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LLUVIA-II: A Program for Two-Dimensional, Transient Flow Through Partially Saturated Porous Media

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Abstract

LLUVIA-II is a program designed for the efficient solution of two-dimensional, transient flow of liquid water through partially saturated, porous media. The code solves Richards equation using the method-of-lines procedure. This document describes the solution procedure employed, input data structure, output, and code verification.

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This work was performed under WBS 1.2.1.4.9.

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1 Introduction

Modeling water flow through highly-fractured volcanic tuffs, such as those found at Yucca Mountain, is computer-time intensive because of the nonlinearities of the material characteristics resulting from variable saturation. Most of the scenarios of interest can, in theory at least, be analyzed using current modeling capabilities, but the costs resulting from the excessive computer requirements are in some cases prohibitive. Using the currently existing general purpose multiphase, multidimensional codes can require on the order of 100 hours of Cray computer time to analyze global Yucca Mountain scenarios. Consequently, alternate numerical methods have been investigated, including boundary integral methods, preconditioned conjugate gradient methods, one-dimensional marching steady-flow, semianalytical methods, and time-dependent one-dimensional method of lines (MOL). In all of these special cases, appreciable computer time savings were experienced over using existing finite element codes. However, in each case simplifications in material characteristics, material interfaces, steady-state limitations, geometry, and/or problem dimensionality had to be imposed.

In a continued effort to investigate other numerical techniques in which fewer restrictions must be applied, a code has been written using the MOL to compute two-dimensional, time-dependent, single phase flow in partially saturated or fully saturated media. The method has been found to be computationally efficient for several applications. The code uses library subroutines to solve the stiff equations that result from the nonlinear material characteristics. Both Neumann and Dirichlet boundary conditions and coordinate stretching have been accounted for.

This report presents the development of the two-dimensional MOL program LLUVIA-II, the input file, and the results of three benchmarking problems. This work was performed under WBS 1.2.1.4.9 of the Yucca Mountain Site Characterization Project.

1.1 Theory and Background

The method-of-lines approach (Hyman, 1979) to solving partial differential equations is particularly well adapted to the solution of nonlinear, parabolic partial differential equations where the material characteristics are such that the equations are mathematically stiff. In this method a set of ordinary differential equations (ODE) are obtained by uncoupling the spatial and temporal discretization of the partial differential equation. The resulting ODEs are solved using the SLATEC library routine DEBDF (Shampine and Watts, 1980; Hindmarsh, 1981). The stability of the solving routine is maintained by a "routine controlled" adaptive time-stepping procedure.

The development of the resulting two-dimensional code outlined in this report is based on a rectangular grid which allows for coordinate stretching in both the z and x directions. The assumption is made that the principle material axes are aligned with the x , z coordinates. Both Neumann and Dirichlet boundary conditions are accounted for.

A brief outline of the code development is given below.

1.2 Numerical Differencing Procedures

Richards' equation (Richards, 1978), which describes the isothermal flow of water through porous media, is given by

$$C_p \frac{\partial P}{\partial t} = \nabla \cdot (K \nabla P), \quad (1)$$

where K = hydraulic conductivity (m/s), P = total effective pressure [$P = \rho g(\psi + z)$, N/m²], C_p = material capacitance (1/m), and t = time (s).

Equation 1 can be written in terms of mass flux for rectangular cartesian coordinates for each i, j node point (Figure 1.1),

$$\frac{\partial P_{i,j}}{\partial t} = \frac{\rho g}{C_p} \left(\frac{\partial q_{x,i,j}}{\partial x} + \frac{\partial q_{z,i,j}}{\partial z} \right), \quad (2)$$

where $q_{x,i,j}$ and $q_{z,i,j}$ are Darcy fluxes in the x and z directions respectively. In finite difference form with fluxes computed at midpoint nodes Equation 2 becomes

$$\frac{\partial P_{x,i,j}}{\partial t} = \frac{\rho g}{C_p} \left(\frac{(q_{z,i+1/2,j} - q_{z,i-1/2,j})}{\Delta x_i} + \frac{(q_{z,i,j+1/2} - q_{z,i,j-1/2})}{\Delta z_j} \right), \quad (3)$$

where

$$\Delta x_i = (x_{i+1} - x_{i-1})/2$$

and

$$\Delta z_j = (z_{j+1} - z_{j-1})/2.$$

The fluxes are given by centered differences approximations,

$$q_{x,i+1/2,j} = \frac{-K_{i+1/2,j}}{\rho g} \frac{(P_{i+1,j} - P_{i,j})}{(x_{i+1} - x_i)} \quad (4a)$$

and

$$q_{z,i,j+1/2} = \frac{-K_{i,j+1/2}}{\rho g} \frac{(P_{i,j+1} - P_{i,j})}{(z_{j+1} - z_j)}. \quad (4b)$$

The hydraulic conductivities at the mid points are evaluated by

and

$$K_{i+1/2,j} = (K_{i+1,j} + K_{i,j})/2$$

$$K_{i,j+1/2} = (K_{i,j+1} + K_{i,j})/2.$$

Figure 1.1. Coordinate System.

For Dirichlet boundary conditions, P is held constant for all times. When Neumann boundary conditions are desired, the water mass flux gradients at the boundary points are determined as follows.

At the right boundary,

$$\frac{\partial q_{x,I,j}}{\partial x} = \frac{2(q_{x,right,j} - q_{x,I-1/2,j})}{(x_I - x_{I-1})}. \quad (5a)$$

At the left boundary,

$$\frac{\partial q_{x,1,j}}{\partial x} = \frac{2(q_{x,3/2,j} - q_{x,1,j})}{(x_2 - x_1)}. \quad (5b)$$

At the top boundary,

$$\frac{\partial q_{z,i,J}}{\partial z} = \frac{2(q_{z,i,top} - q_{z,i,J-1/2})}{(z_J - z_{J-1})}. \quad (5c)$$

At the bottom boundary,

$$\frac{\partial q_{z,i,3/2}}{\partial x} = \frac{2(q_{x,i,3/2} - q_{z,i,1})}{(z_2 - z_1)} \quad (5d)$$

where I = maximum value of i ($nxmax$ in the code), and J = the maximum value of j ($nzmax$ in the code).

The code allows for coordinate stretching in both the x and z directions based on

$$\Delta x_{i+1} = \Delta x_i \times str, \quad (6a)$$

and

$$\Delta z_{j+1} = \Delta z_j \times str, \quad (6a)$$

where str is a user specified stretch factor.

Currently LLUVIA-II is coded to use the van Genuchten (1978) and Mualem (1976) models for describing the conductivity and saturation as a function of pore pressure. These material routines (subroutines CON and FLUIDC) may be rewritten by the user to compute any model desired. The sample problem presented in Appendix C demonstrates the van Genuchten/Mualem models.

1.3 Method of Lines Solution Procedures

The set of stiff ordinary differential equations, given by equation 3, are solved by the method of lines using the SLATEC library subroutine, DEBDF. It employs backward differencing formulas of orders one through five to integrate the system of nonlinear first order ordinary differential equations. Further details regarding this solution routine can be obtained from Shampine and Watts (1980).

2 Program Outline

The code LLUVIA-II is written in FORTRAN 77 and consists of a group of 14 subroutines. A brief discussion of the contents of these routines and the flow of the code are given in Section 4. The code routines can be categorized according to six primary groups.

- Mesh generation. Subroutine GEO generates the x and z spatial locations for the rectangular mesh.
- Boundary and Initial Conditions. Subroutines INPUT and INITPRES assign pressure or flux boundary conditions to the mesh boundaries and initial pressure values to all mesh nodes.
- Solution Procedure. Subroutines CON and FLUIDC evaluate material properties. FF and GRAD evaluate spatial differences and solve the ODEs.
- Calculation of Derived Quantities. Subroutine VELO calculates water velocities.
- Output. Subroutines OUTPUT and FOROUT generate the program output.
- Post-Processing. Subroutines EXO, GENWRT, RESTART, and VSHIFT generate an EXODUS file which can be used with post processing plot programs.

