0., -1., 0., 0., 0., 1., 0., 0., -1., 0.,
1          0., 0., 1., 0., 0., -1. /
NCUT = 6
JTOT = 1
READ (1,*) COR0(1,1), COR0(2,1), COR0(3,1),
1          COAL(1,1), COAL(2,1),
1          COSZ(1,1), COSZ(2,1), COSZ(3,1)
WRITE (8,100) COR0(1,1), COR0(2,1), COR0(3,1),
1          COAL(1,1), COAL(2,1),
1          COSZ(1,1), COSZ(2,1), COSZ(3,1)
100 FORMAT (/, ' SAMPLE CENTER (COR0,1) : ', 3F8.1/
1          ' SAMPLE ANGLE (COAL,1) : ', 2F8.1/
2          ' SAMPLE SIZE (COSZ,1) : ', 3F8.1, /)
DO 10 K1=1, JTOT
ALPP = COAL(1, K1) * DG2RAD
BETT = COAL(2, K1) * DG2RAD
CORA(1,1, K1) = COS(ALPP) * COS(BETT)
CORA(2,1, K1) = SIN(ALPP) * COS(BETT)
CORA(3,1, K1) = SIN(BETT)
CORA(1,2, K1) = -SIN(ALPP)
CORA(2,2, K1) = COS(ALPP)
CORA(3,2, K1) = 0.
CORA(1,3, K1) = -COS(ALPP) * SIN(BETT)
CORA(2,3, K1) = -SIN(ALPP) * SIN(BETT)
CORA(3,3, K1) = COS(BETT)
```

```

DO 9 I=1,3
DO 9 J=1,3
9 CORB(I,J,K1) = CORA(J,I,K1)
10 CONTINUE
DO 30 K1=1, JTOT
DO 25 J=1, NCUT
J4 = J + (K1-1)*NCUT
DO 20 J1=1,3
WKKK = 0.
DO 15 J2=1,3
15 WKKK= WKKK + CORA(J1,J2,K1)*COSZ(J2,K1)*WKYZ(3*(J-1)+J2)/2.
20 XCUT(J1,J4) = COR0(J1,K1)+WKKK
XCUT(4,J4) = COAL(1,K1)*WKALP(2*(J-1)+1) + WKALP(2*(J-1)+2)
XCUT(5,J4) = COAL(2,K1)*WKBTA(2*(J-1)+1) + WKBTA(2*(J-1)+2)
XCUT(6,J4) = 0.0
XCUT(7,J4) = 0.5 * COSZ(NWAL(J),K1)
XCUT(8,J4) = 0.5 * COSZ(NWBT(J),K1)
XCUT(9,J4) = 0.0
25 CONTINUE
30 CONTINUE
NCUT = NCUT * JTOT
RETURN
END

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SUBROUTINE SUBMTRX

PURPOSE: THIS SUBROUTINE PERFORMS THE FOLLOWING TASKS:
 1: SET UP BOUNDARY CONDITION BY CALLING *SUBBOND*;
 2: ASSEMBLE THE GLOBAL MATRIX EQUATION;
 3: SOLVE THE MATRIX EQUATION;
 4: CALCULATE FLUXES ACROSS BOUNDARY SURFACES OR
 PERFORM MASS BALANCE BY CALLING *SUBMSBL*.

ARGUMENTS:

NTS INDEX INDICATING THE TEST NUMBER AND THE BOUNDARY
 SURFACE NUMBER WHICH IS BEING PRESSUREIZED IN
 THE CURRENT TEST.

FLUX (I) VECTOR OF LENGTH NCUT CONTAINING THE STEADY-STATE
 FLUX ACROSS THE BOUNDARY SURFACE I. THIS VECTOR
 IS RETURNED FROM THE SUBPROGRAM *SUBMSBL*.

```

COMMON /FRCT/ NFRCT, NSHP (200), XINP (9, 200), NFR (200), NFRN (1000)
COMMON /CUTT/ NCUT, XCUT (9, 12), NCT (12), NCTN (300)
COMMON /CFCE/ NCF (200), NCFN (300)
COMMON /NODE/ NNODE, NDID (400, 2), NDFR (1000)
COMMON /BOND/ NBOND, NDXD (400, 2), NDCF (300), NDCT (300)
COMMON /XYZZ/ XYZI (400, 4), XYZX (400, 4)
COMMON /MTRX/ PO (400), PX (400)
REAL X0 (4), X1 (4), AA (310), BB, BBX (310, 6), FLUX (12)
REAL AMTRX (47200)
DATA M, IB / 6, 310 /
DATA RHO, UN, UNITCON / 9810., 0.001, 0.01 /
DO 60 NTS=1, M
CALL SUBBOND (NTS)
NSD=INT (REAL (NTS+1)/2.)
SIGN=1.0
IF ( NSD*2 .EQ. NTS) SIGN = -1.0
J5=0
DO 50 I=1, NNODE
BB=0.
DO 5 III=1, NNODE
5 AA (II) =0.
J1=NDID (I, 1)
J2=NDID (I, 2)
DO 40 III=1, 2

```

```

IF (III .EQ. 2) THEN
  JTEMP=J1
  J1=J2
  J2=JTEMP
ENDIF
DO 15 I1=1, IFN(J1, NFR)
  ITT = IFK(J1, NFR) + I1
  IF (J2 .EQ. NFRN (ITT) ) THEN
    JJ2=I1
    DO 10 I2=1,4
      X0(I2)= XYZI (NDFR (ITT), I2)
    ENDIF
  10 CONTINUE
  DO 25 I1=1, IFN(J1, NFR)
    ITT = IFK(J1, NFR) + I1
    IF (I1 .NE. JJ2) THEN
      T2=0.
      DO 20 I2=1,3
        X1(I2) = XYZI (NDFR (ITT), I2)
        T2=T2+(X1(I2)-X0(I2))**2.
      20 CONTINUE
      X1(4)= XYZI (NDFR (ITT), 4)
      X0X1 = SQRT(T2)
      XX = (X1(4) + X0(4))/2.
      XCOEF= XX * (XINP(9, J1)**3.) * RHO
      1 / ( 12. * UN * X0X1 )
      AA(NDFR (ITT))=AA(NDFR (ITT)) + XCOEF
      AA(I)= AA(I) - XCOEF
      BB = BB + SIGN * (X0(NSD)-X1(NSD))*XCOEF
    ENDIF
  25 CONTINUE
  DO 35 I1=1, IFN(J1, NCF)
    T2=0.
    ITT = IFK(J1, NCF) + I1
    DO 30 I2=1,3
      X1(I2) = XYZX (NDCF (ITT), I2)
      T2=T2+(X1(I2)-X0(I2))**2.
    30 CONTINUE
    X1(4)= XYZX (NDCF (ITT), 4)
    X0X1 = SQRT(T2)
    XX = (X1(4) + X0(4))/2.
    XCOEF= XX * (XINP(9, J1)**3.) * RHO
    1 / ( 12. * UN * X0X1 )
    AA(I)= AA(I) - XCOEF
    BB = BB + (SIGN*(X0(NSD)-X1(NSD))-PO(NDCF (ITT)))*XCOEF
  35 CONTINUE
  40 CONTINUE
  DO 45 I1=1, I
    AMTRX(J5+I1) = -AA(I1)
  45 CONTINUE

```

```

J5=J5+I
BBX(I,NTS) = -BB
50 CONTINUE
60 CONTINUE
IER=0
CALL SUBLEQS (AMTRX,M,NNODE,BBX,IB,D1,D2,IER)
IF ( IER .GT. 0 ) THEN
WRITE (8, *) 'ERROR MSG FROM *SUBLEQS* IER =',IER
RETURN
ENDIF
DO 70 NTS = 1, M
CALL SUBBOND (NTS)
DO 65 I1 = 1, NNODE
65 PX(I1) = BBX(I1,NTS)
CALL SUBMSBL (NTS,FLUX)
WRITE (8,100) NTS, (FLUX(J),J=1,6)
100 FORMAT (2X,'NTS=',I1,3X,6F10.2)
70 CONTINUE
RETURN
END

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SUBROUTINE SUBBOND (NT)
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PURPOSE: THIS SUBROUTINE ASSIGNS THE BOUNDARY CONDITIONS FOR
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A SPECIFIC TEST. THE CONTENTS OF THE *PO* VECTOR
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IS CHANGED.
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ARGUMENTS:
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NT INDEX INDICATING THE TEST NUMBER AND THE BOUNDARY
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COMMON /BOND/ NBOND,NDXD(400,2),NDCF(300),NDC(300)
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COMMON /XYZZ/ XYZI(400,4),XYZX(400,4)
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COMMON /MTRX/ PO(400),PX(400)
```

```
1 COMMON /CORD/ COR0(3,2),COSZ(3,2),COAL(2,2),
CORR(3,3,2),CORB(3,3,2)
```

```
NSD=INT(REAL(NT+1)/2.)
```

```
SIGN=1.0
```

```
IF(NSD*2.EQ.NT) SIGN = -1.0
```

```
DO 10 J=1,NBOND
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```
PRES=0.0
```

```
IF(NDXD(J,2).EQ.NT) PRES = COSZ(NSD,1)
```

```
PO(J) = PRES + COSZ(NSD,1)/2. - SIGN * XYZX(J,NSD)
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10 CONTINUE
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RETURN
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END
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SUBROUTINE SUBMSBL (NTS,FLUX)

PURPOSE: THIS SUBROUTINE CALCULATES FLUXES ACROSS BOUNDARY SURFACES
(OR PERFORMS MASS BALANCE).

ARGUMENTS:

NTS INDEX INDICATING THE TEST NUMBER AND THE BOUNDARY
SURFACE NUMBER WHICH IS BEING PRESSUREIZED IN
THE CURRENT TEST.

FLUX(I) VECTOR OF LENGTH NCUT CONTAINING THE STEADY-STATE
FLUX ACROSS THE BOUNDARY SURFACE I.

```

COMMON /FRCT/ NFRCT, NSHP(200), XINP(9,200), NFR(200), NFRN(1000)
COMMON /CUTT/ NCUT, XCUT(9,12), NCT(12), NCTN(300)
COMMON /CFCF/ NCF(200), NCFN(300)
COMMON /NODE/ NNODE, NDID(400,2), NDFR(1000)
COMMON /BOND/ NBOND, NDXD(400,2), NDCE(300), NDCT(300)
COMMON /XYZZ/ XYZI(400,4), XYZX(400,4)
COMMON /MTRX/ PO(400), PX(400)
REAL FLUX(12), X0(4), X1(4)
DATA RHO, UN, UNITCON /9810., 0.001, 0.01 /
NSD=INT(REAL(NTS+1)/2.)
SIGN=1.0
IF( NSD*2 .EQ. NTS) SIGN = -1.0
DO 40 J=1, NCUT
FLUX(J)=0.
DO 35 J1=1, IFN(J,NCT)
IT1 = IFK(J,NCT) + J1
J2=NCTN(IT1)
DO 10 J4=1,4
10 X0(J4) = XYZX (NDCT(IT1), J4)
DO 20 J3=1, IFN(J2,NCF)
ITS = IFK(J2,NCF) + J3
IF (J .NE. NCFN(ITS)) THEN
T2=0.
DO 15 J4=1,3
15 X1(J4) = XYZX (NDCE(ITS), J4)
T2=T2+(X1(J4)-X0(J4))**2.
CONTINUE
X1(4)= XYZX (NDCE(ITS), 4)
X0X1 = SQRT(T2)

```



```

        XX = (X1(4) + X0(4))/2.
        XCOEF= XX * ((XINP(9,J2)*1.00)**3.) * RHO
1         / ( 12. * UN * X0X1 )
        FLUX(J)=FLUX(J)+ XCOEF * ( PO(NDCF(ITS)) + SIGN*X1(NSD)
1         - PO(NDCT(ITT)) - SIGN*X0(NSD) )
        ENDIF
20      CONTINUE
        DO 30 J3=1,IFN(J2,NFR)
            T2=0.
            ITS = IFK(J2,NFR) + J3
            DO 25 J4=1,3
                X1(J4) = XYZI (NDFR(ITS), J4)
                T2=T2+(X1(J4)-X0(J4))**2.
25      CONTINUE
            X1(4) = XYZI (NDFR(ITS), 4)
            X0X1 = SQRT(T2)
            XX = (X1(4) + X0(4))/2.
            XCOEF= XX * ((XINP(9,J2)*1.00)**3.) * RHO
1         / ( 12. * UN * X0X1 )
            FLUX(J)=FLUX(J)+ XCOEF * ( PX(NDFR(ITS)) + SIGN*X1(NSD)
1         - PO(NDCT(ITT)) - SIGN*X0(NSD) )
30      CONTINUE
35      CONTINUE
40      CONTINUE
        RETURN
        END

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SUBROUTINE SUPFRC

PURPOSE FIND ALL INTERSECTIONS AMONG FRACTURES CONTAINED INSIDE
A RECTANGULAR BLOCK OF SAMPLE.

