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LLUVIA: A Program for One-Dimensional, Steady-State Flow Through Partially Saturated Porous Media

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LLUVIA: A Program for One-Dimensional, Steady-State Flow Through Partially Saturated Porous Media

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Abstract

LLUVIA is a program designed for the efficient solution of one-dimensional, steady flow through multiple layers of saturated or partially saturated, fractured, porous media. The original intent of the code was to provide initial pressure conditions to two-dimensional, finite element codes. LLUVIA's capabilities were expanded to meet the needs of analyses in the performance assessment of a proposed, high-level nuclear waste repository. The code is based on an adaptive solution method for Darcy's equation and is structured to accommodate user-defined models for hydraulic conductivity and saturation. Program structure, code input, and output are intended to facilitate the interfacing of LLUVIA with graphical and/or statistical software packages.

This document describes the flow problem of interest, the solution procedure employed, and the content and format of all user-supplied information. A sample problem is also included.

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1 Introduction

In evaluating a geologic site as the potential location for a proposed nuclear waste repository, it is necessary to perform a global performance assessment to determine whether the site is likely to meet regulatory requirements. One requirement involves a minimum time for groundwater travel from a disturbed zone to the accessible environment. Deterministic models based on Richards' equation[1] require details of material characteristics that may never be adequately defined. When information about the distribution of material properties is known, one of the current methodologies for carrying out a global performance assessment is the Monte-Carlo simulation approach. This type of statistically based method attempts to account for the uncertainties in the spatial variability of material properties. The method involves solving the deterministic model repeatedly with model parameters sampled from distributions. A highly efficient computer program is essential to perform the necessary calculations. At present, the simplifying assumption of a one-dimensional, steady flow is required to meet these demands.

LLUVIA is a program designed for the efficient solution of one-dimensional, steady flow through multiple layers of saturated or partially saturated, fractured, porous media. The code is based on an adaptive solution method for Darcy's equation and is structured to accommodate user-defined models for hydraulic conductivity and saturation. LLUVIA takes advantage of the DEPAC library ordinary differential equation solver, DEBDF[2], to solve for the pressure and then computes flux, saturation, velocities, and groundwater travel times. Program structure, code input, and output are intended to facilitate the interfacing of LLUVIA with graphical and/or statistical software packages.

This document serves as the formal documentation of the mathematical models and numerical methods and as a user's guide. A sample problem provides partial test and debug documentation.

2 Problem Definition

LLUVIA was developed to solve efficiently a particular class of flow problems. The isothermal problem involves the steady flux of an incompressible, Newtonian fluid through a one-dimensional domain of saturated or partially saturated layers of rigid, porous media (Figure 1). The media may contain fractures whose properties vary from those of the matrix. The composite matrix/fracture model representation treats the material as a single continuum in solving for the pressure field. The first-order differential equation describing such a flow is Darcy's equation:

$$q = \frac{-K(\psi)}{\rho g}\frac{dP}{dz}, \tag{1}$$

where

q is the specific discharge or infiltration rate
K is the effective hydraulic conductivity
ψ is the pressure head
ρ is the water density
g is the gravitational acceleration
P is the pressure, $P = \rho g(\psi + z)$
z is the elevation.

Conservation of mass is insured by the imposed steady-state condition, and Darcy's equation is a statement of momentum balance. Applications to global performance assessment involve infiltration problems and result in the following applied flux and pressure head boundary conditions:

$$q = q_0 \text{ at } z = z_t$$
$$\psi = \psi_0 \text{ at } z = 0.$$

3 Solution Approach

Equation 1 is the ordinary differential equation to be solved for pressure. For partially saturated conditions, the hydraulic conductivity, K, is a strong function of pressure head, ψ, and Equation 1 can become extremely nonlinear. An example of such a characteristic curve, $K(\psi)$, is shown in Figure 2.[3] This curve represents matrix and fractures in a composite model where both matrix and fracture conductivity are defined by the van Genuchten/Mualem[4] form for the hydraulic conductivity:

$$K(\psi) = n_f K_f + (1 - n_f) K_m \tag{2}$$

$$K = K_s \left[1 + |\alpha\psi|^\beta\right]^{-(\beta-1)/2\beta} \left\{1 - \left[\frac{|\alpha\psi|^\beta}{1 + |\alpha\psi|^\beta}\right]^{(\beta-1)/\beta}\right\}^2, \tag{3}$$

where

n_f is the area fraction of fractures
K_s is saturated hydraulic conductivity
S_r is residual saturation
α, β are curve-fitting parameters
m, f are subscripts referring to matrix and fractures, respectively.

The solver in LLUVIA, DEBDF, is based on A. Hindmarsh's code, LSODE[5]. The implicit solution procedure uses a backward differentiation formula of orders one through five and is interval-oriented. It is particularly well suited to the solution of stiff problems.

The pressure field produced by the solution of Equation 1 is subsequently used to compute the hydraulic conductivity, matrix saturation, and water velocities in both the matrix and fractures (if present) at each nodal location. In these calculations, the matrix and fractures are treated as separate continua. An example of a model for saturation is given in Section 7, and the linear water velocities are defined by[6]

$$v_m = \frac{q_m}{n_m(S_m - S_{m,r})}, \tag{4}$$

$$v_f = \frac{q_f}{n_f(S_f - S_{f,r})}, \tag{5}$$

where S is saturation.

Minimum groundwater travel times (GWTT) are computed from a user-defined starting elevation to the bottom of the domain by always selecting the faster of the velocities at each node.

4 Program Structure

A modular structure is maintained to facilitate code updating and flexibility. There are two major groups to the structure: (1) the main program with subroutines that define problem parameters and compute the solution and (2) a set of user-defined subroutines to evaluate the hydraulic conductivity and saturation as a function of pressure head, to define initial nodal point locations, and to control the format of the output. Figure 3 shows a flow diagram of major program segments. Comments used liberally throughout the code serve as a guide to programmers. The following description provides the user with an explanation of significant program logic and assumptions.

4.1 Parameter Initialization and Definition

The first task is to initialize problem parameters by a call to SUBROUTINE INIT. On the first pass through this routine, the user input file, which must be assigned to logical unit 3, is opened. A problem title of up to 80 characters is read. The next seven input parameters are read and default values assigned if needed (see Section 5.1). If default values are used, appropriate messages will be printed. Units of measure are chosen by the user but must be applied consistently to all input parameters. These six parameters are the number of material units, flux, boundary pressure head, product of water density and gravitational acceleration, tolerance on conductivity change, and mesh definition flag. The corresponding FORTRAN variable names used in Section 5.2 are shown in parentheses in the descriptions below.

The one-dimensional domain may be separated into a number of layers (NMAT) of different materials. The maximum number of layers is currently set at 50 but is easily changed via a PARAMETER statement in the main program. A set of material properties must be defined for each such layer. Layers are numbered consecutively from the bottom to the top of the domain.

The specified flux or infiltration rate, q_0, is an imposed condition and is constant throughout the domain. Flux has the dimensions of volume/unit area/unit time, or length/unit time. A positive input value represents a downward flux. Units of measurement must be consistent with other parameters. The boundary condition at the bottom of the domain is specified as a constant pressure head, ψ_0.

To rid the solution procedure of all dependence on units of measurement, the user must define the product of water density and gravitational acceleration (RHOG).

A tolerance on the allowable percentage change in conductivity between neighboring nodes controls the addition of nodal points. This provides solution refinement without

the need to know *a priori* where significant nonlinearities may occur.

The user defines specific nodal point locations (ZNODE) through SUBROUTINE MESH. During the solution procedure, nodes may be added by the code. If more than one problem is defined in the user input file, the user has the option of redefining the initial nodal point locations through another call to SUBROUTINE MESH or using the augmented locations of the previous problem. If the user expects nonlinearities to vary little between problems, reusing a mesh may be more efficient. Setting the mesh definition flag (IMESH) to zero will force a call to SUBROUTINE MESH; a value of one will not redefine nodal locations. The flag must be set to zero for the first problem.

Next, the material properties, ten for each layer (five for matrix and five for fractures), are read. The meanings of six of these parameters are fixed. They are the matrix porosity, the area fraction of fractures, and the saturated hydraulic conductivity and residual saturation of both the matrix and fractures.

Porosity of the matrix (PORM) is the traditional void-volume-to-total-volume ratio. The area fraction of fractures is the hydraulic aperture times the number of fractures per meter. The sum of the area fraction of matrix and area fraction of fractures is unity.[3] This area fraction of fractures is sometimes referred to as a fracture porosity (PORF). The porosity values are used only to convert matrix and fracture flux values to linear velocities (Equations 4 and 5). If there are no fractures in the material model, the area fraction of fractures is set to zero; provisions for this condition must be made in user SUBROUTINE EVAL (see Section 5.2). Even though there may be no fractures, a value must be assigned to all five fracture parameters, or an appropriate number of commas must exist, since the data file is read in free-field format. By definition, a zero fracture porosity will result in a zero linear velocity in the fractures, *i.e.*, water movement is only through the matrix.