2.1 Mesh Generation

The problem domain must be rectangular in extent. This total domain is made up of one to 20 subregions, as specified by the user. The regions must join so that the rows and columns of mesh points are continuous and orthogonal across the region, as shown in Figure 1.1. Mesh stretching, as specified in the input file, is allowed in both the x and z directions. The code is dimensioned for a maximum of 64 by 64 mesh points. These dimensions may be varied to meet the user's needs.

2.2 Boundary and Initial Conditions

Boundary conditions are specified on the four sides of the total rectangular domain. These conditions can be of two types: (1) Dirichlet - effective liquid pressure, or (2) Neumann - Darcy flux. Initial conditions consisting of effective liquid pressure must be specified throughout each subregion.

2.3 Plotting

LLUVIA-II has no internal plotting capabilities. Instead, an output file is produced in the EXODUS format. This file can then be directed to the graphics package BLOT (Gilkey and Glick, 1989). All properties printed in the output are included on the EXODUS tape for the print-times specified in the input file (see Appendix A through C).

3 Input Guide

The input data file supplies the program with information on the problem geometry, initial pressures, material properties, requested output times, pressure, flux boundary conditions and restart information. A description of the required input is given below. Comments may be located on each line of data after the last required entry. All variables are input in a free-field format, and successive variables are separated by blanks. The contents of each data line given below are indicated by underlining. All quantities associated with a coordinate direction are expressed in terms of the planar (x,z) coordinate system.

The overall geometry is limited to a rectangular region. This total computational region is a composite of 1 to 20 subregions. Each may have unique geometry and/or material requirements and therefore is input separately. The sequence of the input file is as follows.

Region specifiers.

$$\underline{nregx, nregz, \rho g, pflag}$$

where

$nregx$ = the number of subregions in the x direction,
 $nregz$ = the number of subregions in the z direction,
 ρg = water density times gravitational constant (N/m^3), and
 $pflag$ = 1 if initial pressure (pinit) is effective pressure, (N/m^2)
= 2 if pinit is pressure head, ψ , (m).

Region number (repeat next four lines for each subregion).

$$\underline{regn}$$

where

$regn$ = subregion identification number.

$$\underline{nodex, nodez, mat, pinit, pflag}$$

where

$nodex$ = the number nodes in x direction,
 $nodez$ = the number nodes in z direction,

p_{init} = initial effective pressure $P = \rho g(\psi + z)$ if $pflag=0$, and
 p_{init} = initial pressure head, ψ , if $pflag=1$.

$$\underline{xstr, zstr, x0, xmax, z0, zmax}$$

where

$xstr$ = coordinate stretch in the x direction,
 $zstr$ = coordinate stretch in the z direction,
 $x0$ = minimum value of x coordinate,
 $xmax$ = maximum value of x coordinate,
 $z0$ = minimum value of z coordinate, and
 $zmax$ = maximum value of z coordinate.

For stretched geometries the geometric factors, shown in Figure 1.1 are defined by

$$xstr \equiv \frac{\Delta x_{i+1}}{\Delta x_i}, \quad (3.1)$$

and

$$zstr \equiv \frac{\Delta z_{j+1}}{\Delta z_j} \quad (3.2)$$

and the node spacing is given by

$$\Delta m = L \times \left(\frac{g - 1}{g^N - 1} \right) \times g^{(n-1)}, \quad (3.3)$$

where

$\Delta m = \Delta x_i$ or Δz_j ,
 $g = xstr$ or $ystr$,
 L = total length in the i or j direction of
the subregion being generated,
 N = total number of nodes - 1 in the i or j dir, and
 $n = i$ or j index that goes from 1 to N .

Material property card.

The material subroutines CON and FLUIDC currently employ the van Genuchten (1978) and Mualem (1978) models for describing the material characteristics, moisture content and conductivity as functions of pore pressure. The input parameters α and β refer to that formulation. If alternate models are used the α and β storage locations may be used to store other variables.

$$\underline{\alpha, \beta, s_r, s_s, \phi, k}$$

where

$$\begin{aligned}\alpha &= \text{Genuchten air entry parameter (1/m),} \\ \beta &= \text{Genuchten slope parameter,} \\ s_r &= \text{residual saturation,} \\ s_s &= \text{saturated saturation,} \\ \phi &= \text{porosity, and} \\ k &= \text{(m/s).}\end{aligned}$$

It is necessary to have one set of the above four data lines for each region. ($nregx \times nregz$ sets of four data lines/set)

$$\underline{ntimes}$$

where

$ntimes$ = number of times that output data will be printed.

$$\underline{tout}$$

where

$tout$ = value of time where output data will be printed (s).

The number of $tout$ data lines required = $ntimes$.

One set of data lines is necessary for each of the four mesh boundaries. The sets must appear in the following clockwise order; top, right, bottom, left. Each boundary mesh point (i or j) must be assigned either a Dirichlet (fixed pressure) or a Neuman (Darcy flux) value.

ndata

where

ndata = number of data sets for this set,

istart, ifinish, ibctyp, bvalue

where

istart = initial value of *i* for this set,
ifinish = ifinial value of *i* for this set,
ibctyp = 1 then *bvalue* = pressure, and
ibctyp = 2 then *bvalue* = flux (m/s).

For example, if *nxmax* = 10 and the first four *i* values (1 through 4) along the top boundary are to be assigned a fixed pressure of -234.0 N/m² the next four (5 through 8) a flux of 13.0×10^{-7} m/s, and the last two (9 and 10) a fixed pressure of -570.0 N/m² then the four data lines defining this boundary are

3

1 4 1 -234.0

5 8 2 13.0e-7

9 10 1 -570.0.

The code will print and/or read a restart file, depending on the values of *ip* and *ir*.

ip, ir, stime

where

ip = 1 then restart file is written, =0 no file written,
ir = 1 initial pressure field read from restart file,
ir = 0 initial pressures read from input data file, and
stime = restart time, effects printout, but not calculations.

4 Program Description

4.1 Description of Subroutines

A brief description of the subroutines in code LLUVIA-II is given below.

```
subroutine con
```

```
c   Calculates hydraulic conductivity. (m/s)
c   This is a user written subroutine.
```

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
subroutine exo
```

```
c   Translates results of finite difference formulation to
c   format required by EXODUS data file.
```

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
subroutine ff
```

```
c   Calculates numerical spatial differences for right hand
c   side of the differential equation.
```

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
subroutine fluidc
```

```
c   Calculates the moisture content and derivatives of
c   moisture content with respect to pressure.
c   This is a user written subroutine.
```

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
subroutine forout
```

```
c   Prints output.
```

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
subroutine genwrt
```

```
c   Formats data required for the EXODUS file.
```

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
subroutine geom
```

c   Calculates the x and z coordinate location for each node
c   using geometric stretching algorithm.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      subroutine grad

c   Calculates the spatial gradients needed to evaluate the
c   right hand side of the partial differential equations.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      subroutine input

c   Reads required input data such as geometry, computation times,
c   material properties, initial conditions, and boundary conditions.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      subroutine initpres

c   Determines initial pressure distribution.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      subroutine output

c   Prints specifies variables.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      subroutine restart

c   Sets up pressure data file to be used to restart the run.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      subroutine velo

c   Calculates Darcy flux in x and z direction.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
      subroutine vshift

c   Flux components are interpolated at node points for EXODUS file.

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX

4.2 Program Usage

The code has been used on both the CRAY and on SUN workstations. When running on the CRAY the code should be run in single precision. If the code is to run on a SUN workstation, to solve highly nonlinear problems, it is best to use a double precision version of the code. In this version the following card needs to be added to each subroutine except for subroutine genwrt.

```
implicit real*8 (a-h,o-z)
```

The double precision version of the slatec library routines is called by

```
call ddebf(ff,neq,t,f,tout,info,re,ae,id,rwork,lrw,  
1          iwork,liw,rpar,ipar,jac)
```

This call is located in the main program.

4.3 Program Flow

The flow of the subroutines in LLUVIA-II are outlined below.