REMARKS OUTPUT OF THIS SUBROUTINE IS STORED IN THE FOLLOWING
VARIABLES: NFR, NFRN, NNODE, NDID, NDFR, XYZI.

```
COMMON /FRCT/ NFRCT, NSHP(200), XINP(9,200), NFR(200), NFRN(1000)
COMMON /NODE/ NNODE, NDID(400,2), NDFR(1000)
COMMON /XYZZ/ XYZI(400,4), XYZX(400,4)
REAL X1(9), X2(9), TA(3,2)
DATA PI, DG2RAD / 3.141592654, 0.0174532925199433/
DATA TERR / 1.E-9/
NNODE=0
ITT = 0
DO 10 J1=1, NFRCT
10 NFR(J1)=0
DO 50 J1=1, NFRCT
IA = NSHP(J1)
DO 15 J3=1, 9
15 X1(J3)=XINP(J3, J1)
DO 40 J2=1, NFRCT
IB = NSHP(J2)
DO 20 J3=1, 9
20 X2(J3)=XINP(J3, J2)
CALL SUPDRV (IA, X1, IB, X2, ICK, TA)
IF (ICK .EQ. 2) THEN
CALL SUB1 ( TA, ICHK )
IF (ICLK .EQ. 0) THEN
ITT = ITT + 1
NFRN(ITT) = J2
IF ( J2 .GT. J1 ) THEN
NNODE = NNODE + 1
NDFR(ITT) = NNODE
NDID(NNODE, 1) = J1
NDID(NNODE, 2) = J2
TO=0.
CALL SUB1AA (TA)
DO 25 JJ=1, 3
XYZI (NNODE, JJ) = 0.5*(TA (JJ, 1)+TA (JJ, 2))
TO=TO+ (TA (JJ, 1)-TA (JJ, 2)) **2.
25 CONTINUE
XYZI (NNODE, 4) =SQRT (TO)
```

```

ENDIF
IF ( J1 .GT. J2 ) THEN
  JT = NFR(J2)
  IF ( J2 .EQ. 1 ) THEN
    JS = 1
  ELSE
    JS = NFR(J2-1) + 1
  ENDIF
  DO 30 J3 = JS, JT
    IF (NFR(J3) .EQ. J1) NDFR(ITT) = NDFR(J3)
30  CONTINUE
  ENDIF
ENDIF
ENDIF
40  CONTINUE
NFR(J1) = ITT
50  CONTINUE
RETURN
END

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SUBROUTINE SUPCUT

PURPOSE FIND ALL INTERSECTIONS BETWEEN FRACTURES AND THE BOUNDARY SURFACES OF A RECTANGULAR BLOCK OF SAMPLE.

REMARKS OUTPUT OF THIS SUBROUTINE IS STORED IN THE FOLLOWING VARIABLES: NCT, NCTN, NBOND, NXID, NDCF, NDCT, XYZX.

```
COMMON /FRCT/ NFRCT, NSHP(200), XINP(9,200), NFR(200), NFRN(1000)
COMMON /CUTT/ NCUT, XCUT(9,12), NCT(12), NCTN(300)
COMMON /CFCF/ NCF(200), NCFN(300)
COMMON /NODE/ NNODE, NDID(400,2), NDFR(1000)
COMMON /BOND/ NBOND, NDXD(400,2), NDCF(300), NDCT(300)
COMMON /XYZZ/ XYZI(400,4), XYZX(400,4)
REAL X1(9), X2(9), TA(3,2)
DATA PI, DG2RAD / 3.141592654, 0.0174532925199433/
DATA TERR / 1.E-9/
NBOND=0
ITT = 0
DO 10 J1=1, NFRCT
10 NCF(J1)=0
DO 15 J1=1, NCUT
15 NCT(J1)=0
DO 50 J1=1, NCUT
IA = 4
DO 20 J3=1, 9
20 X1(J3)=XCUT(J3, J1)
DO 40 J2=1, NFRCT
IB = NSHP(J2)
DO 25 J3=1, 9
25 X2(J3)=XINP(J3, J2)
CALL SUPDRV (IA, X1, IB, X2, ICK, TA)
IF (ICK .EQ. 2) THEN
  ITT = ITT + 1
  NCTN(ITT) = J2
  NBOND = NBOND + 1
  NDCT(ITT) = NBOND
  NDXD(NBOND, 1) = J2
  NDXD(NBOND, 2) = J1
  TO=0.
  CALL SUB1AA (TA)
  DO 30 JJ=1, 3
  XYZX(NBOND, JJ)=0.5*(TA(JJ, 1)+TA(JJ, 2))
  TO=TO+(TA(JJ, 1)-TA(JJ, 2))**2.
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30      CONTINUE
        XYZX(NBOND,4)=SQRT(TO)
        ENDIF
40      CONTINUE
        NCT(J1) = ITT
50      CONTINUE
        ITT = 0
        DO 60 J1 = 1, NFRCT
        DO 55 J2 = 1, NBOND
        IF ( NDXD(J2,1) .EQ. J1) THEN
            ITT = ITT + 1
            NDCF(ITT) = J2
            NCFN(ITT) = NDXD(J2,2)
        ENDIF
55      CONTINUE
        NCF(J1) = ITT
60      CONTINUE
        RETURN
        END

```



```

IF (II .EQ. 0) THEN
DO 50 I=1,3
IJ=0
I1=1*2
I2=I*2-1
IP1=I+1
IP2=I+2
IF(IP1 .GT. 3) IP1=IP1-3
IF(IP2 .GT. 3) IP2=IP2-3
IF((TP(I,1) .GT. S(I1)) .OR. (TP(I,2) .GT. S(I1))) THEN
IF((TP(I,1) .GT. TP(I,2)) .AND. (TP(I,1) .GT. S(I1)))THEN
TT(I)=S(I1)
IJ=1
ENDIF
IF((TP(I,2) .GT. TP(I,1)) .AND. (TP(I,2) .GT. S(I1)))THEN
TT(I)=S(I1)
IJ=2
ENDIF
TT(IP1)=TP(IP1,1)+(TT(I)-TP(I,1))*(TP(IP1,2)-TP(IP1,1))
1 / (TP(I,2)-TP(I,1))
TT(IP2)=TP(IP2,1)+(TT(I)-TP(I,1))*(TP(IP2,2)-TP(IP2,1))
1 / (TP(I,2)-TP(I,1))
IF((TT(IP1) .GT. S(IP1*2)) .OR. (TT(IP1) .LT. S(IP1*2-1)) .OR.
1 (TT(IP2) .GT. S(IP2*2)) .OR. (TT(IP2) .LT. S(IP2*2-1)))THEN
II=1
ELSE
II=0
DO 35 IK=1,3
35 TP(IK,IJ)=TT(IK)
ENDIF
ENDIF
IF((TP(I,1) .LT. S(I2)) .OR. (TP(I,2) .LT. S(I2))) THEN
IF((TP(I,2) .GT. TP(I,1)) .AND. (TP(I,1) .LT. S(I2)))THEN
TT(I)=S(I2)
IJ=1
ENDIF
IF((TP(I,1) .GT. TP(I,2)) .AND. (TP(I,2) .LT. S(I2)))THEN
TT(I)=S(I2)
IJ=2
ENDIF
TT(IP1)=TP(IP1,1)+(TT(I)-TP(I,1))*(TP(IP1,2)-TP(IP1,1))
1 / (TP(I,2)-TP(I,1))
TT(IP2)=TP(IP2,1)+(TT(I)-TP(I,1))*(TP(IP2,2)-TP(IP2,1))
1 / (TP(I,2)-TP(I,1))
IF((TT(IP1) .GT. S(IP1*2)) .OR. (TT(IP1) .LT. S(IP1*2-1)) .OR.
1 (TT(IP2) .GT. S(IP2*2)) .OR. (TT(IP2) .LT. S(IP2*2-1)))THEN
II=1
ELSE
II=0
DO 40 IK=1,3

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```
40      TP(IK,IJ)=TT(IK)
      ENDIF
      ENDIF
50      CONTINUE
      ENDIF
      DO 65 I=1,2
      DO 60 I1=1,3
      WRK=0.
      DO 55 I2=1,3
55      WRK=WRK+CORA(I1,I2,1)*TP(I2,I)
60      TQ(I1,I)=WRK+COR0(I1,1)
65      CONTINUE
      RETURN
      END
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SUBROUTINE SUBE1AA (TP)

PURPOSE PERFORM COORDINATE TRANSFORMATION FROM THE GLOBAL 3-D COORDINATES DEFINED FOR THE FRACTURE GENERATING REGION TO THE SAMPLE 3-D COORDINATE SYSTEM DEFINED AT THE CENTER OF THE RECTANGULAR BLOCK.

ARGUMENTS:

TP(I,J) INPUT MATRIX OF 3*2 CONTAINING THE GLOBAL X-Y-Z COORDINATES (I=1,3) OF 2 POINTS (J=1,2). AS OUTPUT, TP(I,J) RETURNS THE TRANSFORMED 3-D COORDINATES BASED ON THE CENTER OF THE RECTANGULAR BLOCK.

```
COMMON /CORD/ COR0(3,2),COSZ(3,2),COAL(2,2),
1 CORA(3,3,2),CORB(3,3,2)
REAL TP(3,2),TQ(3,2)
DO 10 I=1,2
DO 10 J=1,3
10 TQ(J,I)=TP(J,I)
DO 40 I=1,2
DO 30 I1=1,3
WRK=0.
DO 20 I2=1,3
20 WRK=WRK+CORB(I1,I2,1)*(TQ(I2,I)-COR0(I2,I))
30 TP(I1,I)=WRK
40 CONTINUE
RETURN
END
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FUNCTION IFN(I,NF)

REMARKS: NUCLEAS CALLED BY VARIOUS SUBPROGRAMS TO UNPACK A
ONE-DIMENSIONAL ARRAY WHERE DATA OF TWO-DIMENSIONAL
NATURE HAVE BEEN STORED.

DIMENSION NF(300)
IF (I .GT. 1) THEN
 IFN = NF(I) - NF(I-1)
ELSE
 IFN = NF(1)
ENDIF
RETURN
END

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FUNCTION IFK(I,NF)

REMARKS: NUCLEAS CALLED BY VARIOUS SUBPROGRAMS TO UNPACK A
ONE-DIMENSIONAL ARRAY WHERE DATA OF TWO-DIMENSIONAL
NATURE HAVE BEEN STORED.

DIMENSION NF(300)
IF (I .GT. 1) THEN
 IFK = NF(I-1)
ELSE
 IFK = 0
ENDIF
RETURN
END

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SUBROUTINE SUPDEAD

PURPOSE DELETE DEAD-END FRACTURES FROM THE FRACTURE NETWORK
 CONTAINED INSIDE THE RECTANGULAR BLOCK OF SAMPLE.
 A DEAD-END FRACTURE IS THE ONE THAT INTERSECTS ONLY ONE
 OTHER FRACTURES AND DOES NOT INTERSECT ANY BOUNDARY SURFACES.

REMARKS RESULTS OF THIS SUBROUTINE MAY CHANGE THE CONTENTS OF THE
 FOLLOWING VARIABLES: NFR, NFRN, NNODE, NDID, NDFR, XYZI.

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```
COMMON /FRCT/ NFRCT, NSHP(200), XINP(9,200), NFR(200), NFRN(1000)
COMMON /CUT/ NCUT, XCUT(9,12), NCT(12), NCTN(300)
COMMON /CFCF/ NCF(200), NCFN(300)
COMMON /NODE/ NNODE, NDID(400,2), NDFR(1000)
COMMON /BOND/ NBOND, NDXD(400,2), NDCF(300), NDCT(300)
COMMON /XYZZ/ XYZI(400,4), XYZX(400,4)
INTEGER IX(2)
CONTINUE
ISOL=0
DO 40 I=1,NFRCT
IF( (IFN(I,NFR) .EQ. 1) .AND. (IFN(I,NCF) .EQ. 0) ) THEN
ISOL = 1
JNODE= NDFR(NFR(I))
JFR1 = I
JFR2 = NFRN(NFR(I))
DO 15 I1 = JNODE+1, NNODE
NDID(I1-1,1)=NDID(I1,1)
NDID(I1-1,2)=NDID(I1,2)
DO 10 I2=1,4
XYZI(I1-1,I2)=XYZI(I1,I2)
CONTINUE
IIJ = 0
DO 20 I2=1,NFR(NFRCT)
IF (NDFR(I2) .EQ. JNODE) THEN
IIJ = IIJ +1
IX(IIJ) = I2
ENDIF
IF (NDFR(I2) .GT. JNODE) NDFR(I2)=NDFR(I2)-1
CONTINUE
IF (IX(1) .GT. IX(2)) THEN
IT = IX(1)
IX(1) = IX(2)
IX(2) = IT
ENDIF
```

```

DO 31 I3 = IX(2)+1, NFR(NFRCT)
NDFR(I3-1)=NDFR(I3)
31 NFRN(I3-1)=NFRN(I3)
DO 32 I3 = IX(1)+1, NFR(NFRCT)
NDFR(I3-1)=NDFR(I3)
32 NFRN(I3-1)=NFRN(I3)
DO 33 I3 = JFR1, NFRCT
33 NFR(I3) = NFR(I3) - 1
DO 34 I3 = JFR2, NFRCT
34 NFR(I3) = NFR(I3) - 1
NNODE = NNODE -1
ENDIF
40 CONTINUE
IF (ISOL .GT. 0) GO TO 5
RETURN
END

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SUBROUTINE RANDLGN (DSEED, NR, XM, S, R)

```

```

PURPOSE      LOG-NORMAL RANDOM DEVIATE GENERATOR.