Hydraulic conductivity values have dimensions of length/unit time. The input values of saturated hydraulic conductivity for matrix (SATM) and fractures (SATF) are supplied to SUBROUTINE EVAL for use in defining a relative hydraulic conductivity. The program uses relative conductivities in Darcy's equation (Equations 1, 6, and 8).

Residual saturation (SRM, SRF) is the limiting value of saturation such that an increase in suction head results in no significant change in saturation.

The use of the remaining material input parameters, two for matrix (PM1, PM2) and two for fractures (PF1, PF2) is at the user's discretion. They, too, are passed to SUBROUTINE EVAL. In the sample problem, these are used as curve-fit parameters for the relative hydraulic conductivity and saturation models. If these are not used, a numerical value must be assigned or a comma inserted to accommodate the free-field input.

Finally, the program reads the interface elevations (ZINTER) and the starting elevation (ZSTART) for groundwater travel-time computation. The interface elevations correspond to the top elevation of each material unit or layer. Interface elevations are defined from the bottom of the domain to the top, as are material layers and the properties attributed to them. These elevations are used in determining which material properties are assigned to a node. If $z(i)$ is the elevation of the i^{th} node and $zint(j)$ represents the j^{th} input interface elevation, then if $zint(j-1) < z(i) \leq zint(j)$, the j^{th} set of material properties are assigned to node i. It is assumed that $zint(0) = 0.0$. Groundwater travel times are summed from this starting elevation down to the bottom of the domain, $z = 0.0$. If the starting elevation is greater than the top of the domain, computation starts at the top.

4.2 Mesh Definition

After parameter initialization and if the mesh definition flag is zero, the main program calls the user SUBROUTINE MESH, which defines the number of nodes and their locations or elevations. Again, consistency of units of measurement should be maintained. The number of material layers and the interface elevations are passed to this subroutine for possible use in computing nodal locations. On return, the program ensures a nodal point at each material interface (SUBROUTINE ADDNODE). The node at the interface is considered to be the topmost node of a layer, *i.e.*, a part of the material below it rather than part of the material above it.

4.3 Solution Procedure

The solution procedure begins by defining several parameters required by the ODE solver, DEBDF. Two of these are error tolerances (RTOL, ATOL) and are initially defined as 10^{-10}. The elevation at which a pressure is to be computed, *i.e.*, a nodal location, is defined and the solver called. The solver may compute a solution at many intermediate points to maintain the requested accuracy but will return the solution only at the requested output location. The solver requires a subroutine (SUBROUTINE F) to evaluate a derivative, given a location and pressure, at many points during its solution algorithm. SUBROUTINE F calls the user-defined SUBROUTINE EVAL to obtain a value of relative conductivity at this point and defines the derivative by

$$\frac{d(\psi + z)}{dz} = \frac{-q_0}{K(\psi)}. \tag{6}$$

Note that during this procedure a flag is set to avoid computing unnecessary saturation values in SUBROUTINE EVAL. Care should be taken by the user to write an

efficient routine for evaluating conductivity if the problem is computationally intensive (generally due to nonlinearities or when many problem solutions are required).

When program execution returns to the main program, the DEBDF status flag (IDID) is checked. A variety of circumstances may present themselves. These are reported and handled as described below.

IDID Value	Result
-1	DEBDF has iterated excessively at this node. Restart the problem here and try again. After four unsuccessful attempts, this simulation stops. The user should verify that nodal locations are in ascending order with no more than one node per elevation.
-2	Error tolerances were deemed too stringent. Adjustments are made by DEBDF and the solution attempted. After four unsuccessful attempts, this simulation stops.
-3	Absolute error tolerance became zero. Value is redefined and the solution attempted. After four unsuccessful attempts, this simulation stops.
<-4	Convergence failed. Relative tolerance is increased and reported and the solution is attempted. After four unsuccessful attempts, this simulation stops.

On rare occasions because of convergence problems, DEBDF will return a solution at a point slightly away from the requested location. If this occurs, the nodal point location is moved and a message printed. Any other messages printed by the code are informational and self-explanatory. If an individual simulation stops because of an error condition described above, no part of the current solution is saved.

SUBROUTINE EVAL is called to evaluate relative conductivity at this latest solution point. The percentage of change in conductivity between this and the previous node is computed and compared against the user input tolerance. If the tolerance is exceeded, a new node is added at the midpoint of these nodes, and the solver is called for a pressure solution at this point. This procedure is repeated until the tolerance is met. The limiting case would be when the node and midpoint node locations are indistinguishable in terms of machine accuracy. At this point, the solver would return a value of IDID=-1 (see above) and stop the simulation. At a material interface, the

conductivity between the interface node and the first node into the next material layer is likely to exceed the specified tolerance. Therefore, the conductivity at the interface node is recomputed, for comparison purposes only, as though it were part of the next material.

The above solution procedure is repeated to compute a pressure at each node.

4.4 Postprocessing

The nodal point and corresponding pressure solution arrays are passed to SUBROUTINE POST along with input parameters including material properties, boundary flux, interface elevations, and starting elevation for groundwater travel time (GWTT). Output pressure head values are computed at each node:

$$\psi = \frac{P}{\rho g} - z. \tag{7}$$

The user SUBROUTINE EVAL is called to evaluate relative conductivity (matrix, fracture, and "total") as well as matrix saturation at each node. The "total," or composite, relative conductivity and matrix saturation are output quantities. With the use of the calculated composite hydraulic conductivity, the specified total flux, and Darcy's equation, the pressure gradient is then computed at each node from

$$\frac{d(\psi + z)}{dz} = \frac{-q_0}{K(\psi)}. \tag{8}$$

Klavetter and Peters [3] suggest that equal pressure in the matrix and fractures is a reasonable assumption under steady flow conditions. This allows the computed pressure pressure gradient to be applied separately to the matrix and fractures. The flux in the matrix and in the fractures is determined by

$$q_m = -K_m(\psi)\frac{d(\psi + z)}{dz}, \tag{9}$$

$$q_f = -K_f(\psi)\frac{d(\psi + z)}{dz}. \tag{10}$$

The linear velocity of the water in the matrix and the fractures at a nodal point are also output and are defined by Equations 4 and 5.

An average matrix and fracture flux through a cell (*i.e.*, between nodal points) is computed as a simple arithmetic average of adjoining, nodal-point flux values. These average fluxes are used to compute average linear velocities through a cell as described below. The average total flux through a cell is the sum of the average matrix and average fracture fluxes. This is the output flux value.

$$q_{m,ave}(i) = \frac{q_m(i+1) + q_m(i)}{2}. \tag{11}$$

$$q_{f,ave}(i) = \frac{q_f(i+1) + q_f(i)}{2}. \tag{12}$$

$$S_{m,ave}(i) = \frac{S_m(i+1) + S_m(i)}{2}. \tag{13}$$

$$S_{f,ave}(i) = \frac{S_f(i+1) + S_f(i)}{2}. \tag{14}$$

$$v_{m,ave}(i) = \frac{q_{m,ave}(i)}{n_m(S_{m,ave}(i) - S_{m,r}(i))}. \tag{15}$$

$$v_{f,ave}(i) = \frac{q_{f,ave}(i)}{n_f(S_{f,ave}(i) - S_{f,r}(i))}. \tag{16}$$

$$q_{total,ave}(i) = q_{m,ave}(i) + q_{f,ave}(i). \tag{17}$$

The more nonlinear the variation of hydraulic conductivity through the cell, the less accurate the average fluxes (total, matrix, and fracture) and, thus, the greater the error in the resulting average velocities. This error can be controlled by the allowable percentage change in conductivity across a cell, which controls cell size (see Section 4.3), or by providing nodal locations at sufficiently small increments. Note that $q_{total,ave}(i)$ is the average total flux through the i^{th} cell, bounded by nodal elevations $z(i)$ and $z(i+1)$ so that there is one less value computed than there are nodes. The input flux value is assigned to $q_{total,ave}(nnode)$ with *nnode* denoting the topmost node of the domain.

With linear water velocities in the matrix and fractures at each node and average linear water velocities in the matrix and fractures across a cell, the minimum groundwater travel time is computed three ways. One uses the average velocities; the other two use both the fastest velocities and then the slowest velocities. Each method compares the matrix water velocity to the water velocity in the fracture and selects the faster to use in computing the minimum travel time through a cell:

$$tmin_{min,i} = \frac{z_{i+1} - z_i}{max(\mid v_m \mid_{max}, \mid v_f \mid_{max})}, \tag{18}$$

$$tmin_{ave,i} = \frac{z_{i+1} - z_i}{max(\mid v_m \mid_{ave}, \mid v_f \mid_{ave})}, \tag{19}$$

$$tmin_{max,i} = \frac{z_{i+1} - z_i}{max(\mid v_m \mid_{min}, \mid v_f \mid_{min})}. \tag{20}$$

Cumulative travel times are reported at each nodal point from the starting elevation specified by the user, $z(istart)$, to the bottom of the domain. The first travel time reported will be at node $istart - 1$ and will represent the time to travel from the node at $z(istart)$ to $z(istart - 1)$. All subsequent travel times will be cumulative. The three values of minimum travel time give the user bounds on the travel time and a basis for judging the sufficiency of the nodal point locations since, in the limit, all three values are equal.