Main program, molc, calls each of the following subroutines.

```
call input
call geom
call initpres
call output
call debdf
call fluidc
call con
call vel
call output
call path
call flux
end
```

subroutine con

Calculates hydraulic conductivity (m/s).
returns to main

subroutine ff

Calculates the right hand side of flow equation.
calls subroutines fluidc, con, and grad.
returns to main

subroutine fluidc

Calculates the moisture content.
returns to main

subroutine flux

Integrates mass flux across each boundary
returns to main

subroutine forout

Formats output data.
returns to main

subroutine geom

Calculates x and z node coordinate location.
returns to main

subroutine grad
Calculates gradients needed for right hand side of equation.
returns to main

subroutine input
Reads all required input data.
returns to main

subroutine initpres
Determines initial pressure distribution.
returns to main

subroutine intrpt
Interpolation routine.
returns to main

subroutine output
Writes output data.
call forout

subroutine path
Calculates the x,z coordinates for pathlines.
calls subroutines xpoints and intrpt.
returns to main

subroutine vel
Calculates the Darcy flux.
returns to main

subroutine xpoints
Determines cell in which pathline points are located.
returns to main

5 Program Verification and Sample Cases

Code verification consists of comparing solutions obtained using LLUVIA-II with analytical solutions and with computational results obtained using the finite element code NORIA-SP (Hopkins *et al.*, 1991). Results for three examples are given. In the first two examples (Case 1a and 1b) the results of LLUVIA-II and NORIA-SP are compared with Fleming's *et al.*, (1986) analytical solution, for one-dimensional time-dependent infiltration into homogeneous porous media. Sand-like material is used for Case 1a and tuff material is used in Case 1b. In Case 2, LLUVIA-II results are compared with NORIA-SP results for infiltration into a multilayered geologic media.

5.1 Comparison with Analytical Numerical Results, Case 1

For vertical, one-dimensional infiltration into a semi-infinite porous medium with a uniform initial moisture content of zero, the analytical solution as given by Fleming is

$$\frac{\theta}{\theta_s} = (1 - e^{\alpha n(\lambda t + z)})^{1/n}. \quad (7)$$

This solution requires the boundary condition at $z = 0$ to be given as either the flux condition,

$$q = K_s(1 - e^{-\alpha n \lambda t})^{1/n}, \quad (8)$$

or the moisture content condition,

$$\theta = \theta_s(1 - e^{-\alpha n \lambda t})^{1/n}. \quad (9)$$

The saturation and conductivity material characteristics are,

$$\theta = \theta_s e^{\alpha \psi}, \quad (10)$$

and

$$K = K_s e^{\alpha \psi (n+1)}, \quad (11)$$

respectively. Where, θ = moisture content, θ_s = saturated moisture content, α and n are parameters of the hydraulic properties, $\lambda = K/\theta_s$, t = time (s), and z = vertical distance (m).

Table 5.1. Material Properties for Case 1

Case	α (1/m)	n (-)	λ (m/s)	K_s (m/s)
1a	2.0	2.0	1.433×10^{-5}	4.3×10^{-6}
1b	0.0046	0.652	1.727×10^{-10}	1.9×10^{-11}

The time-dependent solution domain is given by $0 \leq z \leq \lambda t$. For spatial locations beyond this region the moisture content is specified as zero.

Material characteristics (Table 4-1) were chosen as a fit to generic sand for Case 1a as given by Freeze and Cherry (1979) and for volcanic tuff rock for Case 1b. A listing of the input file, the time-dependent flux boundary condition, the conductivity subroutine, the moisture content subroutine and a partial listing of the output data are given in Appendix A for Case 1a. The input file for Case 1b is given in Appendix B.

LLUVIA-II mesh for Case 1a and 1b consists of two vertical columns of 41 and 81 evenly spaced mesh points extending from $z=0.0$ to $z=-1.0$ m. The NORIA-SP mesh consists of a column of 40, eight-node, equally spaced biquadratic elements.

5.2 Comparison with Analytical Numerical Results, Case 1a, Sand Material

The results for the analytical and both numerical solutions are given in Figure 5.1 for times up to 0.5×10^5 s. Agreement between the LLUVIA-II and NORIA-SP solutions is excellent. Both numerical solutions differ slightly from the analytical solution for saturations less than 0.6. This is a result of the differences in initial conditions. A value of zero saturation is inherent in the analytical solution, while values as large as 0.05 were used in the numerical solutions. Initial saturations appreciably smaller than 0.05 resulted in excessive NORIA-SP computational time requirements. LLUVIA-II computational times requirements increase for under these conditions but are not excessive.

For the case shown in Figure 5.1 the required computer times for the numerical codes LLUVIA-II and NORIA-SP, respectively, were 8 and 250 seconds on the CRAY XMP. LLUVIA-II was also used to compute results using 81 vertical mesh points, with initial saturations less than 0.005, Figure 5.2. The differences in the analytical and LLUVIA-II results decrease appreciably for the reduced initial saturation.

5.3 Comparison With Analytical Numerical Results, Case 1b, Tuff Material

The results for both the analytical and numerical solutions for tuff rock are given in Figure 5.3 for times up to 0.18×10^{13} s. The calculations were terminated before the front reached the bottom boundary. Agreement is excellent except for saturation less than 0.02, where the numerical front diffuses slightly faster than the analytical solution. The required computer times for the numerical codes LLUVIA-II and NORIA-SP were 7 and 273 seconds respectively on the CRAY XMP.

5.4 Comparison with NORIA-SP, Case 2, Multiple Layered Geologic Media

Case 2 represents infiltration into geologic media with five distinctly different material layers. Saturation and conductivity functions for this case were described using the Mualem (1976) and van Genuchten (1978) formulation, Appendix C. The appropriate material constants are given in Table 5-2. The geometry consists of two vertical columns of 201 mesh points extending from $z = 0.0$ m (water table) to $z = 530.4$ m (ground level). Mesh stretching was used to increase resolution near unit interfaces. This sample problem was taken from the code verification exercise, COVE IIA (Carrigan *et al.*, 1991).

A listing of the input data file, conductivity subroutine, moisture content subroutine, and a partial listing of the output data are given in Appendix C.

The case has an initial steady-state Darcy flux of 0.5 mm/yr which is then perturbed by applying a 1.0 mm/yr infiltration at the top boundary. The problem was run in two steps. In the first step a 0.5 mm/yr infiltration was applied to the top boundary and run to a steady-state condition. The "restart" option was then employed using the 0.5 mm/yr steady-state results for initial pressure values while changing the top boundary condition to a flux of 1.0 mm/yr.

Computed vertical flux for times from 10 yr to 1250 yr are given in Figure 5.4. Agreement between NORIA-SP and LLUVIA-II is good except near the infiltration front at $t = 275$ yr. In this region the initial saturation is nearly one. Therefore, the calculated water front location is extremely sensitivity to the calculated pressures. The variation in the LLUVIA and NORIA-SP results are within the scatter of the results of the five numerical codes reported by Dykhuizen, *et al.* (1991).

The results of these three verification cases indicate that the solution procedure in LLUVIA-II is both accurate and computationally efficient. Accumulated experience with the code has shown that it is particularly useful for modeling meter-scale laboratory experiments where initial conditions are dry. These conditions often result in permeability and moisture content values which vary by ten orders of magnitude. The library routines found in the SLATEC package are extremely efficient under these conditions. The results of Case 2 also show that the method-of-lines procedure is good for calculating flow through multilayered geologic media on the scale of hundreds of meters.

Figure 5.1. Comparison of Numerical Results with Analytical Solution, Case 1a for $n = 2.0$, $\theta_s = 0.3$, $\alpha = 2.0$, and $\lambda = 1.433 \times 10^{-5}$, and $S_i \leq 0.005$, 11 Vertical Mesh Points.

Figure 5.2. Comparison of Numerical Results with Analytical Solution Case 1b for $n = 2.0$, $\theta_s = 0.3$, $\alpha = 2.0$, and $\lambda = 1.433 \times 10^{-5}$, and $S_i \leq 0.005$, 81 Vertical Mesh Points.