```

```

REMARKS      NORMAL (0,1) PSEUDO RANDOM DEVIATES U ARE GENERATED BY
              CALLING SUBROUTINE *RANDNRM* AND TRANSFORMED TO LOG-NORMAL
              DEVIATES X, AS  $X = \text{EXP}(XM + S \cdot U)$ .

```

```

ARGUMENTS:

```

```

DSEED        INPUT/OUTPUT DOUBLE PRECISION SEED NUMBER HAVING
              AN INTEGER VALUE IN THE EXCLUSIVE RANGE
              (1.D0, 2147483647.D0). DSEED IS REPLACED BY
              A NEW VALUE TO BE USED IN A SUBSEQUENT CALL.

```

```

NR           NUMBER OF DEVIATES TO BE GENERATED (INPUT).

```

```

XM,S        INPUT PARAMETERS, SEE REMARKS.

```

```

R(I)        OUTPUT VECTOR OF LENGTH NR+1 CONTAINING THE LOG-
              NORMAL DEVIATES IN THE FIRST NR LOCATIONS.
              R(NR+1) IS WORK STORAGE.

```

```

INTEGER NR
REAL R(1), XM, S
DOUBLE PRECISION DSEED
INTEGER I, NN, M
NN = NR
M = MOD(NR, 2)
IF (M.NE.0) NN = NN+1
CALL RANDNRM(DSEED, NN, R)
DO 5 I = 1, NR
R(I) = EXP(XM+S*R(I))
CONTINUE
RETURN
END

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SUBROUTINE RANDNRM (DSEED,NR,R)

PURPOSE NORMAL RANDOM DEVIATE GENERATOR VIA THE POLAR METHOD.

ARGUMENTS:

DSEED INPUT/OUTPUT DOUBLE PRECISION SEED NUMBER HAVING
AN INTEGER VALUE IN THE EXCLUSIVE RANGE OF
(1.D0, 2147483647.D0). DSEED IS REPLACED BY
A NEW VALUE TO BE USED IN A SUBSEQUENT CALL.

NR NUMBER OF DEVIATES TO BE GENERATED (INPUT).
NR MUST BE 2 OR GREATER. IF NR IS ODD, NR-1
DEVIATES ARE GENERATED.

R(I) OUTPUT VECTOR OF LENGTH NR CONTAINING THE NORMAL
DEVIATES. IF NR IS ODD, R(NR) IS NOT USED.

INTEGER NR, I, NN, M
REAL R(NR)
DOUBLE PRECISION DSEED
REAL U, V, SUM, SLN, Z, D2P31M, D2PN31
DATA D2P31M/2147483647.D0/
DATA D2PN31/2147483648.D0/
NN = NR
M = MOD(NR, 2)
IF (M .NE. 0) NN = NN-1
Z = DSEED
5 DO 10 I = 1, NN, 2
Z = AMOD(16807.E0*Z, D2P31M)
U = Z/D2PN31
Z = AMOD(16807.E0*Z, D2P31M)
V = Z/D2PN31
U = U+U-1.0
V = V+V-1.0
SUM = U*U+V*V
IF(SUM .GE. 1.0) GO TO 5
SLN = ALOG(SUM)
SLN = SQRT((-SLN-SLN)/SUM)
R(I) = U*SLN
R(I+1) = V*SLN
10 CONTINUE
DSEED = DBLE(Z)
RETURN
END

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SUBROUTINE RANDUFM (DSEED,NR,R)

PURPOSE BASIC UNIFORM (0,1) PSEUDO-RANDOM NUMBER GENERATOR.

ARGUMENTS:

- DSEED INPUT/OUTPUT DOUBLE PRECISION SEED NUMBER HAVING AN INTEGER VALUE IN THE EXCLUSIVE RANGE OF (1.D0, 2147483647.D0). DSEED IS REPLACED BY A NEW VALUE TO BE USED IN A SUBSEQUENT CALL.
- NR NUMBER OF DEVIATES TO BE GENERATED (INPUT).
- R(I) OUTPUT VECTOR OF LENGTH NR CONTAINING THE PSEUDO-RANDOM UNIFORM (0,1) DEVIATES.

INTEGER NR
REAL R(NR)
DOUBLE PRECISION DSEED
INTEGER I
REAL S2P31,S2P31M,SEED

$$S2P31M = (2^{**}31) - 1$$
$$S2P31 = (2^{**}31)$$

```
DATA S2P31M/2147483647.E0/  
DATA S2P31 /2147483648.E0/  
SEED = DSEED  
DO 5 I=1,NR  
  SEED = AMOD (16807.E0*SEED,S2P31M)  
5 R(I) = SEED / S2P31  
DSEED = SEED  
RETURN  
END
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SUBROUTINE SUPDRV (N1,X1,N2,X2,ICK,P)

PURPOSE FIND THE FINITE LINE INTERSECTION BETWEEN TWO FINITE PLANES.
ON OUTPUT, THE LINE SEGMENT IS REPRESENTED BY TWO END POINTS
OF THE LINE.

ARGUMENTS:

- N1,N2 INDEX DEFINING THE SHAPE OF THE FINITE PLANE;
CIRCLE = 1, ELLIPSE = 2, SQUARE = 3, RECTANGLE = 4.

- X1(I),X2(I) INPUT VECTORS CONTAINING THE GEOMETRY PARAMETERS
USED TO SPECIFY TWO FINITE PLANES.
I=1,3 ARE GLOBAL X-Y-Z COORDINATES DENOTING THE
THE CENTER LOCATION OF THE PLANES.
I=4,6 ARE ANGLES (IN DEGREES) SPECIFYING THE
ORIENTATION OF THE PLANES.
I=7,8 ARE CHARACTERISTIC LENGTH SCALES ASSOCIATED
WITH THE SHAPE OF THE FINITE PLANE.

- ICK OUTPUT INDEX, ICK = 2 IF AN INTERSECTING LINE SEGMENT
EXISTS; ICK = 0 IF TWO FINITE PLANES DO NOT
INTERSECT; ICK = 1 INDICATES POSSIBLE ERROR
CONIDITION IN THIS SUBROUTINE.

- P(I,J) OUTPUT MATRIX OF 3*2 CONTAINING THE GLOBAL X-Y-Z
COORDINATES (I=1,3) OF TWO END POINTS (J=1,2)
OF THE INTERSCTING LINE SEGMENT.

```
REAL X1(9),X2(9),P(3,2)
REAL TG1(3,2),TG2(3,2),TL1(2,2),TL2(2,2),TX(3,2)
REAL TP1(2,2),TP2(2,2),TOUT(3,4)
TERR = 1.E-9
CALL SUPINT(X1,X2,ICK,TX)
IF (ICK .EQ. 0) RETURN
CALL SUPGTL(2,TX,TL1,X1)
CALL SUPGTL(2,TX,TL2,X2)
IF (N1 .LE. 2) THEN
CALL SUPCIR(TL1,X1(7),X1(8),IC1,TP1)
ELSE
CALL SUPRET(TL1,X1(7),X1(8),IC1,TP1)
ENDIF
IF (N2 .LE. 2) THEN
CALL SUPCIR(TL2,X2(7),X2(8),IC2,TP2)
```

```

ELSE
CALL SUPRET (TL2,X2 (7) ,X2 (8) ,IC2,TP2)
ENDIF
ICK = IC1 * IC2
IF (ICK .EQ. 0) RETURN
ICK = 0
CALL SUPLTG (2,TP1,TG1,X1)
CALL SUPLTG (2,TP2,TG2,X2)
CALL SUPGTL (2,TG1,TP1,X2)
CALL SUPGTL (2,TG2,TP2,X1)
DO 10 J = 1 , 2
C   TP1 ON 2
    IIC = 0
    IF (N2 .LE. 2) THEN
    IIC = ICKCIR ( TP1 (1,J) ,TP1 (2,J) ,X2 (7) ,X2 (8) )
    ELSE
    IIC = ICKRET ( TP1 (1,J) ,TP1 (2,J) ,X2 (7) ,X2 (8) )
    ENDIF
    IF ( IIC .EQ. 1) THEN
    ICK = ICK + 1
    DO 12 J1 = 1, 3
12   TOUT (J1,ICK) = TG1 (J1,J)
    ENDIF
C   TP2 ON 1
    IIC = 0
    IF (N1 .LE. 2) THEN
    IIC = ICKCIR ( TP2 (1,J) ,TP2 (2,J) ,X1 (7) ,X1 (8) )
    ELSE
    IIC = ICKRET ( TP2 (1,J) ,TP2 (2,J) ,X1 (7) ,X1 (8) )
    ENDIF
    IF ( IIC .EQ. 1) THEN
    ICK = ICK + 1
    DO 14 J1 = 1, 3
14   TOUT (J1,ICK) = TG2 (J1,J)
    ENDIF
10   CONTINUE
    IF (ICK .EQ. 2) THEN
    DO 20 J1 = 1, 3
    P (J1,1) = TOUT (J1,1)
20   P (J1,2) = TOUT (J1,2)
    ENDIF
    IF (ICK .GT. 2) THEN
    P (1,1) = TOUT (1,1)
    P (2,1) = TOUT (2,1)
    P (3,1) = TOUT (3,1)
    IIC = 1
    DO 22 J1 = 2, ICK
    IF ( (ABS (TOUT (1,J1)-P (1,1)) .LT. TERR) .AND.
1     (ABS (TOUT (2,J1)-P (2,1)) .LT. TERR) .AND.
1     (ABS (TOUT (3,J1)-P (3,1)) .LT. TERR) ) THEN

```

```

IIC = IIC + 1
JC = J1
ENDIF
22 CONTINUE
IF ( IIC .EQ. 2 ) THEN
P(1,2) = TOUT(1,JC)
P(2,2) = TOUT(2,JC)
P(3,2) = TOUT(3,JC)
ICK = IIC
ELSE
ICK = 0
100 WRITE(9,100)
FORMAT(2X,'***** WARNING ON SUBROUTINE SUPDRV ***** ')
ENDIF
ENDIF
IF (ICK .EQ. 1) WRITE (9,100)
RETURN
END

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FUNCTION ICKCIR(X,Y,R1,R2)

PURPOSE CHECK IF A POINT (X,Y) IS LOCATED INSIDE AN ELLIPSE.
IF TRUE, ICKCIR = 1; OTHERWISE ICKCIR = 0.

ARGUMENTS:

X,Y COORDINATES OF A POINT (INPUT).
R1,R2 CHARACTERISTIC LENGTH SCALE DEFINING THE ELLIPSE.
THE BOUNDARY THE ELLIPSE IS GIVEN BY:
 $(X*X)/(R1*R1) + (Y*Y)/(R2*R2) = 1$ (INPUT).

```
REAL X,Y,R1,R2,TEM
ICKCIR = 0
TEM = X*X / (R1*R1) + Y*Y / (R2*R2)
IF ( TEM .LE. 1. ) ICKCIR = 1
RETURN
END
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FUNCTION ICKRET(X,Y,R1,R2)

PURPOSE CHECK IF A POINT (X,Y) IS LOCATED INSIDE A RECTANGLE.
IF TRUE, ICKRET = 1, OTHERWISE ICKRET = 0.