4.5 Program Output

In many cases, the results of this program will be used as input to either a statistical or a graphics software package of the user's choice. To facilitate this interface, the output is controlled by a user-defined SUBROUTINE OUTPUT. Immediately on return from SUBROUTINE POST, the main program passes the computed quantities of interest to SUBROUTINE OUTPUT along with most problem input parameters. The user is free to print only the input/output parameters of interest or may choose to perform additional computations. For example, if a number of problems were supplied in the input data file, SUBROUTINE OUTPUT may include a FORTRAN code that computes the average of some output quantity and reports only that one number. A description of the argument list of this subroutine is given in Section 5.2. After returning to the main program, another call is made to SUBROUTINE INIT to check for input data for another problem. If none are found, the main program ends; otherwise, the above procedure is repeated.

5 User Input

Program input is specified through both a data input file and a set of FORTRAN subroutines. The input file defines problem parameters while the subroutines supply initial nodal locations, hydraulic conductivity and saturation functions, and an output specification for the desired results.

5.1 Input File Format

Any valid file name may be used but must be assigned to logical unit 3 to be read by the code. All data input is in free-field format so that data values may be separated by either spaces, a comma, or a carriage return. The only restriction is that the title, IFLAG, and fracture model parameter 2 must be the last field on their input record (*i.e.*, must be followed by a carriage return). Carriage return is indicated in the following description by the characters CR following the field number.

Units of measure are defined by the user but must be consistent among all input parameters and the user-supplied subroutines. Default values in mks units are defined when certain parameters are input with a value of zero. These parameter values are shown below.

Field No.	Default Value	Input Description
1CR		Title (<= 80 characters).
2		Number of separate material units (maximum currently is 50).
3		Infiltration rate (positive number assumed to be downward).
4	0.0 m	Pressure head at bottom of domain.
5	9810.0 m/s**2	Product of water density and gravitational acceleration.
6	0.10	Limit on acceptable percentage change in conductivity from one node to the next within a unit.

7CR	0	IFLAG, flag to indicate whether nodal locations are to be taken from SUBROUTINE MESH (IFLAG=0) or if locations from the previous calculation are to be reused (IFLAG=1, only when multiple calculations are done). IFLAG must be zero on the first calculation.

Material unit definitions start at the bottom of the domain (i.e., at the water table) and work upward. For example, if three units were being defined, matrix porosity for the bottom unit would be in field 8, matrix porosity for the middle unit would be field 9, and matrix porosity for the top unit would be field 10.

8 -> nmat+7	Matrix porosity for each material.
nmat+8 -> etc,	Matrix saturated hydraulic conductivity for each material.
etc.	Matrix residual saturation for each material.
etc.	Matrix conductivity/saturation model parameter 1 for each material.
etc.	Matrix conductivity/saturation model parameter 2 for each material.
etc.	Fracture ''porosity'' for each material, zero if there are no fractures.
etc.	Fracture saturated hydraulic conductivity for each material.
etc.	Fracture residual saturation for each material.
etc.	Fracture conductivity/saturation model parameter 1 for each material.
etc. CR	Fracture conductivity/saturation model parameter 2 for each material.
etc.	Interface elevations. Bottom is assumed at z=0 (water table).
etc.	Repository elevation (GWTT is computed from this elevation to the water table).

5.2 Subroutines

The user must supply three FORTRAN subroutines. The purpose of these subroutines and their argument lists are described below. Those arguments described as input are values passed to the subroutine, and their values should not be changed.

5.2.1 SUBROUTINE MESH

The purpose of this subroutine is to define the initial number of nodal points at which a solution is to be generated and their corresponding elevation.

```
SUBROUTINE MESH (NINT,ZINTER,NNODE,ZNODE)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION ZNODE(1),ZINTER(1)
   .
   .
   .
RETURN
END
```

Argument list description:

Argument	Input or Output of Subroutine	Integer(I)/ real*8(R)	Description
NINT	input	I	Number of material interfaces, including top and bottom of domain, i.e., number of units plus one.
ZINTER	input	R(*)	Array of interface elevations, ZINTER(1)=0.0.
NNODE	output	I	Number of nodes defined.
ZNODE	output	R(*)	Array of elevations for each node, ZNODE(1) must be zero.

The user may assign nodal-point elevations by using whatever means are most appropriate, *e.g.*, through a DATA statement, executable statements, or a READ statement of an external file.

5.2.2 SUBROUTINE EVAL

The purpose of this subroutine is to evaluate matrix, fracture, and composite conductivities and matrix and fracture saturation for a given nodal pressure head and elevation.

```
      SUBROUTINE EVAL (P,Z,MAT,RHOG,NINT,PORM,KMB,SRM,PM1,PM2,
     1   PORF,KFB,SRF,PF1,PF2,ZINTER,IFLAG,COC,COM,COF,SATM,SATF)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KMB(1),KFB(1)
      DIMENSION PORM(1),SRM(1),PM1(1),PM2(1)
      DIMENSION PORF(1),SRF(1),PF1(1),PF2(1)
      DIMENSION ZINTER(1)
          .
          .
          .
      RETURN
      END
```

Argument list description:

Argument	Input or Output of Subroutine	Integer(I)/ real*8(R)	Description
P	input	R	Total pressure at this node.
Z	input	R	Elevation of this node.
MAT	input	I	The material unit of this node.
RHOG	input	R	Product of water density and gravitational acceleration.
NINT	input	I	Number of material interfaces, including top and bottom of domain, i.e., number of units plus one.
PORM	input	R(*)	Matrix porosity of each unit, PORM(MAT) is the value at this node.

KMB	input	R(*)	Matrix conductivity of each unit, KMB(MAT) is the value at this node.
SRM	input	R(*)	Matrix residual saturation of each unit, SRM(MAT) is the value at this node.
PM1	input	R(*)	Matrix model parameter 1 of each unit, PM1(MAT) is the value at this node.
PM2	input	R(*)	Matrix model parameter 2 of each unit, PM2(MAT) is the value at this node.
PORF	input	R(*)	Fracture porosity of each unit, PORF(MAT) is the value at this node.
KFB	input	R(*)	Fracture conductivity of each unit, KFB(MAT) is the value at this node.
SRF	input	R(*)	Fracture residual saturation of each unit, SRF(MAT) is the value at this node.
PF1	input	R(*)	Fracture model parameter 1 of each unit, PF1(MAT) is the value at this node.
PF2	input	R(*)	Fracture model parameter 2 of each unit, PF2(MAT) is the value at this node.
ZINTER	input	R(*)	Array of interface elevations, ZINTER(1)=0.0.
IFLAG	input	I	If IFLAG=0, there is no need to compute saturation; otherwise, compute saturation.

COC	output	R	Composite hydraulic conductivity.
COM	output	R	Matrix hydraulic conductivity.
COF	output	R	Fracture hydraulic conductivity.
SATM	output	R	Matrix saturation, if IFLAG is not zero.
SATF	output	R	Fracture saturation, if IFLAG is not zero.

The user may use any means or model to define the conductivities and saturation. The composite conductivity is a measure of total material conductivity, *i.e.*, including matrix and fractures. If there are no fractures (PORF=0.0), the composite value and matrix value should be equal.

5.2.3 SUBROUTINE OUTPUT

This subroutine allows the user to output in any desired output format those results or input parameters that are of interest. This facilitates postprocessing of the results with the graphics or statistical package of the user's choice.

```
  SUBROUTINE OUTPUT (TITLE,NNODE,NMAT,PORM,KMB,SRM,PM1,PM2,
1       PORF,KFB,SRF,PF1,PF2,ZINTER,ZSTART,RHOG,
2       Z,PSI,COND,SATM,AVEFLUX,VM,VF,TMIN)
 IMPLICIT REAL*8 (A-H,O-Z)
 DIMENSION PSI(1),Z(1),VM(1),VF(1),ZINTER(1),TMIN(3,NNODE),
1          COND(1),SATM(1),AVEFLUX(1)
 REAL*8 KMB(1),KFB(1)
 DIMENSION PORM(1),SRM(1),PM1(1),PM2(1)
 DIMENSION PORF(1),SRF(1),PF1(1),PF2(1)
 CHARACTER*80 TITLE
    .
    .
    .
 RETURN
 END
```

Argument list description:

Argument	Input or Output of Subroutine	Integer(I)/ real*8(R)	Description
TITLE	input	CHARACTER*80	Title from user input file.
NNODE	input	I	Number of nodal points defined.
NMAT	input	I	Number of material units.
PORM	input	R(*)	Matrix porosity of each unit, PORM(MAT) is the value at this node.
KMB	input	R(*)	Matrix conductivity of each unit, KMB(MAT) is the value at this node.
SRM	input	R(*)	Matrix residual saturation of each unit, SRM(MAT) is the value at this node.
PM1	input	R(*)	Matrix model parameter 1 of each unit, PM1(MAT) is the value at this node.
PM2	input	R(*)	Matrix model parameter 2 of each unit, PM2(MAT) is the value at this node.
PORF	input	R(*)	Fracture porosity of each unit, PORF(MAT) is the value at this node.
KFB	input	R(*)	Fracture conductivity of each unit, KFB(MAT) is the value at this node.
SRF	input	R(*)	Fracture residual saturation of each unit, SRF(MAT) is the value at this node.