Table 5.2. Material Properties for Case 2

	TCw	PTn	TSw1	TSw2-3	CHuv	CHuz
n_m	0.08	0.40	0.11	0.11	0.46	0.28
K_m (m/s)	9.7×10^{-12}	3.9×10^{-7}	1.9×10^{-11}	1.9×10^{-11}	2.7×10^{-7}	2.6×10^{-11}
$S_{r,m}$	0.002	0.100	0.080	0.080	0.041	0.110
α_m (1/m)	0.821×10^{-2}	1.5×10^{-2}	0.567×10^{-2}	0.567×10^{-2}	1.600×10^{-2}	0.308×10^{-2}
β_m	1.558	6.872	1.798	1.798	3.872	1.602
n_f	1.4×10^{-4}	2.7×10^{-5}	4.1×10^{-5}	1.8×10^{-4}	4.6×10^{-5}	4.6×10^{-5}
K_f (m/s)	5.3×10^{-9}	1.6×10^{-8}	0.9×10^{-9}	3.1×10^{-9}	9.2×10^{-9}	9.2×10^{-9}
$S_{r,f}$	0.0395	0.0395	0.0395	0.0395	0.0395	0.0395
α_f (1/m)	1.285	1.285	1.285	1.285	1.285	1.285
β_f	4.23	4.23	4.23	4.23	4.23	4.23
α'_{bulk} (1/m)	6.2×10^{-7}	8.2×10^{-6}	1.2×10^{-6}	5.8×10^{-7}	3.9×10^{-6}	2.6×10^{-6}
$\frac{\partial n_f}{\partial \sigma}$ (1/m)	1.32×10^{-6}	1.9×10^{-7}	5.6×10^{-8}	1.2×10^{-7}	2.8×10^{-8}	2.8×10^{-8}

Where, m = matrix and f = fracture.

Figure 5.3. Comparison of LLUVIA-II and NORIA-SP Numerical Results with Analytical Solution for $n = 0.652$, $\theta_s = 0.11$, $\alpha = 0.0046$, and $\lambda = 1.727 \times 10^{-10}$, and $S_i \leq 0.64 \times 10^{-4}$, 41 Vertical Mesh Points.

Figure 5.4. Comparison of LLUVIA-II Results with NORIA-SP, Case 2. Five Geologic Units.

6 References

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7 Appendix A-Input and Results, Case 1a

7.1 Input, Case 1a

The input file for Case 1a is given below.

```

1  1                                number of regions in x and z directions
1                                region number
2    41    8  -.245e5              no. of x nodes, no. of z nodes, mat, pi
1    1    0.0  0.1  -1.0  0.0    x and z stretch, xo, xmax, zo, zmax
999 999  999  999  999  999    constants overwritten in con and fluidc
5                                number of time prints
1e4                              print output at these 5 times
2e4
3e4
4e4
5e4
1
1 2  2  333                      top boundary over written see next section
1
1 41 2  0.0                      right boundary cond. zero flux
1
1 2  2  0.0                      bottom boundary cond. zero flux
1
1 41 2  0.0                      left boundary cond. zero flux
0  0                              don't print restart, don't read restart file

```

7.2 Time Dependent Boundary Condition, Case 1a

The top boundary condition is time dependent for this sample problem and is therefore defined in subroutine "grad" as follows.

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
      subroutine grad (t)
c      implicit real*8 (a-h,o-z)
      common / bcon / ibctop,ptop,qtop,ibcrt,pright,qright,
1      ibcbot,pbot,qbot,ibclt,pleft,qleft
      common / geo / mat(20),nrx,nrz,nnxr(20),nnzr(20), nxmax,nzmax,
1      strx(20),strz(20),xo(20),xmax(20),x(21),
2      zo(20),zmax(20),z(41),mxz(21,41)
      common / sol / qx(21,41),qz(21,41),qgx(21,41),qgz(21,41)
c Fleming
      data conduct, thetas, ce, an, alpha/ 4.3e-6, .30, 2.7182818,
1 2.0, 2.0/
c calculates the gradients needed in the right hand side of the

```

```

c flow equation.
  do 20 j = 2,nzmax - 1
    do 10 i = 2,nxmax - 1
      qgz(i,j) = 2.*(qz(i,j) - qz(i,j-1))/(z(j+1) - z(j-1))
      qgx(i,j) = 2.*(qx(i,j) - qx(i-1,j))/(x(i+1) - x(i-1))
    10 continue
  20 continue
c top boundary for specified time dependent flux as required by
c fleming's analytic solution.
  alambda = conduct/thetas
  qtop = -conduct*(1-ce**(-alpha*an*alambda*t))*(1/an)
  do 30 i = 2,nxmax-1
    qgz(i,nzmax) = 2.*(qtop - qz(i,nzmax-1))/
    1 (z(nzmax) - z(nzmax-1))
    qgx(i,nzmax) = 2.*(qx(i,nzmax) - qx(i-1,nzmax))/
    1 (x(i+1) - x(i-1))
  30 continue
c right boundary for specified flux

```

7.3 Subroutines for Conductivity and Moisture Content, Case 1a

The material subroutines for conductivity and moisture content for the Fleming analytical solution are given below.

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
      subroutine con(condx,condz,p,x,z,nxmax,nzmax,mxz)
cc this subroutine has fleming's material in it. (7/6/1990)
c
c calculates hydraulic conductivity (m/s)
c units - kg, m, s
c
      dimension af(10),alpm(10),betm(10)
      dimension c(21,41),condx(21,41),condz(21,41),conm(10),conf(10)
      dimension p(21,41),x(21),z(41),mxz(21,41)
      rhog = 9800.
      ce = 2.7182818
c Fleming. remember to change this conductivity value in grad
      conduct = 4.3e-6
      alpha = 2.0
      an = 2.0
c calculate condx and condz
      do 20 j=1,nzmax
        do 10 i=1,nxmax
          mat=mxz(i,j)

```

```

        phm=p(i,j)/rhog - z(j)
        if(phm. gt. -.000001) phm=-.000001
        c(i,j) = conduct*ce**(alpha*(an+1)*phm)
10 continue
20 continue
    do 40 j=1,nzmax
    do 30 i=1,nxmax-1
        condx(i,j)=0.5*(c(i,j)+c(i+1,j))
c      condx(i,j)=c(i,j)*c(i+1,j)/(c(i,j)+c(i+1,j))
30 continue
40 continue
    do 60 j=1,nzmax-1
    do 50 i=1,nxmax
        condz(i,j)=0.5*(c(i,j)+c(i,j+1))
c      condz(i,j)=c(i,j)*c(i,j+1)/(c(i,j)+c(i,j+1))
50 continue
60 continue
    end

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
    subroutine fluidc(cm,th,p,z,mxz,nxmax,nzmax)
c    this subroutine contains fleming's material characteristic curves.
c... this sub calc the moisture content and der of moisture content wrt
c    pressure in units - kg, m, s.
c
    dimension th(21,41),cm(21,41),p(21,41)
    dimension x(21),z(41),mxz(21,41)
    dimension smr(10),anm(10),anf(10),alpm(10),betm(10),alpp(10),
2      fc(10)
c
    dimension thm(21,41)
    rhog = 9800.
    ce=2.7182818
c fleming's material values
    thetas = 0.3
    anm1 = thetas
    anf1 = 1e-10
    smr1 = 0
    sfr = 0
    alpha = 2.0
c
c    loop over nodes
c
    do 100 j=1,nzmax

    do 50 i=1,nxmax
        phm=p(i,j)/rhog - z(j)

```

```

        if (phm.gt.-.000001) phm=-.000001
        th(i,j) = thetas*ce**(alpha*phm)
c compute derivative of moisture content
        cm(i,j) = alpha*th(i,j)
    50 continue
    100 continue
        return
    end

```

7.4 Output, Case 1a

A partial listing of the output for Case 1a follows. In order to hold the total amount of data presented to a reasonable amount a considerable amount of the data has been edited out. These locations are noted by a "several lines of data edited out" comment.