ARGUMENTS:

X,Y COORDINATES OF A POINT (INPUT).
R1,R2 CHARACTERISTIC LENGTH SCALE DEFINING THE RECTANGLE.
THE AREA OF THE RECTANGLE IS BOUND BY
 $ABS(X) <= R1$ AND $ABS(Y) <= R2$ (INPUT).

```
REAL X,Y,R1,R2
ICKRET = 0
IF ( (ABS(X) .LE. R1) .AND. (ABS(Y) .LE. R2) ) ICKRET = 1
RETURN
END
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SUBROUTINE SUPLTG(NI,XYL,XYZG,XINP)
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PURPOSE      PERFORM COORDINATE TRANSFORMATION FROM A LOCAL 2-D
C             COORDINATE SYSTEM DEFINED FOR EACH INDIVIDUAL FINITE
C             PLANE TO THE GLOBAL 3-D COORDINATES.
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ARGUMENTS:
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NI           NO. OF TRANSFORMATIONS (INPUT).
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XYL(I,J)    INPUT MATRIX OF 2*NI CONTAINING THE LOCAL X-Y
C             COORDINATES (I=1,2) OF POINT J.
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XYZG(I,J)   OUTPUT MATRIX OF 3*NI CONTAINING THE GLOBAL X-Y-Z
C             COORDINATES (I=1,3) OF POINT J.
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XINP(I)     INPUT VECTOR CONTAINING THE GEOMETRY PARAMETERS
C             USED TO SPECIFY A FINITE PLANE.
C             I=1,3 ARE GLOBAL X-Y-Z COORDINATES DENOTING THE
C             THE CENTER LOCATION OF THE PLANE.
C             I=4,6 ARE ANGLES (IN DEGREES) SPECIFYING THE
C             ORIENTATION OF THE FINITE PLANE.
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```

INTEGER NI
REAL XYL(2,NI),XYZG(3,NI),XINP(9),XA2(3),XA3(3)
DATA PI,DG2RAD / 3.141592654,0.0174532925199433/
AALP = XINP(4) * DG2RAD
ABTA = XINP(5) * DG2RAD
ATHT = XINP(6) * DG2RAD
XA2(1) = SIN(ABTA)*COS(AALP)
XA2(2) = SIN(ABTA)*SIN(AALP)
XA2(3) = -COS(ABTA)
XA3(1) = -SIN(AALP)
XA3(2) = COS(AALP)
XA3(3) = 0.0
DO 10 N = 1,NI
XB = XYL(1,N)*COS(ATHT) - XYL(2,N)*SIN(ATHT)
YB = XYL(1,N)*SIN(ATHT) + XYL(2,N)*COS(ATHT)
DO 10 J = 1, 3
10 XYZG(J,N) = XINP(J) + XB*XA2(J) + YB*XA3(J)
RETURN
END

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SUBROUTINE SUPGTL(NI,TP,XYL,XCN)

PURPOSE PERFORM COORDINATE TRANSFORMATION FROM THE GLOBAL 3-D
 COORDINATES TO A LOCAL 2-D SYSTEM DEFINED FOR EACH
 INDIVIDUAL FINITE PLANE.

ARGUMENTS:

- NI NO. OF TRANSFORMATIONS (INPUT).
- TP(I,J) INPUT MATRIX OF 3*NI CONTAINING THE GLOBAL X-Y-Z
 COORDINATES (I=1,3) OF POINT J.
- XYL(I,J) OUTPUT MATRIX OF 2*NI CONTAINING THE LOCAL X-Y
 COORDINATES (I=1,2) OF POINT J.
- XCN(I) INPUT VECTOR CONTAINING THE GEOMETRY PARAMETERS
 USED TO SPECIFY A FINITE PLANE.
 I=1,3 ARE GLOBAL X-Y-Z COORDINATES DENOTING THE
 THE CENTER LOCATION OF THE PLANE.
 I=4,6 ARE ANGLES (IN DEGREES) SPECIFYING THE
 ORIENTATION OF THE FINITE PLANE.

```

INTEGER NI
REAL XYL(2,NI),TP(3,NI),XCN(9),XC2(3),XC3(3)
DATA TERR / 1.E-9/
DATA PI,DG2RAD / 3.141592654,0.0174532925199433/
AALP = XCN(4) * DG2RAD
ABTA = XCN(5) * DG2RAD
ATHT = XCN(6) * DG2RAD
XC2(1)= SIN(ABTA)*COS(AALP)
XC2(2)= SIN(ABTA)*SIN(AALP)
XC2(3)=-COS(ABTA)
XC3(1)=-SIN(AALP)
XC3(2)= COS(AALP)
XC3(3)= 0.0
DO 10 N = 1, NI
IF ( ABS(XC2(3)) .GT. TERR ) THEN
XB=(TP(3,N)-XCN(3))/XC2(3)
ELSE
XB=(XC3(2)*(TP(1,N)-XCN(1))-XC3(1)*(TP(2,N)-XCN(2)))
1 / (XC3(2)*XC2(1)-XC3(1)*XC2(2))
ENDIF
IF ( ABS(XC2(3)) .GT. TERR ) THEN

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```
YB=(TP(1,N)-XCN(1)-XB*XC2(1))/XC3(1)
ELSE
YB=(TP(2,N)-XCN(2)-XB*XC2(2))/XC3(2)
ENDIF
XYL(1,N) = XB*COS(ATHT) + YB*SIN(ATHT)
XYL(2,N) =-XB*SIN(ATHT) + YB*COS(ATHT)
10 CONTINUE
RETURN
END
```



```

ENDIF
ELSE
IF ( ABS (B) .LT. TERR) THEN
X = -C / A
IF ( ABS (X) .LE. R1) THEN
ICUT=1
CX(1,1) = X
CX(1,2) = X
CX(2,1) = R2
CX(2,2) =-R2
ELSE
ICUT=0
ENDIF
ELSE
XX(1) = R1
YY(1) = (-A*R1-C)/B
XX(2) =-R1
YY(2) = ( A*R1-C)/B
YY(3) = R2
XX(3) = (-3*R2-C)/A
YY(4) =-R2
XX(4) = ( B*R2-C)/A
ICCT=0
DO 10 IC = 1,4
IF ((ABS (XX (IC)) .LE. R1) .AND. (ABS (YY (IC)) .LE. R2)) THEN
ICCT = ICCT + 1
CT(1, ICCT) = XX (IC)
CT(2, ICCT) = YY (IC)
ENDIF
10 CONTINUE
IF (ICCT .EQ. 0) THEN
ICUT = 0
ELSE
CX(1,1) = CT(1,1)
CX(2,1) = CT(2,1)
JCT = 1
DO 15 J= 2, ICCT
IF ( CT(1,J) .NE. CT(1,1)) THEN
CX(1,2) = CT(1,J)
CX(2,2) = CT(2,J)
JCT = 2
ENDIF
15 CONTINUE
ICUT = 1
IF (JCT .EQ. 1) ICUT=0
ENDIF
ENDIF
ENDIF
RETURN
END

```



```

ELSE
ICUT=0
ENDIF
ELSE
RLA = R1*R1*A*A
AX = 1./(R2*R2) + B*B / RLA
BX = 2.*B*C / RLA
CX = C*C / RLA - 1
BAC = BX*BX - 4.*AX*CX
IF (BAC .GT. 0) THEN
ICUT=1
CT(2,1) = (-BX + SQRT(BAC)) / (2.*AX)
CT(1,1) = (- B*CT(2,1) - C) / A
CT(2,2) = (-BX - SQRT(BAC)) / (2.*AX)
CT(1,2) = (- B*CT(2,2) - C) / A
ELSE
ICUT=0
ENDIF
ENDIF
RETURN
END

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SUBROUTINE SUPINT (XAN,XBN,INCT,P)

PURPOSE FIND THE LINE INTERSECTION BETWEEN TWO INFINITE PLANES.
ON OUTPUT, THE LINE INTERSECTION IS REPRESENTED BY TWO
DISTINCT POINTS ON THE LINE.

ARGUMENTS:

XAN (I),XBN (I) INPUT VECTORS CONTAINING THE GEOMETRY PARAMETERS
USED TO SPECIFY TWO INFINITE PLANES.
I=1,3 ARE GLOBAL X-Y-Z COORDINATES DENOTING THE
THE CENTER LOCATION OF THE PLANES.
I=4,6 ARE ANGLES (IN DEGREES) SPECIFYING THE
ORIENTATION OF THE PLANES.

INCT OUTPUT INDEX, INCT = 1 IF A LINE INTERSECTION EXISTS;
OTHERWISE INCT = 0.

P (I,J) OUTPUT MATRIX OF 3*2 CONTAINING THE GLOBAL X-Y-Z
COORDINATES (I=1,3) OF TWO DISTINCT POINTS (J=1,2)
ON THE LINE INTERSECTION.

```
REAL XAN (9),XBN (9),P (3,2)
REAL XA (4),XB (4),R1 (3),R2 (3)
DATA TERR / 1.E-9/
DATA PI,DG2RAD / 3.141592654,0.0174532925199433/
XA (1)=COS (XAN (5)*DG2RAD)*COS (XAN (4)*DG2RAD)
XA (2)=COS (XAN (5)*DG2RAD)*SIN (XAN (4)*DG2RAD)
XA (3)=SIN (XAN (5)*DG2RAD)
XA (4)=XA (1)*XAN (1)+XA (2)*XAN (2)+XA (3)*XAN (3)
XB (1)=COS (XBN (5)*DG2RAD)*COS (XBN (4)*DG2RAD)
XB (2)=COS (XBN (5)*DG2RAD)*SIN (XBN (4)*DG2RAD)
XB (3)=SIN (XBN (5)*DG2RAD)
XB (4)=XB (1)*XBN (1)+XB (2)*XBN (2)+XB (3)*XBN (3)
IF ((ABS (XA (1)*XB (2)-XB (1)*XA (2)) .LT. TERR) .AND.
1 (ABS (XA (2)*XB (3)-XB (2)*XA (3)) .LT. TERR) .AND.
2 (ABS (XA (3)*XB (1)-XB (3)*XA (1)) .LT. TERR)) THEN
  INCT=0
ELSE
  INC1=1
  R00=XA (1)*XB (2)-XB (1)*XA (2)
  IF (ABS (R00) .GT. TERR) THEN
    R1 (1)=(XB (3)*XA (2)-XA (3)*XB (2))/R00
    R1 (2)=(XB (1)*XA (3)-XA (1)*XB (3))/R00
```

```

R1(3)=1.
R2(1)=(XB(2)*XA(4)-XA(2)*XB(4))/R00
R2(2)=(XB(4)*XA(1)-XA(4)*XB(1))/R00
R2(3)=0.
ELSE
R00=XA(2)*XB(3)-XB(2)*XA(3)
IF (ABS(R00) .GT. TERR) THEN
R1(1)=1.
R1(2)=(XB(1)*XA(3)-XA(1)*XB(3))/R00
R1(3)=(XB(1)*XA(2)-XA(1)*XB(2))/R00
R2(1)=0.
R2(2)=(XB(3)*XA(4)-XA(3)*XB(4))/R00
R2(3)=(XB(4)*XA(2)-XA(4)*XB(2))/R00
ELSE
R00=XA(3)*XB(1)-XB(3)*XA(1)
R1(1)=(XB(3)*XA(2)-XA(3)*XB(2))/R00
R1(2)=1.
R1(3)=(XB(2)*XA(1)-XA(2)*XB(1))/R00
R2(1)=(XB(4)*XA(3)-XA(4)*XB(3))/R00
R2(2)=0.
R2(3)=(XB(1)*XA(4)-XA(1)*XB(4))/R00
ENDIF
ENDIF
DO 10 J=1,3
P(J,1)= R1(J) * 1.0 + R2(J)
P(J,2)=-R1(J) * 1.0 + R2(J)
CONTINUE
ENDIF
RETURN
END

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SUBROUTINE SUBLEQS (A,M,N,B,IB,D1,D2,IER)
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PURPOSE      LINEAR EQUATION SOLUTION OF A SYMMETRIC, POSITIVE DEFINITE
C             MATRIX.
```

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ARGUMENTS:
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A(I)         INPUT VECTOR OF LENGTH N(N+1)/2 CONTAINING THE N BY N
C             COEFFICIENT MATRIX OF THE EQUATION AX = B. A IS
C             A POSITIVE DEFINITE SYMMETRIC MATRIX STORED IN
C             SYMMETRIC STORAGE MODE.
```

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M            NUMBER OF RIGHT HAND SIDES OR COLUMNS IN B (INPUT).
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N            ORDER OF A AND NUMBER OF ROWS IN B (INPUT).
```

```
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C
B(I,J)       INPUT MATRIX OF N * M CONTAINING THE RIGHT-HAND SIDES
C             OF THE EQUATION AX = B.
C             ON OUTPUT, THE N BY M SOLUTION MATRIX X REPLACES B.
```

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IB           ROW DIMENSION OF B EXACTLY AS SPECIFIED IN THE
C             DIMENSION STATEMENT IN THE CALLING PROGRAM (INPUT).
```

```
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D1,D2        COMPONENTS OF THE DETERMINANT OF A, WHERE:
C             DETERMINANT(A) = D1*2.**D2 (OUTPUT).
```

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IER          ERROR PARAMETER (OUTPUT).
C             IER = 1 INDICATES THAT THE INPUT MATRIX A IS
C             ALGORITHMICALLY NOT POSITIVE DEFINITE.
```