PF1	input	R(*)	Fracture model parameter 1 of each unit, PF1(MAT) is the value at this node.
PF2	input	R(*)	Fracture model parameter 2 of each unit, PF2(MAT) is the value at this node.
ZINTER	input	R(*)	Array of interface elevations, ZINTER(1)=0.0.
ZSTART	input	R	Starting elevation for groundwater travel-time computation.
RHOG	input	R	Product of water density and gravitational acceleration.
Z	input	R(*)	Array of nodal point elevations.
PSI	input	R(*)	Array of pressure head at nodes.
COND	input	R(*)	Array of composite hydraulic conductivity at nodes.
SATM	input	R(*)	Array of matrix saturation at nodes.
AVEFLUX	input	R(*)	Array of average flux through cells (cumulative). Note that AVEFLUX(1) is the average flux through the bottom cell, AVEFLUX(NNODE-1) is the flux through the top cell, and AVEFLUX(NNODE) is the top boundary flux.
VM	input	R(*)	Array of matrix water velocity at nodes.
VF	input	R(*)	Array of fracture water velocity at nodes.

TMIN	input	R(*)	Array of three values for minimum travel time. TMIN(1,*) is minimum, TMIN(2,*) is average, and TMIN(3,*) is maximum.

6 Program Execution

LLUVIA is written in FORTRAN and is currently running under a VAX VMS environment. Three program modules must be linked to execute LLUVIA. These are (1) the main program, postprocessing, and input/output subroutines; (2) the solver, DEBDF; and (3) the user-supplied FORTRAN subroutines. The source or object (compiled source) file for the first module, LLUVIA, may be obtained from the authors or the current Department 1510 contact. The solver resides in the SLATEC[7] library. If access to this library is not possible, the appropriate subroutines can be made available. Finally, the user-supplied subroutines MESH, EVAL, and OUTPUT (assumed to exist together as USER.FOR for illustration) are compiled to form the third module. These three modules are then linked to form the executable. Under VAX VMS with the symbol SLATEC defining the library's location and the object files LLUVIA.OBJ and USER.OBJ in the current default directory, the following command is appropriate:

```
$ LINK LLUVIA,USER,SLATEC/LIB
```

The executable file LLUVIA.EXE should now exist in the directory. The user input file (assumed LLUVIA.INP for illustration) must be assigned to unit 3; printed LLUVIA output is written to unit 6. During interactive sessions, unit 6 defaults to the terminal screen but in batch mode, the default is the file FOR006.DAT. Other file assignments may be needed by the user-supplied routines. A standard batch execution would include the following VAX DCL commands:

```
$ ASSIGN LLUVIA.INP FOR003
$ ASSIGN LLUVIA.OUT FOR006
$ RUN LLUVIA
```

7 Sample Problem

The sample problem is taken from the COVE 2A Benchmarking Activity (Case 2) of the Nuclear Waste Repository Technology Department at Sandia National Labs. Details can be found in the Problem Definition Memo written by R. W. Prindle in 1986 (PDM #72-01). The problem involves five hydrologic units (Figure 4) with a steady flux of 0.1 mm/yr with the water table at $z = 0$. The input data file is shown in Figure 5. SUBROUTINE MESH (Figure 6) defined initial nodal locations at the 75 elevations requested in the COVE 2A problem statement with no further attempt to refine at the material interfaces. With the restriction of a 10% conductivity change across a cell, the code added 136 nodes for a total of 211 nodes. The van Genuchten[8] model for saturation and van Genuchten/Mualem[4] form for the hydraulic conductivity were used in SUBROUTINE EVAL (Figure 7) and are defined as

$$K = K_s \left[1 + |\alpha\psi|^{\beta}\right]^{-(\beta-1)/2\beta} \left\{1 - \left[\frac{|\alpha\psi|^{\beta}}{1 + |\alpha\psi|^{\beta}}\right]^{(\beta-1)/\beta}\right\}^2, \tag{21}$$

$$S = (1 - S_r)\left\{\frac{1}{1 + |\alpha\psi|^{\beta}}\right\}^{(\beta-1)/\beta} + S_r \tag{22}$$

where

K is effective hydraulic conductivity
K_s is saturated hydraulic conductivity
ψ is pressure head
z is elevation
S_r is residual saturation
α, β are curve-fitting parameters.

Examination of the input file reveals extreme differences (up to five orders of magnitude) in matrix saturated conductivity between material layers. The nonlinearity of their characteristic curves is similar to that of Figure 2. These attributes produce computational difficulties, typically at material interfaces, for many solution schemes. Total central processing unit time was 20 seconds (VAX 8650). Approximately 13 seconds of this time involved adding nodes. SUBROUTINE OUTPUT wrote program results at each node to a separate file. This file was then used as input to a plotting program. Plots were generated of the requested output quantities: normalized flux, pressure head, matrix saturation, hydraulic conductivity, and the magnitude of water velocity in the matrix and fractures (Figures 8-13). Symbols appear for every fifth nodal point. Figure 11 shows the varying total hydraulic conductivity throughout the domain. Figure 10

indicates high matrix saturation near the water table, which results in significant water velocity in the fractures (Figure 13) relative to the matrix velocity. These results compared well with other finite-element and finite-difference codes that participated in the COVE 2A effort. The minimum groundwater travel times were 1.252850×10^{13}, 1.262358×10^{13}, and 1.284412×10^{13} seconds. This represents a variation of only 2.5% of the minimum travel time based on average flux.

8 References

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8. van Genuchten, R., "Calculating the Unsaturated Hydraulic Conductivity with a New Closed-Form Analytical Model," Water Resources Bulletin, Princeton University Press, Princeton University, Princeton, NJ (1978). (HQS.880517.1859)