A partial listing of the output for Case 1a is given below.

```

subroutine input
number of regions in x and z dir.=2*1

region number
no. of x and z nodes in region, mat, initial press
stretch in x and z direction, xo, xmzx, zo, zmax
    1
    2   41   8-0.24500E+05
    0.10000E+01 0.10000E+01 0.00000E+00 0.10000E+00-0.10000E+01 0.00000E+00
    0.99900E+03 0.99900E+03 0.99900E+03 0.99900E+03 0.99900E+03 0.99900E+03

ptop=0.      qtop=333.
pright=0.    qright=0.
pbot=0.      qbot=0.
pleft=0.     qleft=0.

nxmax=, xzmax= 2, 41
x coordinates
    0.000E+00  0.100E+00
z coordinates
    -0.100E+01 -0.975E+00 -0.950E+00 -0.925E+00 -0.900E+00 -0.875E+00
    -0.850E+00 -0.825E+00 -0.800E+00 -0.775E+00 -0.750E+00 -0.725E+00
    -0.700E+00 -0.675E+00 -0.650E+00 -0.625E+00 -0.600E+00 -0.575E+00
    -0.550E+00 -0.525E+00 -0.500E+00 -0.475E+00 -0.450E+00 -0.425E+00
    -0.400E+00 -0.375E+00 -0.350E+00 -0.325E+00 -0.300E+00 -0.275E+00

```

```

-0.250E+00 -0.225E+00 -0.200E+00 -0.175E+00 -0.150E+00 -0.125E+00
-0.100E+00 -0.750E-01 -0.500E-01 -0.250E-01 -0.471E-13
material
  8 8
  8 8
  8 8
  8 8

```

‘several lines of data edited out’

```

time=10000.
converged solution

```

```

.      xxxxxx pressure field xxxxxx

          0.0000E+00  1.0000E-01

-4.707E-14 -2.0709E+03 -2.0709E+03
-2.500E-02 -2.6901E+03 -2.6901E+03
-5.000E-02 -3.4268E+03 -3.4268E+03
-7.500E-02 -4.3562E+03 -4.3562E+03
-1.000E-01 -5.6507E+03 -5.6507E+03
-1.250E-01 -7.8127E+03 -7.8127E+03
-1.500E-01 -1.2521E+04 -1.2521E+04
-1.750E-01 -2.2699E+04 -2.2699E+04
-2.000E-01 -2.4499E+04 -2.4499E+04
-2.250E-01 -2.4500E+04 -2.4500E+04
-2.500E-01 -2.4500E+04 -2.4500E+04
-2.750E-01 -2.4500E+04 -2.4500E+04

```

‘several lines of data edited out’

```

.      xxxxxx qx flux xxxxxx

          0.0000E+00  1.0000E-01

-4.707E-14 -1.7985E-20  0.0000E+00
-2.500E-02 -2.8613E-20  0.0000E+00
-5.000E-02 -2.1183E-20  0.0000E+00
-7.500E-02 -1.3941E-20  0.0000E+00
-1.000E-01 -7.3431E-21  0.0000E+00
-1.250E-01 -1.8236E-20  0.0000E+00

```

```

-1.500E-01 -3.3021E-21 0.0000E+00
-1.750E-01 -1.1012E-23 0.0000E+00
-2.000E-01 0.0000E+00 0.0000E+00
-2.250E-01 0.0000E+00 0.0000E+00
-2.500E-01 0.0000E+00 0.0000E+00

```

‘several lines of data edited out’

.   xxxxxx qz flux xxxxxx

```

0.0000E+00 1.0000E-01

-4.707E-14 0.0000E+00 0.0000E+00
-2.500E-02 -2.7462E-06 -2.7462E-06
-5.000E-02 -2.5187E-06 -2.5187E-06
-7.500E-02 -2.2407E-06 -2.2407E-06
-1.000E-01 -1.8899E-06 -1.8899E-06
-1.250E-01 -1.4255E-06 -1.4255E-06
-1.500E-01 -7.8275E-07 -7.8275E-07
-1.750E-01 -1.0517E-07 -1.0517E-07
-2.000E-01 -5.9852E-11 -5.9852E-11
-2.250E-01 -1.5876E-14 -1.5876E-14
-2.500E-01 -4.6261E-18 -4.6261E-18
-2.750E-01 -1.4140E-21 -1.4140E-21
-3.000E-01 0.0000E+00 0.0000E+00
-3.250E-01 0.0000E+00 0.0000E+00
-3.500E-01 0.0000E+00 0.0000E+00

```

‘several lines of data edited out’

.   xxxxx moisture xxxxx

```

0.0000E+00 1.0000E-01

-4.707E-14 1.9660E-01 1.9660E-01
-2.500E-02 1.8214E-01 1.8214E-01
-5.000E-02 1.6475E-01 1.6475E-01
-7.500E-02 1.4327E-01 1.4327E-01
-1.000E-01 1.1565E-01 1.1565E-01
-1.250E-01 7.8206E-02 7.8206E-02
-1.500E-01 3.1453E-02 3.1453E-02

```


-1.750E-01	4.1428E-03	4.1428E-03
-2.000E-01	3.0160E-03	3.0160E-03
-2.250E-01	3.1702E-03	3.1702E-03
-2.500E-01	3.3327E-03	3.3327E-03
-2.750E-01	3.5036E-03	3.5036E-03
-3.000E-01	3.6832E-03	3.6832E-03

“several lines of data edited out”

xxxxx condx field xxxxx

0.0000E+00

-4.707E-14	1.2101E-06
-2.500E-02	9.6235E-07
-5.000E-02	7.1218E-07
-7.500E-02	4.6839E-07
-1.000E-01	2.4635E-07
-1.250E-01	7.6177E-08
-1.500E-01	4.9554E-09
-1.750E-01	1.1323E-11
-2.000E-01	4.3693E-12
-2.250E-01	5.0740E-12
-2.500E-01	5.8951E-12
-2.750E-01	6.8492E-12
-3.000E-01	7.9576E-12
-3.250E-01	9.2454E-12
-3.500E-01	1.0742E-11
-3.750E-01	1.2480E-11

“several lines of data edited out”

xxxxx condz field xxxxx

0.0000E+00 1.0000E-01

-2.500E-02	1.0862E-06	1.0862E-06
-5.000E-02	8.3727E-07	8.3727E-07
-7.500E-02	5.9028E-07	5.9028E-07
-1.000E-01	3.5737E-07	3.5737E-07
-1.250E-01	1.6126E-07	1.6126E-07
-1.500E-01	4.0566E-08	4.0566E-08

-1.750E-01	2.4834E-09	2.4834E-09
-2.000E-01	7.8464E-12	7.8464E-12
-2.250E-01	4.7217E-12	4.7217E-12
-2.500E-01	5.4846E-12	5.4846E-12
-2.750E-01	6.3721E-12	6.3721E-12
-3.000E-01	7.4034E-12	7.4034E-12
-3.250E-01	8.6015E-12	8.6015E-12
-3.500E-01	9.9935E-12	9.9935E-12

‘several lines of data edited out’

.   xxxxx cap field xxxxx

	0.0000E+00	1.0000E-01
-4.707E-14	3.9319E-01	3.9319E-01
-2.500E-02	3.6428E-01	3.6428E-01
-5.000E-02	3.2950E-01	3.2950E-01
-7.500E-02	2.8655E-01	2.8655E-01
-1.000E-01	2.3130E-01	2.3130E-01
-1.250E-01	1.5641E-01	1.5641E-01
-1.500E-01	6.2905E-02	6.2905E-02
-1.750E-01	8.2855E-03	8.2855E-03
-2.000E-01	6.0321E-03	6.0321E-03
-2.250E-01	6.3403E-03	6.3403E-03
-2.500E-01	6.6654E-03	6.6654E-03
-2.750E-01	7.0071E-03	7.0071E-03
-3.000E-01	7.3664E-03	7.3664E-03
-3.250E-01	7.7441E-03	7.7441E-03

‘several lines of data edited out’

8 Appendix B—Input and Results, Case 1b

8.1 Input, Case 1b

The geometry for Case 1b is the same as that used in Case 1a. The material properties represent a generic volcanic tuff rock.

```
1  1
1
2      21      8  -2.45e7
1      1      0.0      1.0  -400.0  0.0
999 999      999      999      999      999  These values are overwritten in
3                                              Subroutines CON and FLUDIC
.6e12
.12e13
.18e13
1
1 2  2      333                                top boundary over written see next section
1
1 41 2      0.0                                right boundary cond. zero flux
1
1 2  2      0.0                                bottom boundary cond. zero flux
1
1 41 2      0.0                                left boundary cond. zero flux
0  0
0  0                                don't print restart, don't read restart file
```

8.2 Subroutines for Conductivity and Moisture Content, Case 1b

The material subroutines for conductivity and moisture content for the Fleming analytical solution used in Case 1b are the same as those used in Case 1a except for the material constants (Table 1). Therefore, they will not be included here.