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C
DIMENSION A(1),B(IB,1)
```

```
IER = 0
```

```
                DECOMPOSE A
```

```
CALL SUBDECP (A,A,N,D1,D2,IER)
```

```
IF (IER.NE.0) RETURN
```

```
                PERFORM ELIMINATION
```

```
DO 5 I = 1,M
```

```
    CALL SUBLUEM (A,B(1,I),N,B(1,I))
```

```
CONTINUE
```

```
RETURN
```

```
END
```



```

D1 = D1*X
IF (A(IP) + X*RN .LE. A(IP)) GO TO 50
15 IF (ABS(D1).LE.ONE) GO TO 20
D1 = D1 * SIXTH
D2 = D2 + FOUR
GO TO 15
20 IF (ABS(D1) .GE. SIXTH) GO TO 25
D1 = D1 * SIXTN
D2 = D2 - FOUR
GO TO 20
25 UL(IP) = ONE/SQRT(X)
GO TO 35
30 UL(IP) = X * UL(IR)
35 IP1 = IP
IP = IP+1
IR = IR+1
40 CONTINUE
45 CONTINUE
RETURN
50 IER = 1
RETURN
END

```



```
IS=IP
IQ=II+1
T=X(II)
IF (N.LT.IQ) GO TO 25
KK = N
DO 20 K=IQ,N
  T = T - A(IS) * X(KK)
  KK = KK-1
  IS = IS-KK
20 CONTINUE
25 X(II)=T*A(IS)
30 CONTINUE
RETURN
END
```

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A.4 SAMPLE INPUT/OUTPUT FOR EXPERIMENT 1

SAMPLE OF INPUT DECK SETUP FOR EXPERIMENT 1

#EOR		(END OF RECORD)
200., 200., 200., 200.		(NFRCT, FRX, FRY, FRZ)
50., 10.		(FRCTLTH, FRCAPTR)
918., 35., 763., 849.		(DS1, DS2, DS3, DS4)
3		(NSET)
100., 100., 130., 0., 0., 100., 100., 100.	(COR0, COAL, COSZ)	
100., 100., 125., 0., 0., 110., 110., 110.	(COR0, COAL, COSZ)	
100., 100., 120., 0., 0., 120., 120., 120.	(COR0, COAL, COSZ)	
#EOR		(END OF RECORD)
#EOF		(END OF FILE)

*
* SAMPLE OUTPUT FROM EXPERIMENT 1
*

* ECHO INPUT PARAMETERS
*

NFRCT,FRX,FRY,FRZ : 200 200.0 200.0 200.0
FRCTLTH, FRCAPR : 50.0 10.0
SEED—DS1,DS2,DS3,DS4 : 918.0 35.0 763.0 849.0

*
* ISOLATED SAMPLE # 1 AND THE FLUXES ACROSS THE BOUNDARY SURFACES.
* NTS INDICATES DIFFERENT SAMPLE ORIENTATIONS, NEGATIVE FLUX IMPLIES
* THE FLUX INTO THE SAMPLE BLOCK.
*

SAMPLE CENTER (COR0,1) : 100.0 100.0 130.0
SAMPLE ANGLE (COAL,1) : .0 .0
SAMPLE SIZE (COSZ,1) : 100.0 100.0 100.0

(BONDARY	+X	-X	+Y	-Y	+Z	-Z)
NTS=1	-2668.66	127.62	489.19	1183.36	739.63	128.86
NTS=2	127.62	-1594.47	168.68	387.45	435.84	474.89
NTS=3	489.19	168.68	-1165.08	28.51	445.85	32.85
NTS=4	1183.36	387.45	28.51	-3228.39	1070.14	558.93
NTS=5	739.63	435.84	445.85	1070.14	-2821.24	129.78
NTS=6	128.86	474.89	32.85	558.93	129.78	-1325.30

*
* ISOLATED SAMPLE # 2 AND THE TEST RESULTS.
*

SAMPLE CENTER (COR0,1) : 100.0 100.0 125.0
SAMPLE ANGLE (COAL,1) : .0 .0
SAMPLE SIZE (COSZ,1) : 110.0 110.0 110.0

(BONDARY	+X	-X	+Y	-Y	+Z	-Z)
NTS=1	-1940.17	33.40	393.26	712.43	697.57	103.51
NTS=2	33.40	-1405.49	155.85	496.35	274.94	444.95
NTS=3	393.26	155.85	-1564.32	29.73	623.12	362.37
NTS=4	712.43	496.35	29.73	-3296.71	1382.42	675.77
NTS=5	697.57	274.94	623.12	1382.42	-3144.93	166.88
NTS=6	103.51	444.95	362.37	675.77	166.88	-1753.49

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```
COMMON /FRCT/ NFRCT, NSHF (200), XINP (9, 200), NFR (200), NFRN (1000)
COMMON /CUTP/ NCUT, XCUT (9, 12), NCT (12), NCTN (300)
COMMON /CFCF/ NCF (200), NCFN (300)
COMMON /NODE/ NNODE, NDID (400, 2), NDFR (1000)
COMMON /BOND/ NBOND, NDXD (400, 2), NDCF (300), NDCT (300)
COMMON /XYZZ/ XYZI (400, 4), XYZX (400, 4)
COMMON /MTRX/ PO (400), PX (400)
CALL INPFRCT
CALL INPCUT
CALL SUPFRCT
CALL SUPCUT
CALL SUPDEAD
CALL SUBBOND
CALL SUBMTRX
CALL OUTRUN2
STOP
END
```

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SUBROUTINE INPCUT

PURPOSE: THIS SUBROUTINE READS IN THE CENTER LOCATION (COR0),
ROTATION (COAL) AND SIZE (COSZ) OF A RECTANGULAR BLOCK
OF SAMPLE (K1=1) AND A RECTANGULAR ZONE OF INJECTION
(K1=2) AND GENERATES THE GEOMETRIC PARAMETERS FOR EACH
OF THE RECTANGULAR BOUNDARY SURFACES. THUS, BOUNDARY
SURFACES 1-6 ARE THOSE OF THE SAMPLE BLOCK AND THE SURFACES
7-12 ARE INJECTION PLANES. THIS SUB-PROGRAM CHANGES THE
CONTENTS OF THE FOLLOWING VARIABLES: NCUT, COR0, COAL,
COSZ, X CUT, CORA, CORB.

```

COMMON /FRCT/ NFRCT, NSHP (200), XINP (9, 200), NFR (200), NFRN (1000)
COMMON /CUTT/ NCUT, X CUT (9, 12), NCT (12), NCTN (300)
COMMON /CORD/ COR0 (3, 2), COSZ (3, 2), COAL (2, 2),
1          CORA (3, 3, 2), CORB (3, 3, 2)
REAL WKALP (12), WKBTA (12), WKX (3), WKYZ (18)
INTEGER NWAL (6), NWBT (6)
DATA PI, DG2RAD / 3.141592654, 0.0174532925199433/
DATA WKALP /1., 0., 1., 180., 1., 90., 1., 270., 1., 0., 1., 0./
DATA WKBTA /1., 0., -1., 0., 0., 0., 0., 0., 1., 90., 1., 270./
DATA NWAL / 3, 3, 3, 3, 1, 1 /
DATA NWBT / 2, 2, 1, 1, 2, 2 /
DATA WKYZ /1., 0., 0., -1., 0., 0., 0., 1., 0., 0., -1., 0.,
1          0., 0., 1., 0., 0., -1. /
NCUT = 6
JTOT = 2
READ (1, *) COR0 (1, 1), COR0 (2, 1), COR0 (3, 1),
1          COAL (1, 1), COAL (2, 1),
2          COSZ (1, 1), COSZ (2, 1), COSZ (3, 1)
WRITE (8, 100) COR0 (1, 1), COR0 (2, 1), COR0 (3, 1),
1          COAL (1, 1), COAL (2, 1),
2          COSZ (1, 1), COSZ (2, 1), COSZ (3, 1)
100 FORMAT (//, ' SAMPLE CENTER (COR0, 1) : ', 3F8.1/
1          ' SAMPLE ANGLE (COAL, 1) : ', 2F8.1/
2          ' SAMPLE SIZE (COSZ, 1) : ', 3F8.1)
READ (1, *) COR0 (1, 2), COR0 (2, 2), COR0 (3, 2),
1          COAL (1, 2), COAL (2, 2),
2          COSZ (1, 2), COSZ (2, 2), COSZ (3, 2)
WRITE (8, 110) COR0 (1, 2), COR0 (2, 2), COR0 (3, 2),
1          COAL (1, 2), COAL (2, 2),
2          COSZ (1, 2), COSZ (2, 2), COSZ (3, 2)
110 FORMAT (//, ' INJECT CENTER (COR0, 2) : ', 3F8.1/
1          ' INJECT ANGLE (COAL, 2) : ', 2F8.1/
2          ' INJECT SIZE (COSZ, 2) : ', 3F8.1)

```

```

DO 10 K1=1, JTOT
ALPP = COAL(1, K1) * DG2RAD
BETT = COAL(2, K1) * DG2RAD
CORA(1, 1, K1) = COS(ALPP) * COS(BETT)
CORA(2, 1, K1) = SIN(ALPP) * COS(BETT)
CORA(3, 1, K1) = SIN(BETT)
CORA(1, 2, K1) = -SIN(ALPP)
CORA(2, 2, K1) = COS(ALPP)
CORA(3, 2, K1) = 0.
CORA(1, 3, K1) = -COS(ALPP) * SIN(BETT)
CORA(2, 3, K1) = -SIN(ALPP) * SIN(BETT)
CORA(3, 3, K1) = COS(BETT)
DO 9 I=1, 3
DO 9 J=1, 3
9 CORB(I, J, K1) = CORA(J, I, K1)
10 CONTINUE
DO 30 K1=1, JTOT
DO 25 J=1, NCUT
J4 = J + (K1-1)*NCUT
DO 20 J1=1, 3
WKKK = 0.
DO 15 J2=1, 3
15 WKKK = WKKK + CORA(J1, J2, K1) * COSZ(J2, K1) * WKYZ(3*(J-1)+J2)/2.
20 XCUT(J1, J4) = COR0(J1, K1) + WKKK
XCUT(4, J4) = COAL(1, K1) * WKALP(2*(J-1)+1) + WKALP(2*(J-1)+2)
XCUT(5, J4) = COAL(2, K1) * WKBTA(2*(J-1)+1) + WKBTA(2*(J-1)+2)
XCUT(6, J4) = 0.0
XCUT(7, J4) = 0.5 * COSZ(NWAL(J), K1)
XCUT(8, J4) = 0.5 * COSZ(NWBT(J), K1)
XCUT(9, J4) = 0.0
25 CONTINUE
30 CONTINUE
NCUT = NCUT * JTOT
RETURN
END

```


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SUBROUTINE SUBBOND

PURPOSE: THIS SUBROUTINE ASSIGNS THE BOUNDARY CONDITIONS FOR
THE HYDRAULIC INJECTION TEST. THE CONTENTS OF THE VECTOR
PO IS CHANGED.

ARGUMENTS:

PRES (I) VECTOR OF LENGTH NCUT CONTAINING THE PRESSURE
HEAD VALUES (IN LENGTH UNITS) FOR THE BOUNDARY
SURFACE I.

NOTE THAT BOUNDARY SURFACES 7-12 ARE INJECTION
PLANES AND A PRESSURE HEAD OF 100 LENGTH UNITS
IS ASSIGNED FOR THIS EXPERIMENT.