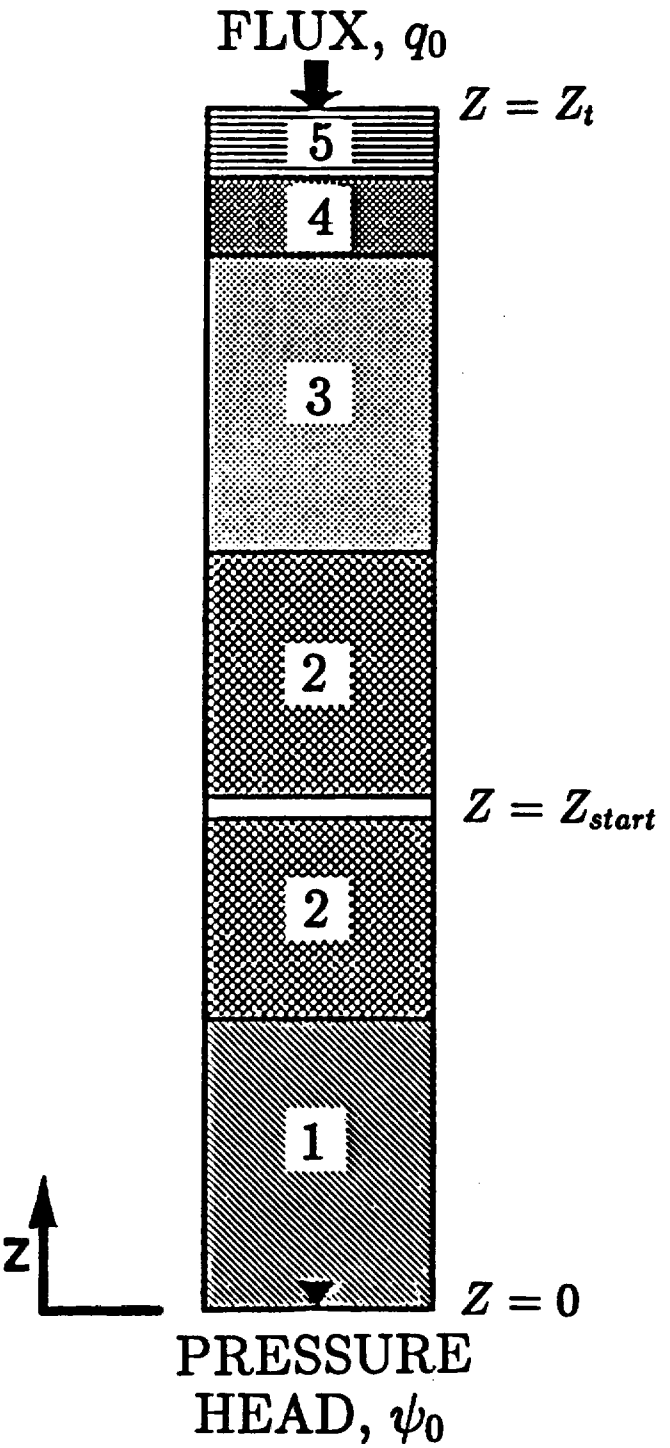


Figure 1: Schematic of Typical Domain

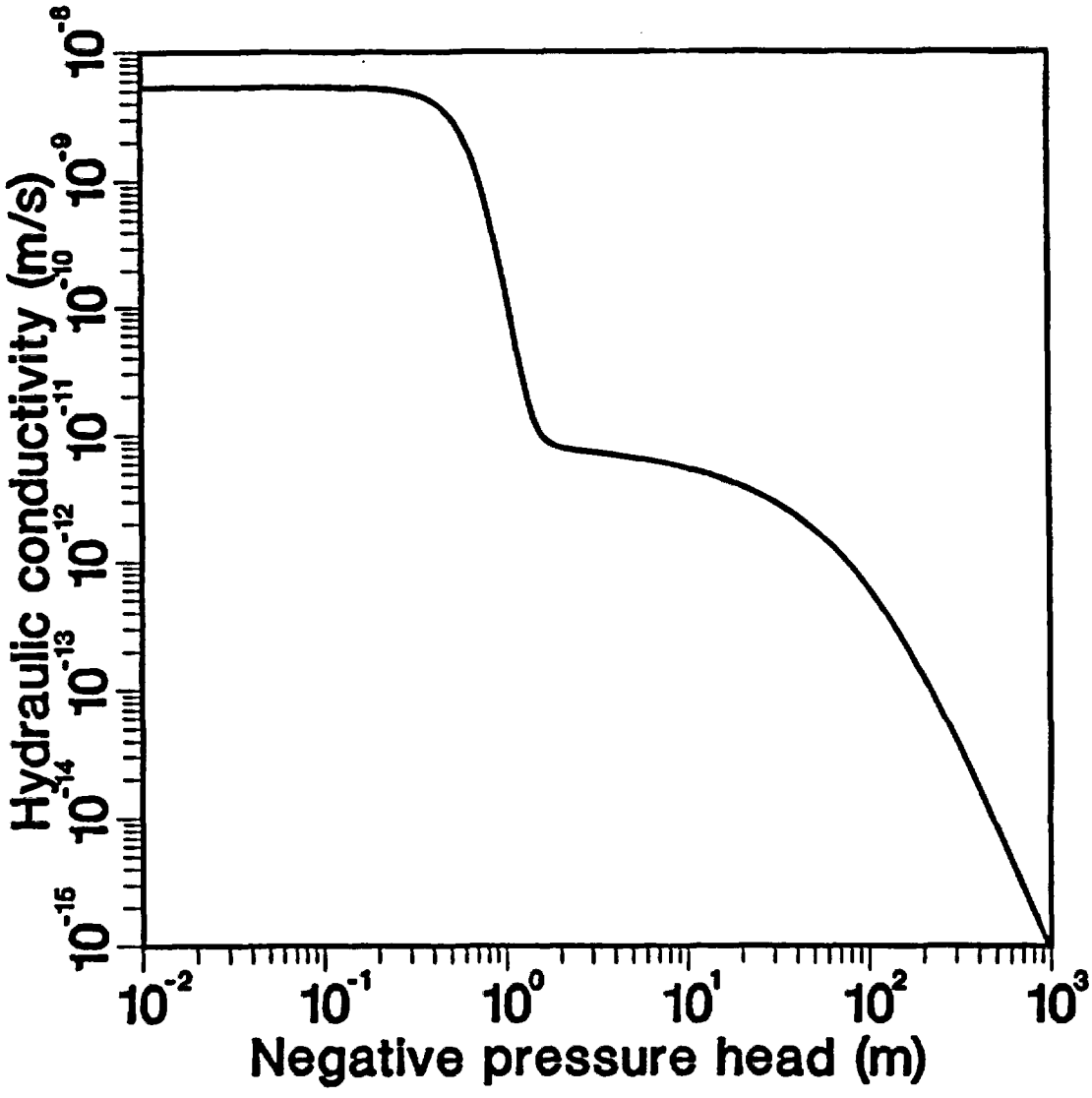


Figure 2: Composite Hydraulic Conductivity
(Source: Reference 3)

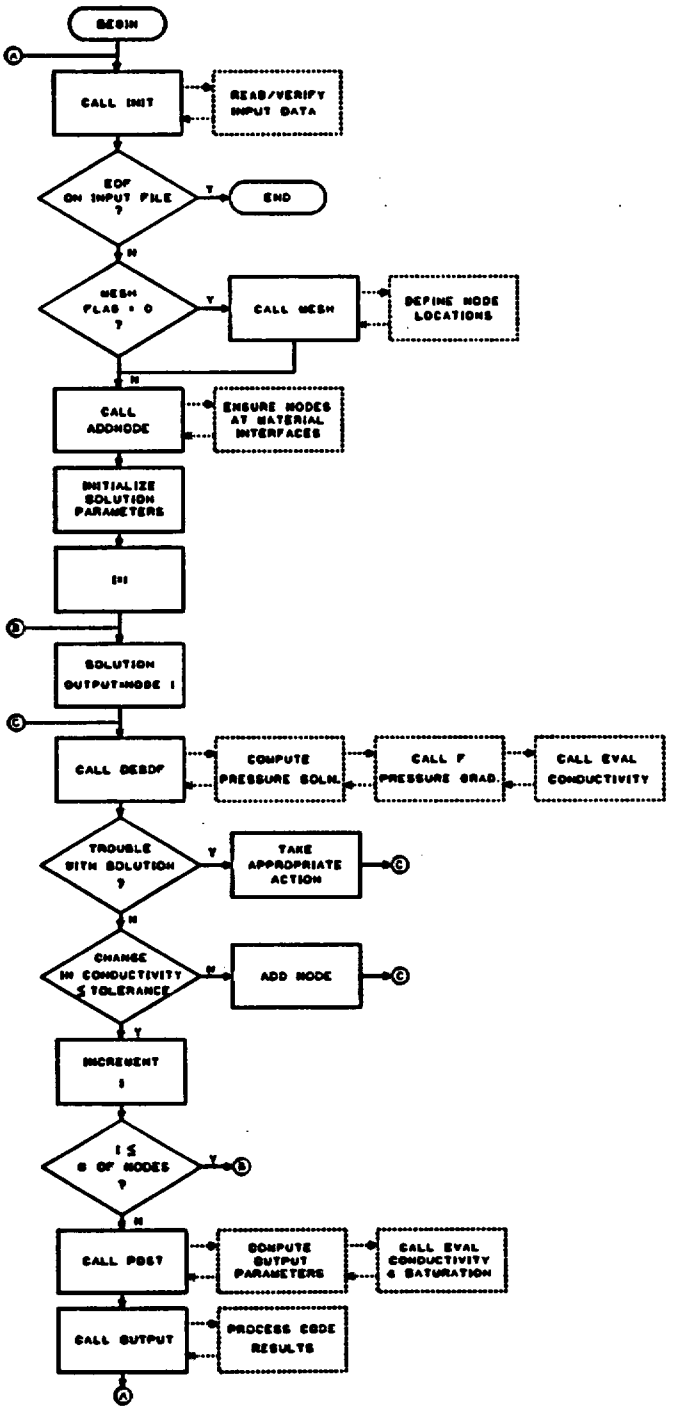
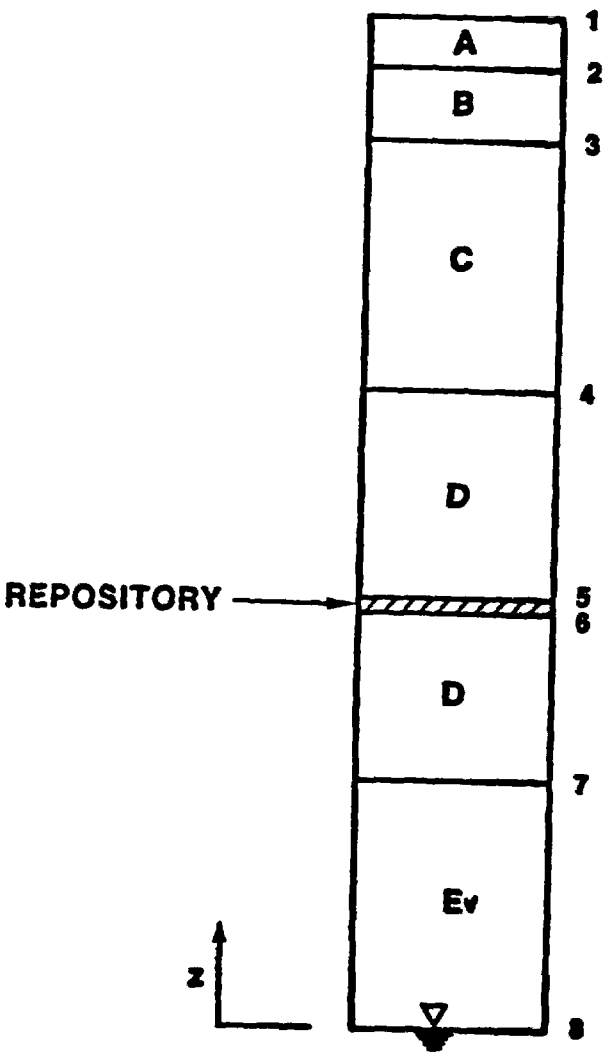