8.3 Output, Case 1b

Results of Case 1B are given in Figure 4.3.

9 Appendix C—Input and Results, Case 2

9.1 Input, Case 2

The input for the 5 geologic layers are divided into 17 different material regions in the z direction to allow for adequate mesh stretching near region boundaries and material interfaces.

1	17						
1							
2	7	1	9.8				
1	1.2291	0.0	10.0	0.0	10.0		
0.016	3.872	0.041	1.0	0.46	2.7e-7	chnv	
2							
2	31	2	9.8				
1	1.0	0.0	10.0	10.0	117.3		
0.016	3.872	0.041	1.0	0.46	2.7e-7	chnv	
3							
2	9	3	9.8				
1	.86036	0.0	10.0	117.3	130.3		
0.016	3.872	0.041	1.0	0.46	2.7e-7	chnv	
4							
2	16	4	9.8				
1	1.10431	0.0	10.0	130.3	150.8		
.00567	1.798	0.080	1.0	0.11	1.9e-11	tsw2	
5							
2	16	5	9.8				
1	1	0.0	10.0	150.8	202.3		
.00567	1.798	0.080	1.0	0.11	1.9e-11	tsw2	
6							
2	9	6	9.8				
1	0.89033	0.0	10.0	202.3	219.5		
.00567	1.798	0.080	1.0	0.11	1.9e-11	tsw2	
7							
2	10	7	9.8				
1	1	0.0	10.0	219.5	224.0		
.00567	1.798	0.080	1.0	0.11	1.9e-11	tsw2	
8							
2	7	8	9.8				
1	1.34644	0.0	10.0	224.0	240.0		
.00567	1.798	0.080	1.0	0.11	1.9e-11	tsw2	
9							
2	19	9	9.8				
1	1	0.0	10.0	240.0	314.9		
.00567	1.798	0.080	1.0	0.11	1.9e-11	tsw2	
10							
2	8	10	9.8				
1	0.8575	0.0	10.0	314.9	335.4		
.00567	1.798	0.080	1.0	0.11	1.9e-11	tsw2	
11							
2	7	11	9.8				
1	1.55085	0.0	10.0	335.4	348.4		
.00567	1.798	0.080	1.0	0.11	1.9e-11	tsw1	
12							

```

2      26      12      9.8
1      1      0.0      10.0  348.4  452.5
.00567 1.798  0.080  1.0  0.11  1.9e-11  tws1
13
2      8      13      9.8
1      0.80355 0.0      10.0  452.5  465.5
.00567 1.798  0.080  1.0  0.11  1.9e-11  tws1
14
2      11      14      9.8
1      1.30911 0.0      10.0  465.5  484.55
.015  6.872  0.100  1.0  0.40  3.9e-7   ptn
15
2      11      15      9.8
1      0.86324 0.0      10.0  484.55  503.6
.015  6.872  0.100  1.0  0.40  3.9e-7   ptn
16
2      11      16      9.8
1      1.3091 0.0      10.0  503.6  517.0
.00821 1.558  0.002  1.0  0.08  9.7e-12  tcw
17
2      11      17      9.8
1      0.86324 0.0      10.0  517.0  530.4
.00821 1.558  0.002  1.0  0.08  9.7e-12  tcw
12      number of times printed
100
3.1558e8
3.1558e9
7.8890e9
8.678e9
9.467e9
1.1045e10
1.5779e10
2.3668e10
3.1558e10
3.9447e10
4.7336e10
1
1 2 2 -3.1688088e-11 ( infiltration in top boundary m/s)
1
1 201 2 0.0 ( zero flux through right boundary )
1
1 2 1 9.8005 ( fixed pressure, p=rho*g(psi+z)=9805*(0.001 + 0) )
1
1 201 2 0.0 ( zero flux through left boundary )
1 0 ( ip=1, print restart file, ir=0 read restart file )
end data

```

9.2 Subroutines for Conductivity and Saturation, Case 2

Saturation and conductivity functions for this case were described using the Mualem (1976) and van Genuchten (1978) formulation. Subroutines CON and FLUIDC which contain these formulations are given below.

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
      subroutine con(condx,condz,p,x,z,nxmax,nzmax,mxz)
cc
c
c   calculates hydraulic conductivity (m/s)
c   units - kg,m,s.
c
c       implicit real*8 (a-h,o-z)
c       common /mat /alpm(20),betm(20),smr(20),sms(20),anm(20),conm(20)
c       dimension af(20)
c       dimension c(5,202),condx(5,202),condz(5,202),conf(20)
c       dimension p(5,202),x(5),z(202),mxz(5,202)
c   fracture properties
c       data(af(i), i=1,3 ) / 4.6e-5, 4.6e-5, 4.6e-5 /
c       data(af(i), i=4,10 ) / 18.e-5, 18.e-5, 18.e-5, 18.e-5,
1          18.e-5, 18.e-5, 18.e-5 /
c       data(af(i), i=11,13) / 4.1e-5, 4.1e-5, 4.1e-5 /
c       data(af(i), i=14,15) / 2.7e-5, 2.7e-5 /
c       data(af(i), i=16,17) / 14.e-5, 14.e-5 /
c
c       data(conf(i),i=1,3) / 20.e-5, 20.e-5, 20.e-5 /
c       data(conf(i),i=4,10) / 1.7e-5, 1.7e-5, 1.7e-5,
1          1.7e-5, 1.7e-5, 1.7e-5, 1.7e-5 /
c       data(conf(i),i=11,13) / 2.2e-5, 2.2e-5, 2.2e-5 /
c       data(conf(i),i=14,15) / 61.e-5, 61.e-5 /
c       data(conf(i),i=16,17) / 3.8e-5, 3.8e-5 /
c   conductive function statement
c       confu(al,ap)=(1.+ap)**(-al/2.)*(1.-(ap/(1.+ap))**al)**2
c   fracture properties
c       alpf=1.2851
c       betf=4.23
c       rhog=9800.0
c   calculate condx and condz
c       do 20 j=1,nzmax
c       do 10 i=1,nxmax
c       mat=mxz(i,j)
c       phm=p(i,j)/rhog - z(j)
c       if(phm.gt. -.000001) phm=-.000001
c       apm=(alpm(mat)*(-phm))**betm(mat)
c       alm=(1-1./betm(mat))

```

```

      apf=(alf*      (-phm))*betf
      alf=(1-1/betf)
      com=confu(alm,apm)*conm(mat)
      cof=confu(alf,apf)*conf(mat)
      c(i,j) = (1.0-af(mat))*com + af(mat)*cof
10  continue
20  continue
    do 40 j=1,nzmax
    do 30 i=1,nxmax-1
      condx(i,j)=0.5*(c(i,j)+c(i+1,j))
30  continue
40  continue
    do 60 j=1,nzmax-1
    do 50 i=1,nxmax
      condz(i,j)=0.5*(c(i,j)+c(i,j+1))
50  continue
60  continue
    end

```

```

cxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxxx
      subroutine fluidc(cm,th,p,z,mxz,nxmax,nzmax)

```

```

cc
c... This sub calc the moisture content and der of moisture content wrt
c    phm. (units - kg,m,s)
c
c    variables:

```

```

c    betp      water compressibility (beta prime)
c    alpp      rock compressibility (alpha prime)
c    anf       fracture porosity
c    anm,phi   material porosity
c    th        moisture content (fracture and matrix averaged)
c    smr       residual saturation of the matrix
c    sfr       residual saturation of the fracture
c    sm        saturation of matrix
c    sf        saturation of fracture
c    fc        fracture compressibility

```

```

c    implicit real*8 (a-h,o-z)
c    common /mat /alpm(20),betm(20),smr(20),sms(20),anm(20),conm(20)
c    dimension th(5,202),cm(5,202),p(5,202)
c    dimension x(5),z(202),mxz(5,202)
c    dimension anf(20),alpp(20),fc(20)

```