COMMON /BOND/ NBOND,NDXD(400,2),NDCF(300),NDCT(300)

COMMON /XYZZ/ XYZI(400,4),XYZX(400,4)

COMMON /MTRX/ PO(400),PX(400)

1 COMMON /CORD/ COR0(3,2),COSZ(3,2),COAL(2,2),
CORA(3,3,2),CORB(3,3,2)

REAL PRES(12)

DATA PRES /0.,0.,0.,0.,0.,0.,100.,100.,100.,100.,100.,100./

DO 10 J=1,NBOND

PO(J)=PRES(NDXD(J,2))+COSZ(3,1)/2.-XYZX(J,3)

10 CONTINUE

RETURN

END

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SUBROUTINE SUBMTRX

PURPOSE: THIS SUBROUTINE ASSEMBLES THE GLOBAL MATRIX EQUATION
AND SOLVES THE HEAD DISTRIBUTION IN THE SAMPLE.

```
COMMON /FRCT/ NFRCT, NSHP(200), XINP(9,200), NFR(200), NFRN(1000)
COMMON /CUTT/ NCUT, XCUT(9,12), NCT(12), NCTN(300)
COMMON /CFCF/ NCF(200), NCFN(300)
COMMON /NODE/ NNODE, NDID(400,2), NDFR(1000)
COMMON /BOND/ NBOND, NDXD(400,2), NDCF(300), NDCT(300)
COMMON /XYZZ/ XYZI(400,4), XYZX(400,4)
COMMON /MTRX/ PO(400), PX(400)
REAL X0(4), X1(4), AA(400), BB
REAL AMTRX(50000)
DATA M, IB / 1, 400/
DATA RHO, UN, UNITCON /9810., 0.001, 0.01 /
J5=0
DO 50 I=1, NNODE
  BB=0.
  DO 5 I1=1, NNODE
    AA(I1)=0.
    J1=NDID(I,1)
    J2=NDID(I,2)
    DO 40 III=1,2
      IF (III .EQ. 2) THEN
        JTEMP=J1
        J1=J2
        J2=JTEMP
      ENDIF
    DO 15 I1=1, IFN(J1, NFR)
      ITT = IFK(J1, NFR, + I1)
      IF (J2 .EQ. NFRN(ITT) ) THEN
        JJ2=I1
        DO 24 I2=1,4
          X0(I2)= XYZI (NDFR(ITT), I2)
        ENDIF
        CONTINUE
        DO 25 I1=1, IFN(J1, NFR)
          ITT = IFK(J1, NFR) + I1
          IF (I1 .NE. JJ2) THEN
            T2=0.
            DO 20 I2=1,3
              X1(I2) = XYZI (NDFR(ITT), I2)
              T2=T2+(X1(I2)-X0(I2))**2.
            CONTINUE
          20
```

```

X1(4) = XYZI (NDFR(ITT), 4)
X0X1 = SQRT(T2)
XX = (X1(4) + X0(4))/2.
XCOEF= XX * (XINP(9,J1)**3.) * RHO
1      / ( 12. * UN * X0X1 )
AA(NDFR(ITT))=AA(NDFR(ITT)) + XCOEF
AA(I) = AA(I) - XCOEF
BB = BB + (X0(3)-X1(3))*XCOEF
ENDIF
25 CONTINUE
DO 35 I1=1, IFN(J1,NCF)
T2=0.
ITT = IFK(J1,NCF) + I1
DO 30 I2=1,3
X1(I2) = XYZX (NDCF(ITT), I2)
T2=T2+(X1(I2)-X0(I2))**2.
30 CONTINUE
X1(4) = XYZX (NDCF(ITT), 4)
X0X1 = SQRT(T2)
XX = (X1(4) + X0(4))/2.
XCOEF= XX * (XINP(9,J1)**3.) * RHO
1      / ( 12. * UN * X0X1 )
AA(I) = AA(I) - XCOEF
BB = BB + (X0(3)-X1(3)-PO(NDCF(ITT)))*XCOEF
35 CONTINUE
40 CONTINUE
DO 45 I1=1,I
AMTRX(J5+I1) = -AA(I1)
45 CONTINUE
J5=J5+I
PX(I) = -BB
50 CONTINUE
IER = 0
CALL SUBLEQS (AMTRX,M,NNODE,PX,IB,D1,D2,IER)
IF ( IER .GT. 0) THEN
WRITE (8, *) 'ERROR MSG FROM *SUBLEQS* IER =',IER
ENDIF
RETURN
END

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SUBROUTINE OUTRUN2

PURPOSE: THIS SUBROUTINE WRITES THE FRACTURE NETWORK INFORMATION AND THE HYDRAULIC DATA INTO A TEMPORARY FILE TO BE USED IN RUN2 OF THE EXPERIMENT.

```
COMMON /FRCT/ NFRCT, NSHP(200), XINP(9,200), NFR(200), NFRN(1000)
COMMON /CUT/ NCUT, XCUT(9,12), NCT(12), NCTN(300)
COMMON /CFCF/ NCF(200), NCFN(300)
COMMON /NODE/ NNODE, NDID(400,2), NDFR(1000)
COMMON /BOND/ NBOND, NDXD(400,2), NDCF(300), NDCT(300)
COMMON /XYZZ/ XYZI(400,4), XYZX(400,4)
COMMON /MTRX/ PO(400), PX(400)
WRITE (10,*) NFRCT, NFR(NFRCT), NCF(NFRCT), NNODE, NBOND
DO 10 J = 1, NFRCT
WRITE (10,*) J, XINP(9,J),
1 IFN(J,NFR), (NDFR(K),K=IFK(J,NFR)+1,NFR(J)),
2 IFN(J,NCF), (NDCF(K),K=IFK(J,NCF)+1,NCF(J))
10 CONTINUE
DO 20 J = 1, NNODE
WRITE (10,*) J, PX(J), NDID(J,1), NDID(J,2), (XYZI(J,K),K=1,4)
20 CONTINUE
DO 30 J = 1, NBOND
WRITE (10,*) J, PO(J), NDXD(J,1), NDXD(J,2), (XYZX(J,K),K=1,4)
30 CONTINUE
RETURN
END
```



```

C      TCHK(I)          VECTOR OF LENGTH N+1, WHERE N IS THE NUMBER OF
C      CHECK POINTS, CONTAINING THE CHARACTERISTIC
C      TIME SCALES CORRESPONDING TO THE RELATIVE BT
C      VALUES DEFINED BY VEATOR *CCHK*.
C
C      NIJET           TOTAL NUMBER OF BOUNDARY SURFACES WHERE THE
C      TRACER WILL BE APPLIED AT TIME UNIT 0.
C
C      NJET(I)         VECTOR OF LENGTH NIJET CONTAINING THE BOUNDARY
C      SURFACE NUMBER OF WHICH A TRACER IS APPLIED AT
C      TIME 0.
C
C      AVGVEL          AVERAGE VELOCITY OF THE FRACTURE NETWORK.
C
C      VOLSUM          TOTAL VOLUME OF THE FLOWING FLUID IN THE NETWORK.
C
C
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```

```

COMMON /FRCT/ NFRCT,APER(200),NFR(200),NCF(200)
COMMON /NODE/ NNODE,NDID(300,2),PX(300),XYZI(300,4)
COMMON /BOND/ NBOND,NDXD(200,2),PO(200),XYZX(200,4)
COMMON /FLNT/ INET(300),FINND(300)
COMMON /FBND/ INXT(200),FEXND(200)
COMMON /RFDN/ NDFR(700),NDCF(300)
COMMON /ERTI/ ITRE(1800),FTRE(1800),TYMIN(1800)
COMMON /XRTI/ ITRX(800),FTRX(800),TYMEX(800)
COMMON /IJET/ NIJET, NJET(12)
DIMENSION BTCV(2050),TCHK(7),CCHK(7),NDCHK(6)
DATA NCHK,NDCHK / 6, -1, -2, -3, -4, -5, -6/
DATA TBEG,TEND,NSTP / 0.0, 2000.0, 2000 /
DATA CCHK / 0.0, 0.1, 0.25, 0.5, 0.75, 0.90, 1.5/
DATA NIJET,NJET / 6, 7, 8, 9, 10, 11, 12, 0,0,0,0,0,0 /
CALL INPDATA
CALL FLOWNET (AVGVEL,VOLSUM)
WRITE (10,100) AVGVEL,VOLSUM
100  FORMAT (/2X,'***** GLOBAL VOLUME AVERAGED VELOCITY = ',
1     F14.4,/ 2X,'***** GLOBAL VOLUME = ',
2     F14.4,/)
CALL OUTFLNT
DO 20 I = 1, NCHK
CALL TRACER ( NDCHK(I), TBEG, TEND, NSTP, BTCV)
J1=1
TYMST = (TBEG - TEND) / REAL(NSTP)
DO 10 J0 = 2,NSTP+1
IF( (BTCV(J0)-CCHK(J1)) .GT. 1.E-9 ) THEN
TCHK(J1) = TYMST * (REAL (J0-2) + (CCHK(J1) - BTCV(J0-1))
1     / (BTCV(J0)-BTCV(J0-1)) )
J1=J1+1
ENDIF
10  CONTINUE

```

```
J1=J1-1
WRITE (10,110) NDCHK(I),TEND,BTCV(NSTP+1),
1      (NINT(100.*CCHK(J0)),TCHK(J0),J0=1,J1)
110  FORMAT (/2X,'NODE, T-END, BT-TEND: ',15,4X,F6.0,
1      4X,F7.4/(3(2X,'T',12,' = ',F6.1,2X)) )
20   CONTINUE
STOP
END
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SUBROUTINE INPDATA

PURPOSE: THIS SUBROUTINE READS IN THE FRACTURE NETWORK INFORMATION, INCLUDING HYDRAULIC HEAD DISTRIBUTIONS, FROM A DATA FILE. THE DATA FILE IS CREATED IN PROGRAM *EXP2R1*, OR RUN 1 OF THE HYDRAULIC-TRACER INJECTION EXPERIMENT. INPUT DATA ARE STORED IN COMMON BLOCKS /FRCT/, /NODE/, /BOND/ AND /RFND/.

```

COMMON /FRCT/ NFRCT,APER(200),NFR(200),NCF(200)
COMMON /NODE/ NNODE,NDID(300,2),PX(300),XYZI(300,4)
COMMON /BOND/ NBOND,NDXD(200,2),PO(200),XYZX(200,4)
COMMON /RFND/ NDFR(700),NDCF(300)
DIMENSION NTEM(25),NTEN(25)
READ (1,*) NFRCT,NFRSUM,NCFSUM,NNODE,NBOND
NFRJ=0
NCFJ=0
DO 20 J = 1, NFRCT
  NFRJP1 = NFRJ + 1
  NCFJP1 = NCFJ + 1
  READ (1,*) J1,APER(J), NFRJ1, (NTEM(J2),J2=1,NFRJ1),
1      NCFJ1, (NTEN(J2),J2=1,NCFJ1)
  DO 6 K=NFRJP1,NFRJP1+NFRJ1
6      NDFR(K) = NTEM(K-NFRJP1+1)
  DO 7 K=NCFJP1,NCFJP1+NCFJ1
7      NDCF(K) = NTEN(K-NCFJP1+1)
  IF ( J1 .NE. J) THEN
    WRITE (10,100) J, J1
100    FORMAT (2X,'*** INPUT DATA ERROR IN INBNL LOOP 20 *****',
1      'J = ',I5,5X,'J1 = ',I5)
    RETURN
  ENDIF
  NFRJ = NFRJ + NFRJ1
  NCFJ = NCFJ + NCFJ1
  NFR(J) = NFRJ
  NCF(J) = NCFJ
20  CONTINUE
  IF ((NFR(NFRCT) .NE. NFRSUM) .OR. (NCF(NFRCT) .NE. NCFSUM)) THEN
    WRITE (10,110) NFRSUM,NFR(NFRCT),NCFSUM,NCF(NFRCT)
110    FORMAT (2X,'*** INPUT DATA ERROR IN INBNL LOOP 20 *****',
1      'NFRS,NFR(S)=' ,2I5,5X,'NCF(S),NCF(S)=' ,2I5)
  ENDIF
  DO 30 J = 1, NNODE
  READ (1,*) J1, PX(J1), NDID(J1,1),NDID(J1,2), (XYZI(J1,K),K=1,4)
  IF ( J1 .NE. J) THEN

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        WRITE (10,120) J, J1
120     FORMAT (2X,'*** INPUT DATA ERROR IN INBNL LOOP 30 *****',
1         'J = ',I5,5X,'J1 = ',I5)
        RETURN
        ENDIF
30     CONTINUE
        DO 40 J = 1, NBOND
        READ (1,*) J1, PO(J1), NDXD(J1,1),NDXD(J1,2), (XYZX(J1,K),K=1,4)
        IF ( J1 .NE. J) THEN
130     WRITE (10,130) J, J1
        FORMAT (2X,'*** INPUT DATA ERROR IN INBNL LOOP 40 *****',
1         'J = ',I5,5X,'J1 = ',I5)
        RETURN
        ENDIF
40     CONTINUE
        RETURN
        END

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SUBROUTINE FLOWNET (VELOAGE,VOLSUM)

PURPOSE: THIS SUBROUTINE GENERATES A COMPLETE FLOW NETWORK FOR THE FRACTURE SYSTEM. THE OUTPUT OF THIS PROGRAM IS STORED IN COMMON BLOCKS /FLNT/, /FBND/, /ERTI/ AND /XRTI/.

ARGUMENTS:

AVGVEL AVERAGE VELOCITY OF THE FRACTURE NETWORK.
VOLSUM TOTAL VOLUME OF THE FLOWING FLUID IN THE NETWORK.