Figure 3: Code Flow Diagram



Point	Elevation, z (m)
1	530.4
2	503.6
3	465.5
4	335.4
5	224.0
6	219.5
7	130.3
8	0.0

Figure 4: Problem Domain

```
Case 2 of COVE2A, VITRIC, FLUX=.1 mm/yr
5
3.1688e-12, 0.0, 9806.65, 0.10, 0
0.46,   0.11,    0.11,    0.40,   0.08
2.7D-7, 1.9D-11, 1.9D-11, 3.9D-7, 9.7D-12
0.041,  0.08,    0.08,    0.10,   0.002
0.016,  0.00567, 0.00567, 0.015,  0.00821
3.872,  1.798,   1.798,   6.872,  1.558
4.6D-5, 1.8D-4,  4.1D-5,  2.7D-5, 1.4D-4
2.0D-4, 1.7D-5,  2.2D-5,  6.1D-4, 3.8D-5
0.0395, 0.0395,  0.0395,  0.0395, 0.0395
1.285,  1.285,   1.285,   1.285,  1.285
4.23,   4.23,    4.23,    4.23,   4.23
130.3, 335.4, 465.5, 503.6, 530.4
219.5
```

Figure 5: Input File

```
      SUBROUTINE MESH (NINT,ZINTER,NNODE,ZNODE)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 ZNODE(1),ZINTER(1)
      DIMENSION ZP(75)
C
C  This routine defines the number of nodes and their elevations
C  according to the specifications of the problem statement
C
C   Input variables
C   NINT   number of interfaces-not used here
C   ZINTER interface elevations-not used here
C
C   Output variables
C   NNODE  is the number of nodes
C   ZNODE  nodal elevations returned to main program
C
C   Routine variables
C   ZP     is an array holding the specified elevations
C
      DATA ZP /   0.0,  0.5,  1.0,  2.0,  5.0, 10.0, 20.0, 30.0,
     1           50.0, 70.0, 90.0,110.0,120.0,125.0,128.0,129.0,
     2    129.5,130.0,130.2,130.4,130.6,131.0,132.0,135.0,
     3          140.0,150.0,170.0,190.0,210.0,219.0,224.0,230.0,
     4    250.0,270.0,290.0,310.0,330.0,335.0,336.0,340.0,
     5          350.0,370.0,390.0,410.0,430.0,440.0,450.0,455.0,
     6    460.0,463.0,464.0,465.0,465.4,465.6,466.0,467.0,
     7          468.0,470.0,475.0,480.0,490.0,495.0,500.0,502.0,
     8    502.5,503.0,503.5,503.7,504.0,505.0,507.0,510.0,
     9          520.0,530.0,530.4/
C
C  Define the nodal points
C
      NNODE=75
      DO 10 I=1,NNODE
         ZNODE(I)=ZP(I)
  10  CONTINUE
C
      RETURN
      END
```

Figure 6: SUBROUTINE MESH

```
      SUBROUTINE EVAL (P,Z,MAT,RHOG,NINT,PORM,KMB,SRM,ALPM,BETM,
     1   PORF,KFB,SRF,ALPF,BETF,ZINTER,IFLAG,AKB,COM,COF,SATM,SATF)
      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 KMB(1),KFB(1)
      DIMENSION PORM(1),SRM(1),ALPM(1),BETM(1)
      DIMENSION PORF(1),SRF(1),ALPF(1),BETF(1)
      DIMENSION ZINTER(1)
C
C     Calculates hydraulic conductivity (m/sec) and saturation
C     according to the van Genuchten/Mualem model
C
C     Input variables
C     P     total pressure at node
C     Z     elevation of node
C     MAT   material unit number at node
C     RHOG water density times gravitational acceleration
C     ALPM matrix alpha of van Genuchten model
C     BETM matrix beta of van Genuchten model
C     ALPF fracture alpha of van Genuchten model
C     BETF fracture beta of van Genuchten model
C     PORM KMB SRM PORF KFB SRF are as described in manual
C     IFLAG  =1 if conductivity only, =2 if saturation too
C     Other input variable are described in the manual but not needed
C     in this application.
C
C     Output variables
C     AKB   composite hydraulic conductivity
C     COM   conductivity of the matrix
C     COF   conductivity of the fractures
C     SATM matrix saturation
C     SATF fracture saturation
C
C     Routine variables
C     PHM   pressure head at node
C     CONFU,SAT   function statements
C
C  Conductivity function statement
      CONFU(AL,AP)=(1.+AP)**(-AL/2.)*(1.-(AP/(1.+AP))**AL)**2
C  Saturation function statement
      SAT (AL,AP)= (1. / (1.+AP))**AL
C
      PHM=P/RHOG-Z
      IF(PHM.GT. -.000001)  PHM=-.000001
      APM=(ALPM(MAT)*(-PHM))**BETM(MAT)
      ALM=(1.-1./BETM(MAT))
      APF=(ALPF(MAT) * (-PHM))**BETF(MAT)
      ALF=(1.-1./BETF(MAT))
C  Compute and area-weight the matrix and fracture conductivity
      COM=CONFU(ALM,APM)*KMB(MAT)*(1-PORF(MAT))
      COF=CONFU(ALF,APF)*KFB(MAT)*PORF(MAT)
C  Compute the composite conductivity from the matrix and fracture values
      AKB=COM + COF
      IF (IFLAG.EQ.1) RETURN
C
C  If IFLAG =2, go on to compute saturation too.
C
      SATM = (1.-SRM(MAT))*SAT(ALM,APM) + SRM(MAT)
      SATF = (1.-SRF(MAT))*SAT(ALF,APF) + SRF(MAT)
      RETURN
      END
```