```

c
c    properties
c

```

```

data(anf(i), i=1,3 ) / 4.6e-5, 4.6e-5, 4.6e-5 /
data(anf(i), i=4,10) / 18.e-5, 18.e-5, 18.e-5, 18.e-5,
1      18.e-5, 18.e-5, 18.e-5 /
data(anf(i), i=11,13) / 4.1e-5, 4.1e-5, 4.1e-5 /
data(anf(i), i=14,15) / 2.7e-5, 2.7e-5 /
data(anf(i), i=16,17) / 14.e-5, 14.e-5 /

c
data(alpp(i),i=1,3) / 39.e-7, 39.e-7, 39.e-7 /
data(alpp(i),i=4,10) / 5.8e-7, 5.8e-7, 5.8e-7, 5.8e-7,
1      5.6e-7, 5.8e-7, 5.8e-7 /
data(alpp(i),i=11,13) / 12.e-7, 12.e-7, 12.e-7 /
data(alpp(i),i=14,15) / 82.e-7, 82.e-7 /
data(alpp(i),i=16,17) / 6.2e-7, 6.2e-7 /

c
data(fc(i) ,i=1,3) / 2.8e-8, 2.8e-8, 2.8e-8 /
data(fc(i) ,i=4,10) / 12.e-8, 12.e-8, 12.e-8, 12.e-8,
1      12.e-8, 12.e-8, 12.e-8 /
data(fc(i) ,i=11,13) / 5.6e-8, 5.6e-8, 5.6e-8 /
data(fc(i) ,i=14,15) / 19.e-8, 19.e-8 /
data(fc(i) ,i=16,17) / 132.e-8, 132.e-8 /
data rhog/ 9800./

c
c saturation function statement
c
satfu(sr,ss,al,ap)=(ss-sr)*(1+ap)**(-al) + sr

c
c derivative of saturation function statement
c
chfu(sr,ss,al,ap,bet,a,phm)=(ss-sr)*al*(1+ap)**(-al-1.)
1 *bet*a**bet*(-phm)**(bet-1)

c
c fracture properties
c
sfr=3.950e-2

alpf=1.2851
betf=4.23

c
c matrix properties
c
betp=9.8e-7

c
c evaluate moisture content
c
alf=(1.-1./betf)

c
c loop over nodes

```



```

c
do 100 j=1,nzmax
  do 50 i=1,nxmax
    mat = mxz(i,j)
    alm=(1.0-1.0/betm(mat))
    phm=p(i,j)/rhog - z(j)
    if (phm.gt.-.000001) phm=-.000001
    apm=(alpm(mxz(i,j))*(-phm))*betm(mat)
    apf=(alpf*      (-phm))*betf
    sm=satfu(smr(mat),sms(mat),alm,apm)
    sfs=1.0
    sf=satfu(sfr,sfs ,alf,apf)

c
c   convert saturation to moisture content
c
    th(i,j)=sm*anm(mat)*(1.-anf(mat)) + sf*anf(mat)

c
c   these effects need to be incorporated into the capacitance term
c
    watcomp=betp*th(i,j)
    rokcomp=alpp(mat)*th(i,j)/(anf(mat)+anm(mat))*
2    (sm-anf(mat)*(sm-sf))
    fracomp=fc(mat)*th(i,j)/(anf(mat)+anm(mat))*(sm-sf)

c
c   compute the derivative of saturation wrt psi
c
    chm=chfu(smr(mat),sms(mat),alm,apm,betm(mat),
2    alpm(mat),phm)
    sfs = 1.0
    chf=chfu(sfr ,sfs,alf,apf,betf      ,alpf      ,phm)

c
c   convert to moisture content and sum terms for total capacitance
c
    cm1=chm*anm(mat)*(1.-anf(mat)) + chf*anf(mat)
    cm(i,j)=cm1 + watcomp + rokcomp + fracomp
  50 continue
100 continue

c
  return
end

```

9.3 Output, Case 2

A partial listing of the output for Case 2 follows. To keep the total amount of data presented to a reasonable amount a considerable amount of the data has been edited out. These locations are noted by an 'several lines of data edited out' comment.

subroutine input

number of regions in x and z dir.=1, 17

region number

no. of x and z nodes in region, mat, initial press

stretch in x and z direction, xo, xmzx, zo, zmax

```
1
 2   7   1 0.98000E+01
0.10000E+01 0.12291E+01 0.00000E+00 0.10000E+02 0.00000E+00 0.10000E+02
0.16000E-01 0.38720E+01 0.41000E-01 0.10000E+01 0.46000E+00 0.27000E-06
2
 2  31   2 0.98000E+01
0.10000E+01 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+02 0.11730E+03
0.16000E-01 0.38720E+01 0.41000E-01 0.10000E+01 0.46000E+00 0.27000E-06
337f
 2   9   3 0.98000E+01
0.10000E+01 0.86036E+00 0.00000E+00 0.10000E+02 0.11730E+03 0.13030E+03
0.16000E-01 0.38720E+01 0.41000E-01 0.10000E+01 0.46000E+00 0.27000E-06
4
 2  16   4 0.98000E+01
0.10000E+01 0.11043E+01 0.00000E+00 0.10000E+02 0.13030E+03 0.15080E+03
0.56700E-02 0.17980E+01 0.80000E-01 0.10000E+01 0.11000E+00 0.19000E-10
5
 2  16   5 0.98000E+01
0.10000E+01 0.10000E+01 0.00000E+00 0.10000E+02 0.15080E+03 0.20230E+03
0.56700E-02 0.17980E+01 0.80000E-01 0.10000E+01 0.11000E+00 0.19000E-10
6
 2   9   6 0.98000E+01
0.10000E+01 0.89033E+00 0.00000E+00 0.10000E+02 0.20230E+03 0.21950E+03
0.56700E-02 0.17980E+01 0.80000E-01 0.10000E+01 0.11000E+00 0.19000E-10
```

‘several lines of data edited out’

ptop=0. qtop=-3.1688088E-11

pright=0. qright=0.

pbot=9.8005 qbot=0.

pleft=0. qleft=0.

subroutine geom