9

```
COMMON /FRCT/ NFRCT,APER(200),NFR(200),NCF(200)
COMMON /NODE/ NNODE,NDID(300,2),PX(300),XYZI(300,4)
COMMON /BOND/ NBOND,NDXD(200,2),PO(200),XYZX(200,4)
COMMON /FLNT/ INET(300),FINND(300)
COMMON /FBND/ INXT(200),FEXND(200)
COMMON /ERTI/ ITRE(1800),FTRE(1800),TYMIN(1800)
COMMON /XRTI/ ITRX(800),FTRX(800),TYMEX(800)
COMMON /REFN/ NDFR(700),NDCF(300)
DIMENSION X0(4),X1(4),XFLUX(40),JFL(40),XTYM(40)
DIMENSION XVELO(40)
VOLSUM=0.0
VOLVEL=0.0
DO 40 J = 1, NNODE
  FINND(J) = 0.
  JCNT = 0
  FLUXPOS = 0.
  FLUXNEG = 0.
  DO 9 J5 = 1, 4
    X0(J5) = XYZI(J,J5)
  DO 30 J0 = 1, 2
    JSD = NDID(J,J0)
    IF (JSD .EQ. 1) THEN
      NFRJML=0
      NCFJML=0
    ELSE
      NFRJML=NFR(JSD-1)
      NCFJML=NCF(JSD-1)
    ENDIF
    DO 15 J1 = 1,NFR(JSD)-NFRJML
      JND = NDFR(NFRJML+J1)
      IF ( JND .NE. J ) THEN
        JCNT = JCNT + 1
```

```

DO 12 J5 = 1, 4
X1 (J5) = XYZI (JND,J5)
12 CONTINUE
CALL FLXCAL( X0, PX (J), X1, PX (JND), APER (JSD), XFLUX (JCNT),
1 XVELO (JCNT), XTYM (JCNT), VOLM, FLUXPOS, FLUXNEG )
VOLSUM = VOLSUM + VOLM
VOLVEL = VOLVEL + XVELO (JCNT)*VOLM
JFL (JCNT) = JND
ENDIF
15 CONTINUE
DO 20 J1 = 1,NCF (JSD)-NCFJM1
JXD = NDCF (NCFJM1+J1)
JCNT = JCNT + 1
DO 17 J5 = 1, 4
X1 (J5) = XYZX (JXD,J5)
17 CONTINUE
CALL FLXCAL( X0, PX (J), X1, PO (JXD), APER (JSD), XFLUX (JCNT),
1 XVELO (JCNT), XTYM (JCNT), VOLM, FLUXPOS, FLUXNEG )
VOLSUM = VOLSUM + VOLM
VOLVEL = VOLVEL + XVELO (JCNT)*VOLM
JFL (JCNT) = -JXD
20 CONTINUE
30 CONTINUE
FINND (J) = FLUXPOS
IF ( ABS (FLUXPOS+FLUXNEG) .GT. 1.E-4 ) THEN
WRITE (10,100) J, FLUXPOS, FLUXNEG
100 FORMAT (5X,'*** WARNING ON SUBROUTINE *FLOWNET* ',/
1 5X,'INODE = ',I3,5X,'FLUXPOS = ',F8.4,5X,
2 'FLUXNEG = ',F8.4)
ENDIF
IF (J .EQ. 1) THEN
JJM1= 0
ELSE
JJM1= INET (J-1)
ENDIF
IF (FLUXPOS .LT. 1.E-5) THEN
JA = 0
ELSE
JA = 0
DO 35 J5 = 1, JCNT
IF (XFLUX (J5) .GT. 1.E-6) THEN
FTREJJA = XFLUX (J5)/FLUXPOS
IF (FTREJJA .GT. 1.E-5) THEN
JA = JA + 1
JJM2 = JJM1 + JA
FTRE (JJM2) = FTREJJA
TYMIN (JJM2) = XTYM (J5)
ITRE (JJM2) = JFL (J5)
ENDIF
ENDIF
ENDIF

```

```

35     CONTINUE
      ENDIF
      INET(J) = JJM1 + JA
40     CONTINUE
      DO 70 J = 1, NBOND
      FEXND(J) = 0.
      JCNT = 0
      FLUXPOS = 0.
      FLUXNEG = 0.
45     DO 45 J5 = 1, 4
      X0(J5) = XYZX(J,J5)
      JSD = NDXD(J,1)
      IF (JSD .EQ. 1) THEN
          NFRJM1=0
          NCFJM1=0
      ELSE
          NFRJM1=NFR(JSD-1)
          NCFJM1=NCF(JSD-1)
      ENDIF
      DO 55 J1 = 1,NFR(JSD)-NFRJM1
      JND = NDFR(NFRJM1+J1)
      JCNT = JCNT + 1
      DO 52 J5 = 1, 4
      X1(J5) = XYZI(JND,J5)
52     CONTINUE
      CALL FLXCAL( X0, PO(J), X1, PX(JND), APER(JSD), XFLUX(JCNT),
1          XVELO(JCNT), XTYM(JCNT), VOLM, FLUXPOS, FLUXNEG )
      VOLSUM = VOLSUM + VOLM
      VOLVEL = VOLVEL + XVELO(JCNT)*VOLM
      JFL(JCNT) = JND
55     CONTINUE
      DO 60 J1 = 1,NCF(JSD)-NCFJM1
      JXD = NDCF(NCFJM1+J1)
      IF ( JXD .NE. J) THEN
          JCNT = JCNT + 1
          DO 57 J5 = 1, 4
          X1(J5) = XYZX(JXD,J5)
57     CONTINUE
      CALL FLXCAL( X0, PO(J), X1, PO(JXD), APER(JSD), XFLUX(JCNT),
1          XVELO(JCNT), XTYM(JCNT), VOLM, FLUXPOS, FLUXNEG )
      VOLSUM = VOLSUM + VOLM
      VOLVEL = VOLVEL + XVELO(JCNT)*VOLM
      JFL(JCNT) = -JXD
      ENDIF
60     CONTINUE
      FLUXNET = FLUXPOS + FLUXNEG
      FEXND(J) = FLUXNET
      IF (J .EQ. 1) THEN
          JJM1= 0
      ELSE

```

```

    JJM1= INXT(J-1)
  ENDIF
  IF (FLUXNET .LT. 1.E-5) THEN
    JA=0
  ELSE
    JA=0
    DO 65 J5 = 1, JCNT
      FTRXJA = XFLUX(J5) / FLUXPOS
      IF (FTRXJA .GT. 1.0E-5) THEN
        JA = JA + 1
        JJM2 = JJM1 + JA
        FTRX (JJM2) = FTRXJA
        TYMEX (JJM2) = XTYM(J5)
        ITRX (JJM2) = JFL(J5)
      ENDIF
65    CONTINUE
    ENDIF
    INXT(J) = JJM1 + JA
70  CONTINUE
    VELOAGE = VOLVEL / VOLSUM
    RETURN
  END

```


20

```

IF (JTRDE .LT. 0 ) THEN
  KWRK1 (1) = NNTRCX (-JTRDE, INXT)
  KMTHR (1) = JTRDE
ELSE
  KWRK1 (1) = NNTRCX (JTRDE, INET)
  KMTHR (1) = JTRDE
ENDIF
IF (KWRK1 (1) .EQ. 0) GO TO 30
  KWRK2 (1) = 1
JLEV=1
CONTINUE
IF (JLEV .GT. 1) THEN
  IF (KMTHR (JLEV-1) .LT. 0 ) THEN
    NTEM = NNTRCX (-KMTHR (JLEV-1), INXT) + KWRK2 (JLEV-1)
    KMTHR (JLEV) = ITRX (NTEM)
  ELSE
    NTEM = NNTRCX ( KMTHR (JLEV-1), INET) + KWRK2 (JLEV-1)
    KMTHR (JLEV) = ITRE (NTEM)
  ENDIF
  IF (KMTHR (JLEV) .LT. 0 ) THEN
    KWRK1 (JLEV) = NNTRCX (-KMTHR (JLEV), INXT)
  ELSE
    KWRK1 (JLEV) = NNTRCX ( KMTHR (JLEV), INET)
  ENDIF
ENDIF
IF (KWRK2 (JLEV) .LE. KWRK1 (JLEV)) THEN
  IF (KMTHR (JLEV) .LT. 0) THEN
    NTEM = NNTRCX (-KMTHR (JLEV), INXT) + KWRK2 (JLEV)
    TTTT = TYMEX (NTEM)
    FFFF = FTRX (NTEM)
    IIII = ITRX (NTEM)
  ELSE
    NTEM = NNTRCX ( KMTHR (JLEV), INET) + KWRK2 (JLEV)
    TTTT = TYMIN (NTEM)
    FFFF = FTRE (NTEM)
    IIII = ITRE (NTEM)
  ENDIF
  IF (FFFF .LT. 1.E-6) FFFF = 1.E-6
  TT0 = TT0 + TTTT
  TTX = TTX * DBLE (FFFF)
  IF ( (TTX .LT. 1.D-6) .OR. (TT0 .GT. TYMR1) ) THEN
    TT0 = TT0 - TTTT
    TTX = TTX / DBLE ( FFFF )
    KWRK2 (JLEV)=KWRK2 (JLEV)+1
    JLEV=JLEV-1
  ELSE
    IF ( IIII .LT. 0 ) THEN
      KCONT=KCONT + 1
      KKMM=NDXD (-IIII, 2)
      CFATOR = 0.0
    
```

```

22      GO TO 22 KLMM = 1, NIJET
        IF (KKMM .EQ. NJET(KLMM) ) CFATOR = 1.0
        CONTINUE
        IDX = INT( (TT0-TYMR0)/ TYMST ) +2
        IF (TT0 .LE. TYMR0)  IDX = 1
        IF (TT0 .GT. TYMR1)  IDX = NTYM +2
        WRKCG (IDX) = WRKCG (IDX) + CFATOR * REAL(TTX)
        TRAVLT = TRAVLT + CFATOR * REAL(TTX) * TT0
        TT0 = TT0 - TPTT
        TTX = TTX / DBLE( FFFF )
        KWRK2 (JLEV)=KWRK2 (JLEV)+1
        JLEV=JLEV-1
    ENDIF
    ENDIF
    JLEV=JLEV+1
ELSE
    KWRK2 (JLEV)=1
    JLEV=JLEV-1
    IF (KMTHR(JLEV) .LT. 0) THEN
        NTEM = NNTRCR(-KMTHR(JLEV), INXT) + KWRK2 (JLEV)
        TPTT = TYMEX (NTEM)
        FFFF = PTRX (NTEM)
    ELSE
        NTEM = NNTRCR( KMTHR(JLEV), INET) + KWRK2 (JLEV)
        TPTT = TYMIN (NTEM)
        FFFF = FTRE (NTEM)
    ENDIF
    IF (FFFF .LT. 1.E-6) FFFF = 1.E-6
    TT0 = TT0 - TPTT
    TTX = TTX / DBLE(FFFF)
    KWRK2 (JLEV)=KWRK2 (JLEV)+1
ENDIF
IF (KWRK2(1) .LE. KWRK1(1)) GO TO 20
30  CONTINUE
    TEMC(1)=WRKCG(1)
    J1=1
    DO 50 J0 = 2,NTYM+1
        TEMC(J0) = TEMC(J0-1) + WRKCG(J0)
50  CONTINUE
    RETURN
    END

```


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FUNCTION NNTRCR(N, NR)

REMARKS: NUCLEAS CALLED BY VARIOUS SUBPROGRAMS TO UNPACK A
ONE-DIMNSIONAL ARRAY WHERE DATA OF TWO-DIMENSIONAL
NATURE HAVE BEEN STORED.

DIMENSION NR(300)
IF (N .EQ. 1) THEN
NNTRCR=0
ELSE
NNTRCR=NR(N-1)
ENDIF
RETURN
END

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FUNCTION NNTRCX(N, NR)

REMARKS: NUCLEAS CALLED BY VARIOUS SUBPROGRAMS TO UNPACK A
ONE-DIMNSIONAL ARRAY WHERE DATA OF TWO-DIMENSIONAL
NATURE HAVE BEEN STORED.

DIMENSION NR(300)
IF (N .EQ. 1) THEN
NNTRCX=NR(1)
ELSE
NNTRCX=NR(N)-NR(N-1)
ENDIF
RETURN
END

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SUBROUTINE FLXCAL (X0,P0,X1,P1,AP,FLX,VEL,TYM,VOL,FLXP,FLXN)

REMARKS: NUCLEAS CALLED BY SUBROUTINE *FLOWNET* TO CALCULATE
THE FLUX BETWEEN TWO NODAL POINTS.