Figure 7: SUBROUTINE EVAL

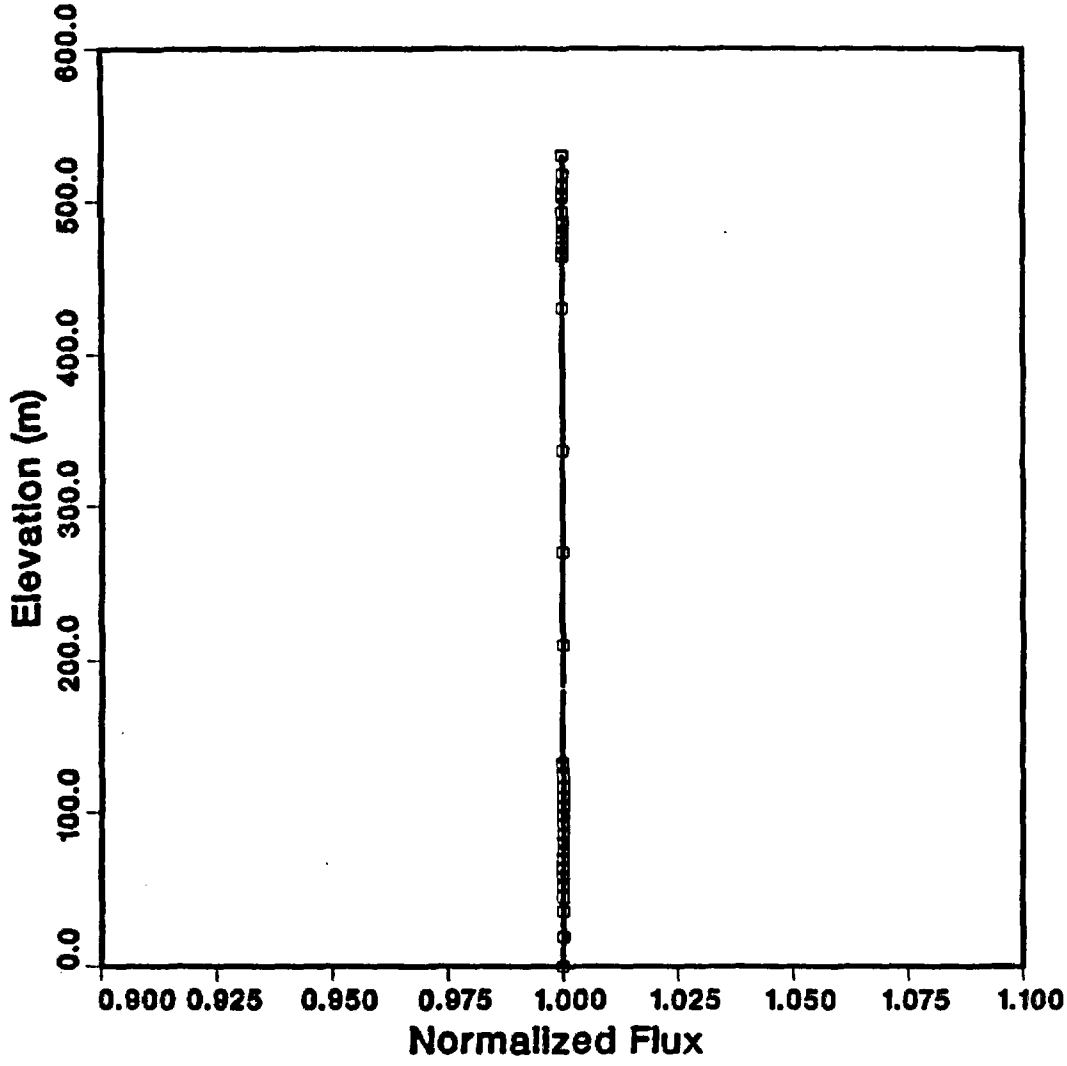


Figure 8: Normalized Average Flux

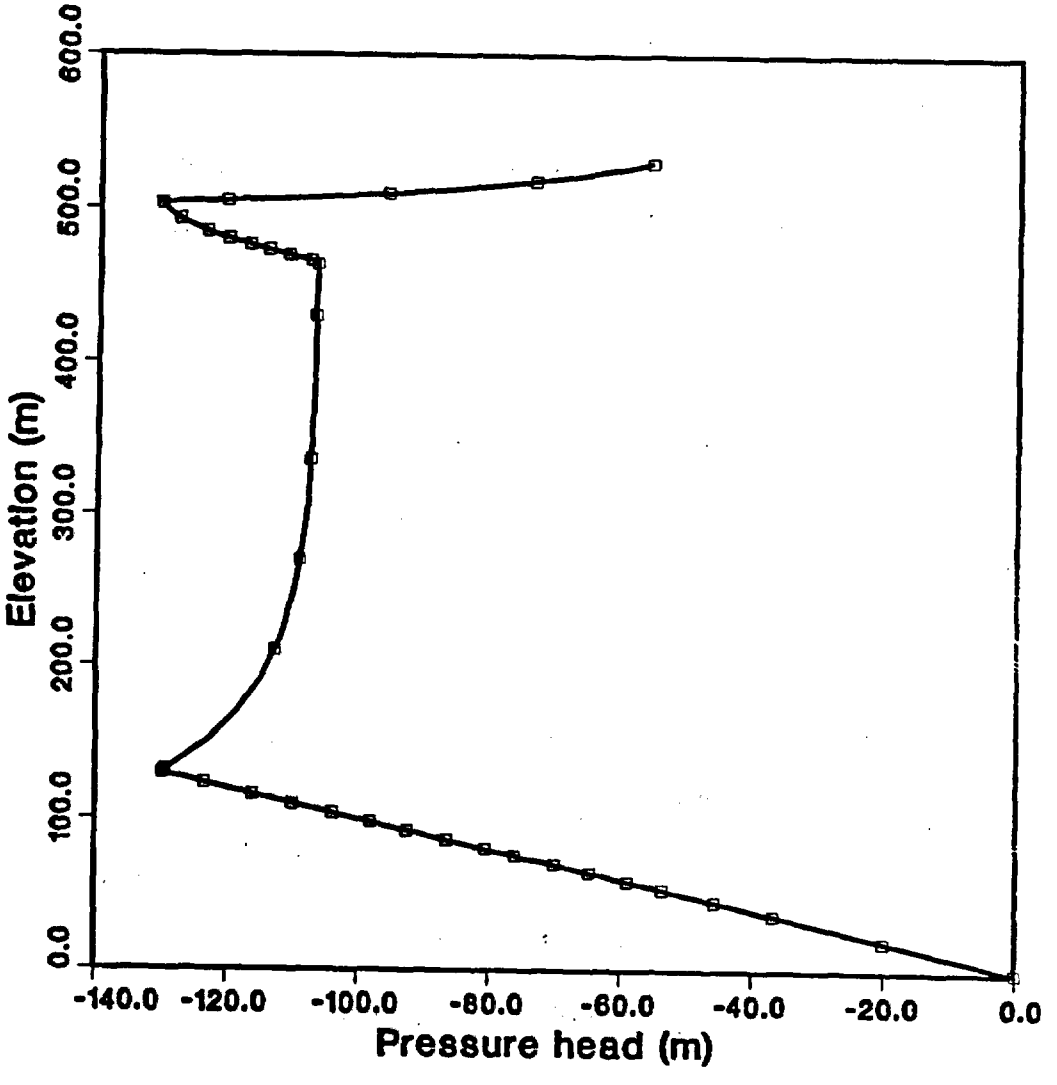


Figure 9: Pressure Head

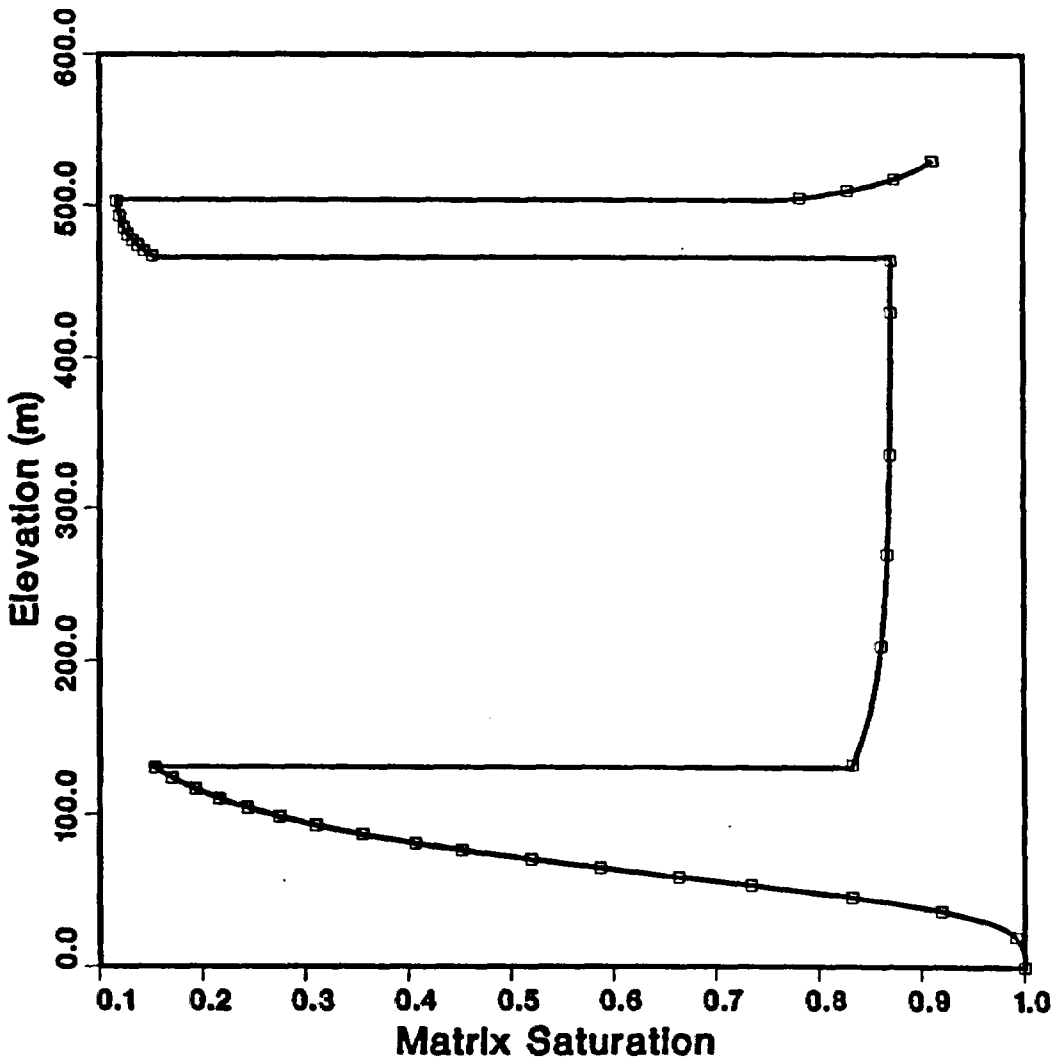


Figure 10: Matrix Saturation

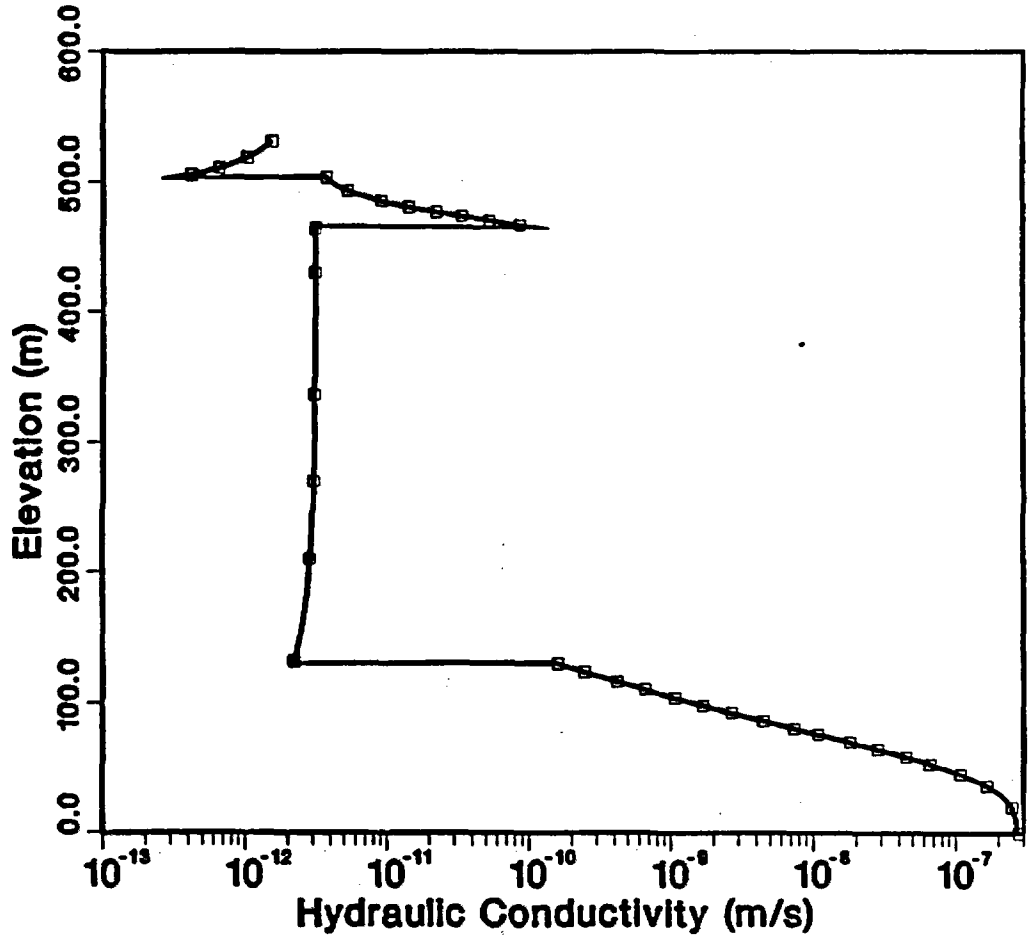