REAL X0(4), X1(4)
DATA RHO,UN,UNITCON / 9810., 0.001, 0.01 /
VOL = 0.
T2 = 0.
DO 10 J5 = 1, 3
T2 = T2 + (X1(J5)-X0(J5))**2.
10 CONTINUE
X0X1 = SQRT (T2)
XX = (X1(4) + X0(4))/2.
COEF = XX * AP**3. * RHO /
1 (12. * UN * X0X1)
FLX = COEF * (P1+X1(3) - (P0+X0(3)))
VEL = FLX / (XX * AP)
IF (FLX .EQ. 0.) THEN
TYM = 1.0E+12
ELSE
TYM = X0X1 / VEL.
ENDIF
IF (FLX .GT. 0.) THEN
FLXP = FLXP + FLX
VOL = X0X1 * XX * AP
ELSE
FLXN = FLXN + FLX
ENDIF
RETURN
END

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SUBROUTINE OUTFLNT

PURPOSE: THIS SUBROUTINE PRINTS OUT THE FLOW NETWORK OF THE FRACTURE SYSTEM.

```
COMMON /FRCT/ NFRCT,APER(200),NFR(200),NCF(200)
COMMON /NODE/ NNODE,NDID(300,2),PX(300),XYZI(300,4)
COMMON /BOND/ NBOND,NDXD(200,2),PO(200),XYZX(200,4)
COMMON /FLNT/ INET(300),FINND(300)
COMMON /FBND/ INXT(200),FEXND(200)
COMMON /RFDN/ NDFR(700),NDCF(300)
COMMON /ERTI/ ITRE(1800),FTRE(1800),TYMIN(1800)
COMMON /XRTI/ ITRX(800),FTRX(800),TYMEX(800)
DO 10 J = 1, 10, 1
IF (J .EQ. 1) THEN
  JJM1 = 0
ELSE
  JJM1 = INET(J-1)
ENDIF
WRITE (10,110) J, INET(J)-JJM1, FINND(J)
WRITE (10,111) (ITRE(J0), J0=JJM1+1,INET(J))
WRITE (10,112) (FTRE(J0), J0=JJM1+1,INET(J))
WRITE (10,113) (TYMIN(J0), J0=JJM1+1,INET(J))
110  FORMAT (/2X,'** INODE= ',I3,5X,'# OF INFLOWS= ',I2,
1      5X,'INFLOW FLUX = ',F10.4)
111  FORMAT (2X,'INFLOW NODE : ',5I10,/,
1      (2X,' ',5I10))
112  FORMAT (2X,'REL. FLUX : ',5F10.4,/,
1      (2X,' ',5F10.4))
113  FORMAT (2X,'TRAVEL TIME : ',5F10.2,/,
1      (2X,' ',5F10.2))
10  CONTINUE
DO 20 J = 1, 10, 1
IF (J .EQ. 1) THEN
  JJM1 = 0
ELSE
  JJM1 = INXT(J-1)
ENDIF
WRITE (10,120) J, INXT(J)-JJM1, FEXND(J)
WRITE (10,111) (ITRX(J0), J0=JJM1+1,INXT(J))
WRITE (10,112) (FTRX(J0), J0=JJM1+1,INXT(J))
WRITE (10,113) (TYMEX(J0), J0=JJM1+1,INXT(J))
120  FORMAT (/2X,'** XNODE= ',I3,5X,'# OF INFLOWS= ',I2,
1      5X,'INFLOW FLUX = ',F10.4)
20  CONTINUE
RETURN
END
```

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SAMPLE OUTPUT FROM RUN 2 OF EXPERIMENT 2

***** GLOBAL VOLUME AVERAGED VELOCITY = 4.0684
***** GLOBAL VOLUME = 11840.6511

*
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*
*

FLOW NETWORK STRUCTURE DEPICTED FROM INTERNAL NODAL POINTS.

** INODE= 1 # OF INFLOWS= 1 INFLOW FLUX = .6409
INFLOW NODE : 3
REL. FLUX : 1.0000
TRAVEL TIME : 1.24

** INODE= 2 # OF INFLOWS= 3 INFLOW FLUX = .4145
INFLOW NODE : 1 3 4
REL. FLUX : .3439 .5477 .1083
TRAVEL TIME : 10.32 7.20 57.81

*
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*

DATA CONTINUES ...

** INODE= 9 # OF INFLOWS= 4 INFLOW FLUX = .0069
INFLOW NODE : 5 6 10 85
REL. FLUX : .0935 .1530 .0138 .7397
TRAVEL TIME : 633.74 3006.22 19512.33 115.27

** INODE= 10 # OF INFLOWS= 2 INFLOW FLUX = .0033
INFLOW NODE : 5 6
REL. FLUX : .0478 .9522
TRAVEL TIME : 8943.19 291.83

*
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*

DATA CONTINUES UNTIL INNODE = NNODE.

*
 * FLOW NETWORK STRUCTURE DEPICTED FROM EXTERNAL NODAL POINTS.
 *
 *

** XNODE=	1	# OF INFLOWS=	6	INFLOW FLUX =	.8679
INFLOW NODE :	22	62	63	64	65
	66				
REL. FLUX :	.2127	.0637	.3035	.0774	.1936
	.1491				
TRAVEL TIME :	64.93	114.79	43.36	97.03	44.76
	51.32				

** XNODE=	2	# OF INFLOWS=	3	INFLOW FLUX =	.1445
INFLOW NODE :	87	88	89		
REL. FLUX :	.3924	.2881	.3195		
TRAVEL TIME :	75.20	92.18	20.07		

*
 * DATA CONTINUES ...
 *

** XNODE=	5	# OF INFLOWS=	7	INFLOW FLUX =	.1627
INFLOW NODE :	124	125	126	127	128
	129	130			
REL. FLUX :	.0983	.2615	.0731	.0467	.1328
	.1894	.1982			
TRAVEL TIME :	101.39	45.15	284.64	305.93	42.94
	139.51	127.05			

*
 * DATA CONTINUES UNTIL XNODE = NBOND.
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CHARACTERISTIC TIME SCALES ASSOCIATED WITH EACH INDIVIDUAL
BREAKTHROUGH (BT) CURVE DETERMINED AT SPECIFIC NODE.
NEGATIVE NODAL INDEX IMPLIES AN EXTERNAL NODE IS BEING EXAMINED.
BT-TEND IS THE DEGREE OF BT (C/CO) AT THE END OF A SPECIFIED
TIME INTERVAL, T-END.
T0 IS THE TIME WHEN THE FIRST TRACE OF THE INJECTED MASS IS
DETECTED AT THE OUTFLOW BOUNDARY. T50 IS THE TIME WHEN
C/CO = 0.5.

NODE, T-END, BT-TEND: -1 2000. .6980
T 0 = 66.0 T10 = 76.1 T25 = 96.1
T50 = 129.9

NODE, T-END, BT-TEND: -2 2000. .9540
T 0 = 137.0 T10 = 148.8 T25 = 230.6
T50 = 334.1 T75 = 516.2 T90 = 934.6

NODE, T-END, BT-TEND: -3 2000. .9534
T 0 = 334.0 T10 = 332.5 T25 = 346.8
T50 = 433.0 T75 = 680.9 T90 = 854.7

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DATA CONTINUES UNTIL THE DESIRED NUMBER OF BT CURVES ARE
REACHED.

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A.7 SAMPLE INPUT/OUTPUT OF EXPERIMENT 2

SAMPLE INPUT DATA SETUP FOR EXPERIMENT 2

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#EOR	(END OF RECORD)
200., 200., 200., 200.	(NERCT, FRX, FRY, FRZ)	
50., 10.	(FRCTLTH, FRCAPTR)
342., 1468., 325., 6406.	(DS1, DS2, DS3, DS4)
100., 100., 100., 0., 0., 180., 180., 180.	(SAMPLE INFORMATION)
100., 100., 100., 0., 0., 20., 20., 20.	(INJECTION ZONE INFO)
#EOR	(END OF RECORD)
#EOF	(END OF FILE)

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*

SAMPLE OUTPUT FROM RUN 2 OF EXPERIMENT 2

***** GLOBAL VOLUME AVERAGED VELOCITY = 4.0684
***** GLOBAL VOLUME = 11840.6511

*
*
*
*

FLOW NETWORK STRUCTURE DEPICTED FROM INTERNAL NODAL POINTS.

** INODE= 1 # OF INFLOWS= 1 INFLOW FLUX = .6409
INFLOW NODE : 3
REL. FLUX : 1.0000
TRAVEL TIME : 1.24

** INODE= 2 # OF INFLOWS= 3 INFLOW FLUX = .4145
INFLOW NODE : 1 3 4
REL. FLUX : .3439 .5477 .1083
TRAVEL TIME : 10.32 7.20 57.81

*
*
*

DATA CONTINUES ...

** INODE= 9 # OF INFLOWS= 4 INFLOW FLUX = .0069
INFLOW NODE : 5 6 10 85
REL. FLUX : .0935 .1530 .0138 .7397
TRAVEL TIME : 633.74 3006.22 19512.33 115.27

** INODE= 10 # OF INFLOWS= 2 INFLOW FLUX = .0033
INFLOW NODE : 5 6
REL. FLUX : .0478 .9522
TRAVEL TIME : 8943.19 291.83

*
*
*

DATA CONTINUES UNTIL INNODE = NNODE.

*
 * FLOW NETWORK STRUCTURE DEPICTED FROM EXTERNAL NODAL POINTS.
 *
 *

** XNODE=	1	# OF INFLOWS=	6	INFLOW FLUX =	.8679
INFLOW NODE :	22	62	63	64	65
	66				
REL. FLUX :	.2127	.0637	.3035	.0774	.1936
	.1491				
TRAVEL TIME :	64.93	114.79	43.36	97.03	44.76
	51.32				

** XNODE=	2	# OF INFLOWS=	3	INFLOW FLUX =	.1445
INFLOW NODE :	87	88	89		
REL. FLUX :	.3924	.2881	.3195		
TRAVEL TIME :	75.23	92.18	20.07		

*
 * DATA CONTINUES ...
 *

** XNODE=	5	# OF INFLOWS=	7	INFLOW FLUX =	.1627
INFLOW NODE :	124	125	126	127	128
	129	130			
REL. FLUX :	.0983	.2615	.0731	.0467	.1328
	.1894	.1982			
TRAVEL TIME :	101.39	45.15	284.64	305.93	42.94
	139.51	127.05			

*
 * DATA CONTINUES UNTIL XNODE = NBOND.
 *

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CHARACTERISTIC TIME SCALES ASSOCIATED WITH EACH INDIVIDUAL
BREAKTHROUGH (BT) CURVE DETERMINED ST SPECIFIC NODE.
NEGATIVE NODAL INDEX IMPLIES AN EXTERNAL NODE IS BEING EXAMINED.
BT-TEND IS THE DEGREE OF BT (C/CO) AT THE END OF A SPECIFIED
TIME INTERVAL, T-END.
T0 IS THE TIME WHEN THE FIRST TRACE OF THE INJECTED MASS IS
DETECTED AT THE OUTFLOW BOUNDARY. T50 IS THE TIME WHEN
C/CO = 0.5.

NODE, T-END, BT-TEND:	-1	2000.	.6980
T 0 =	66.0	T10 = 76.1	T25 = 96.1
T50 =	129.9		
NODE, T-END, BT-TEND:	-2	2000.	.9540
T 0 =	137.0	T10 = 148.8	T25 = 230.6
T50 =	334.1	T75 = 516.2	T90 = 934.6
NODE, T-END, BT-TEND:	-3	2000.	.9534
T 0 =	334.0	T10 = 332.5	T25 = 346.8
T50 =	433.0	T75 = 680.9	T90 = 854.7

*
*
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DATA CONTINUES UNTIL THE DESIRED NUMBER OF BT CURVES ARE
REACHED.

BIBLIOGRAPHIC DATA SHEET

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12 SUPPLEMENTARY NOTES

13 ABSTRACT (200 words or less)

A 3-dimensional fracture generating scheme is presented which can be used to simulate water flow and contaminant (solute) transport through fracture system of a rock. It is presently limited to water saturated conditions, zero permeability for the rock matrix, and steady state water flow, but allows for transient solute transport. The scheme creates finite planar plates of uniform thickness which represent fractures in 3-dimensional space. A given fracture (plate) has the following descriptors: center location, orientation, shape, areal extent and aperture. Each parameter can be described by an appropriate probability distribution. Individual fractures are generated to form an assemblage of a certain fracture density. All fracture intersections and boundary/fracture intersections are determined and deadend fractures are eliminated. Flow through the fracture assemblage is considered laminar and described by Poiseuille's law. The principle of mass conservation at each intersection is used to develop the global matrix equation, which is solved subject to specified boundary conditions to yield the head and flow distribution at each intersection. Solute transport is considered to be advective between intersections with complete mixing at each intersection. Solutes added to the flow system can be explicitly followed and concentration vs. time relationships can be determined anywhere in the system. Some examples are included.

14 DOCUMENT ANALYSIS - a KEYWORDS/DESCRIPTORS

rock, fracture, water flow, solute transport computer model

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CONTAMINANT TRANSPORT THROUGH A ROCK FRACTURE SYSTEM