Figure 11: Hydraulic Conductivity

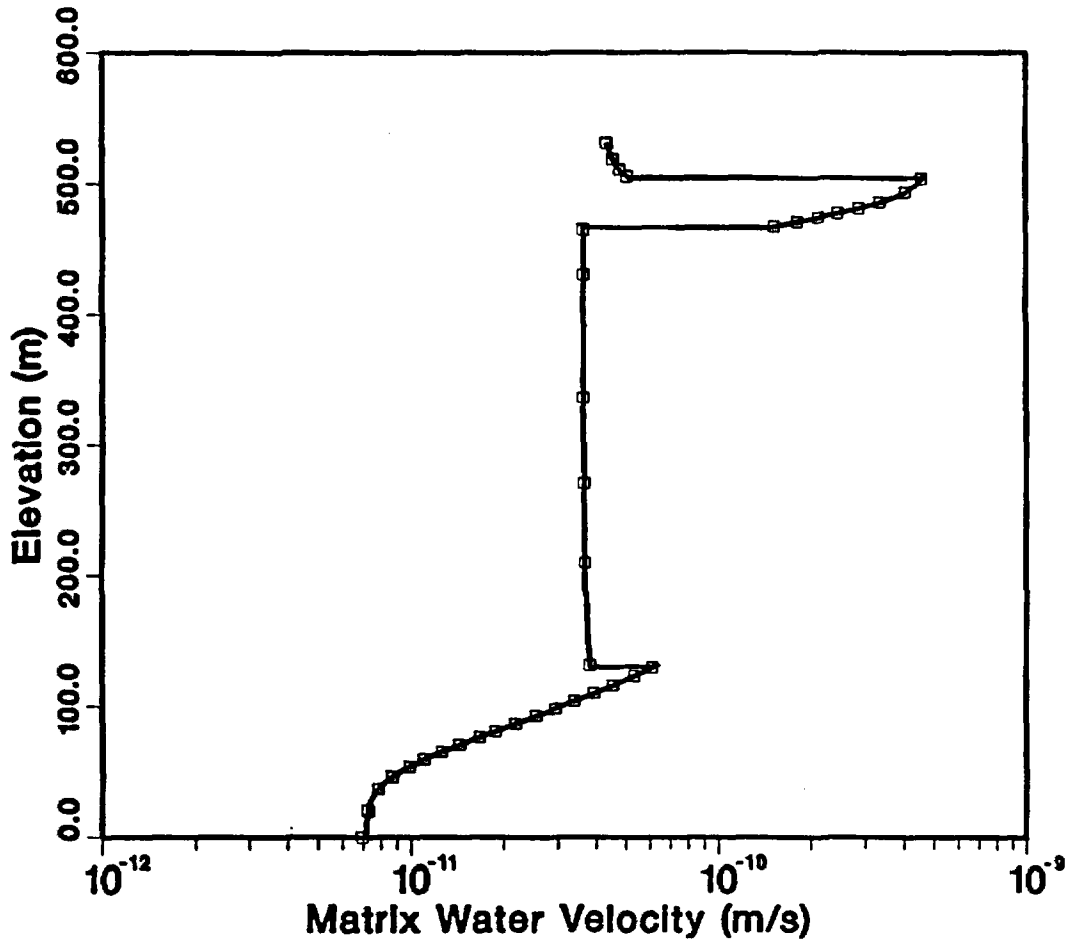


Figure 12: Water Velocity in the Matrix

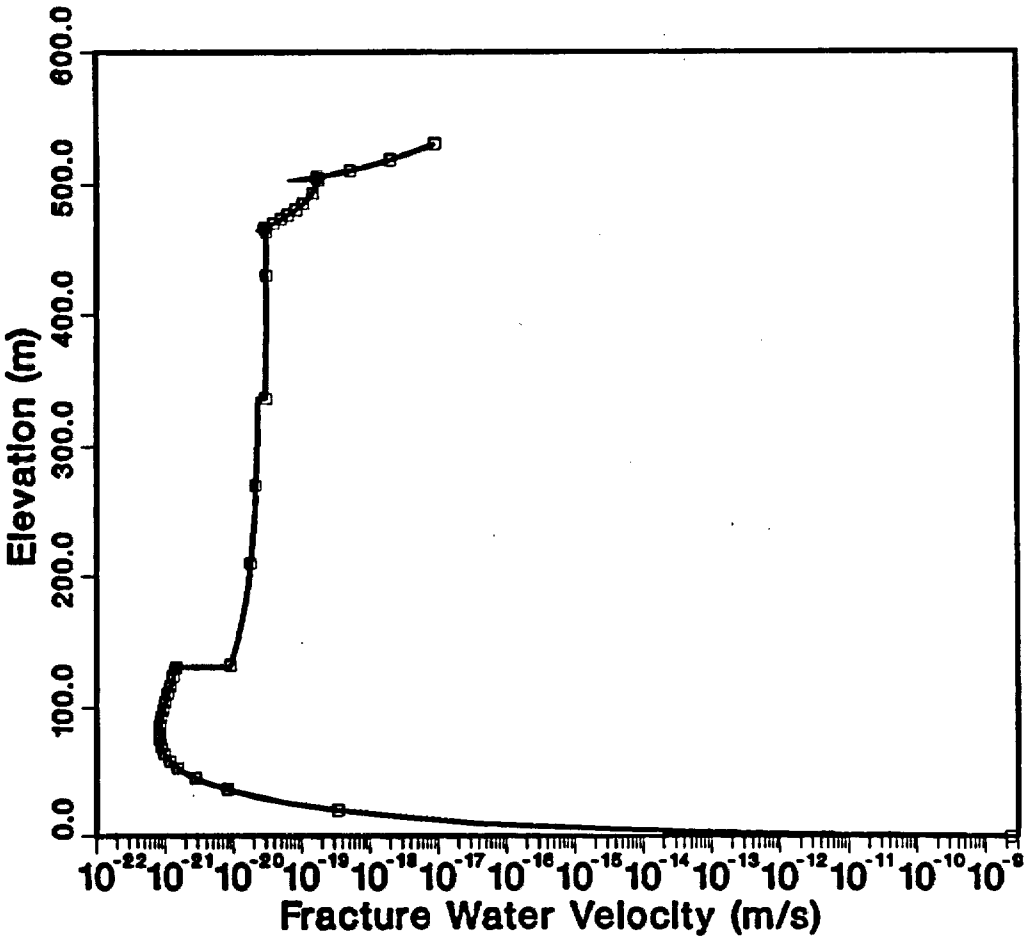


Figure 13: Water Velocity in the Fractures

9 RIB/SEPDB Data

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