```

xmax(nrt)=, zmax(nrt=10., 530.4
nxmax=, xznax=,2, 201
x coordinates
  0.0000E+00  0.1000E+02
z coordinates
  0.0000E+00  0.9360E+00  0.2086E+01  0.3500E+01  0.5238E+01  0.7375E+01
  0.1000E+02  0.1358E+02  0.1715E+02  0.2073E+02  0.2431E+02  0.2788E+02
  0.3146E+02  0.3504E+02  0.3861E+02  0.4219E+02  0.4577E+02  0.4934E+02
  0.5292E+02  0.5650E+02  0.6007E+02  0.6365E+02  0.6723E+02  0.7080E+02
  0.7438E+02  0.7796E+02  0.8153E+02  0.8511E+02  0.8869E+02  0.9226E+02
  0.9584E+02  0.9942E+02  0.1030E+03  0.1066E+03  0.1101E+03  0.1137E+03
  0.1173E+03  0.1199E+03  0.1221E+03  0.1240E+03  0.1257E+03  0.1271E+03
  0.1283E+03  0.1294E+03  0.1303E+03  0.1309E+03  0.1316E+03  0.1324E+03
  0.1332E+03  0.1341E+03  0.1352E+03  0.1363E+03  0.1375E+03  0.1389E+03
  0.1404E+03  0.1421E+03  0.1440E+03  0.1460E+03  0.1483E+03  0.1508E+03
  0.1542E+03  0.1577E+03  0.1611E+03  0.1645E+03  0.1680E+03  0.1714E+03
  0.1748E+03  0.1783E+03  0.1817E+03  0.1851E+03  0.1886E+03  0.1920E+03
  0.1954E+03  0.1989E+03  0.2023E+03  0.2054E+03  0.2082E+03  0.2107E+03
  0.2129E+03  0.2148E+03  0.2166E+03  0.2181E+03  0.2195E+03  0.2200E+03
  0.2205E+03  0.2210E+03  0.2215E+03  0.2220E+03  0.2225E+03  0.2230E+03
  0.2235E+03  0.2240E+03  0.2251E+03  0.2266E+03  0.2286E+03  0.2314E+03
  0.2351E+03  0.2400E+03  0.2442E+03  0.2483E+03  0.2525E+03  0.2566E+03
  0.2608E+03  0.2650E+03  0.2691E+03  0.2733E+03  0.2774E+03  0.2816E+03
  0.2858E+03  0.2899E+03  0.2941E+03  0.2983E+03  0.3024E+03  0.3066E+03
  0.3107E+03  0.3149E+03  0.3193E+03  0.3231E+03  0.3264E+03  0.3292E+03
  0.3316E+03  0.3336E+03  0.3354E+03  0.3360E+03  0.3368E+03  0.3381E+03
  0.3402E+03  0.3434E+03  0.3484E+03  0.3526E+03  0.3567E+03  0.3609E+03
  0.3651E+03  0.3692E+03  0.3734E+03  0.3775E+03  0.3817E+03  0.3859E+03
  0.3900E+03  0.3942E+03  0.3984E+03  0.4025E+03  0.4067E+03  0.4109E+03
  0.4150E+03  0.4192E+03  0.4234E+03  0.4275E+03  0.4317E+03  0.4358E+03
  0.4400E+03  0.4442E+03  0.4483E+03  0.4525E+03  0.4558E+03  0.4584E+03
  0.4605E+03  0.4622E+03  0.4635E+03  0.4646E+03  0.4655E+03  0.4659E+03
  0.4665E+03  0.4672E+03  0.4682E+03  0.4694E+03  0.4711E+03  0.4732E+03
  0.4760E+03  0.4797E+03  0.4845E+03  0.4879E+03  0.4909E+03  0.4934E+03
  0.4955E+03  0.4974E+03  0.4990E+03  0.5004E+03  0.5017E+03  0.5027E+03
  0.5036E+03  0.5039E+03  0.5043E+03  0.5048E+03  0.5055E+03  0.5064E+03
  0.5075E+03  0.5090E+03  0.5110E+03  0.5136E+03  0.5170E+03  0.5194E+03
  0.5214E+03  0.5232E+03  0.5247E+03  0.5261E+03  0.5272E+03  0.5282E+03
  0.5290E+03  0.5298E+03  0.5304E+03
material
  17  17
  17  17
  17  17
  17  17
  17  17
  17  17
  17  17

```

17 17
17 17
17 17
17 17
16 16
16 16

‘several lines of data edited out’

output solution   time
                    3   0.316E+10

time=3155800000.
converged solution

xxxxxx pressure field xxxxxx

	0.0000E+00	1.0000E+01
5.304E+02	5.1859E+06	5.1859E+06
5.298E+02	5.1797E+06	5.1797E+06
5.290E+02	5.1725E+06	5.1725E+06
5.282E+02	5.1642E+06	5.1642E+06
5.272E+02	5.1545E+06	5.1545E+06
5.261E+02	5.1434E+06	5.1434E+06
5.247E+02	5.1303E+06	5.1303E+06
5.232E+02	5.1155E+06	5.1155E+06
5.214E+02	5.0977E+06	5.0977E+06
5.194E+02	5.0782E+06	5.0782E+06
5.170E+02	5.0539E+06	5.0539E+06
5.136E+02	5.0218E+06	5.0218E+06
5.110E+02	4.9941E+06	4.9941E+06
5.090E+02	4.9369E+06	4.9369E+06
5.075E+02	4.8570E+06	4.8570E+06
5.064E+02	4.7797E+06	4.7797E+06
5.055E+02	4.7072E+06	4.7072E+06
5.048E+02	4.6409E+06	4.6409E+06
5.043E+02	4.5817E+06	4.5817E+06
5.039E+02	4.5299E+06	4.5299E+06
5.036E+02	4.4855E+06	4.4855E+06
5.027E+02	4.4855E+06	4.4855E+06
5.017E+02	4.4855E+06	4.4855E+06
5.004E+02	4.4855E+06	4.4855E+06
4.990E+02	4.4855E+06	4.4855E+06

4.974E+02 4.4855E+06 4.4855E+06
4.955E+02 4.4855E+06 4.4855E+06
4.934E+02 4.4855E+06 4.4855E+06
4.909E+02 4.4855E+06 4.4855E+06
4.879E+02 4.4855E+06 4.4855E+06

‘several lines of data edited out’

xxxxxx qz flux xxxxxx

0.0000E+00 1.0000E+01

5.304E+02 0.0000E+00 0.0000E+00
5.298E+02 -3.1688E-11 -3.1688E-11
5.290E+02 -3.1688E-11 -3.1688E-11
5.282E+02 -3.1688E-11 -3.1688E-11
5.272E+02 -3.1688E-11 -3.1688E-11
5.261E+02 -3.1688E-11 -3.1688E-11
5.247E+02 -3.1688E-11 -3.1688E-11
5.232E+02 -3.1688E-11 -3.1688E-11
5.214E+02 -3.1688E-11 -3.1688E-11
5.194E+02 -3.1688E-11 -3.1688E-11
5.170E+02 -3.1688E-11 -3.1688E-11
5.136E+02 -3.1688E-11 -3.1688E-11
5.110E+02 -3.1688E-11 -3.1688E-11
5.090E+02 -3.1686E-11 -3.1686E-11
5.075E+02 -3.1666E-11 -3.1666E-11
5.064E+02 -3.1635E-11 -3.1635E-11
5.055E+02 -3.1598E-11 -3.1598E-11
5.048E+02 -3.1557E-11 -3.1557E-11
5.043E+02 -3.1517E-11 -3.1517E-11
5.039E+02 -3.1479E-11 -3.1479E-11
5.036E+02 -3.1445E-11 -3.1445E-11
5.027E+02 -3.1378E-11 -3.1378E-11
5.017E+02 -2.9523E-11 -2.9523E-11
5.004E+02 -2.7617E-11 -2.7617E-11
4.990E+02 -2.5708E-11 -2.5708E-11
4.974E+02 -2.3856E-11 -2.3856E-11
4.955E+02 -2.2130E-11 -2.2130E-11
4.934E+02 -2.0600E-11 -2.0600E-11
4.909E+02 -1.9329E-11 -1.9329E-11
4.879E+02 -1.8356E-11 -1.8356E-11
4.845E+02 -1.7688E-11 -1.7688E-11
4.797E+02 -1.7240E-11 -1.7240E-11
4.760E+02 -1.7078E-11 -1.7078E-11

4.732E+02 -1.7022E-11 -1.7022E-11
 4.711E+02 -1.6997E-11 -1.6997E-11
 4.694E+02 -1.6983E-11 -1.6983E-11
 4.682E+02 -1.6973E-11 -1.6973E-11
 4.672E+02 -1.6966E-11 -1.6966E-11
 4.665E+02 -1.6960E-11 -1.6960E-11
 4.659E+02 -1.6956E-11 -1.6956E-11
 4.655E+02 -1.6953E-11 -1.6953E-11

‘several lines of data edited out’

xxxxx moisture xxxxx

	0.0000E+00	1.0000E+01
5.304E+02	8.0000E-02	8.0000E-02
5.298E+02	8.0000E-02	8.0000E-02
5.290E+02	8.0000E-02	8.0000E-02
5.282E+02	8.0000E-02	8.0000E-02
5.272E+02	8.0000E-02	8.0000E-02
5.261E+02	8.0001E-02	8.0001E-02
5.247E+02	7.9999E-02	7.9999E-02
5.232E+02	8.0001E-02	8.0001E-02
5.214E+02	7.9997E-02	7.9997E-02
5.194E+02	8.0003E-02	8.0003E-02
5.170E+02	7.9994E-02	7.9994E-02
5.136E+02	8.0005E-02	8.0005E-02
5.110E+02	7.9986E-02	7.9986E-02
5.090E+02	7.9781E-02	7.9781E-02
5.075E+02	7.9244E-02	7.9244E-02
5.064E+02	7.8513E-02	7.8513E-02
5.055E+02	7.7679E-02	7.7679E-02
5.048E+02	7.6818E-02	7.6818E-02
5.043E+02	7.5984E-02	7.5984E-02
5.039E+02	7.5217E-02	7.5217E-02
5.036E+02	7.4538E-02	7.4538E-02
5.027E+02	3.8056E-01	3.8056E-01
5.017E+02	3.8330E-01	3.8330E-01
5.004E+02	3.8609E-01	3.8609E-01
4.990E+02	3.8884E-01	3.8884E-01
4.974E+02	3.9145E-01	3.9145E-01
4.955E+02	3.9382E-01	3.9382E-01
4.934E+02	3.9586E-01	3.9586E-01
4.909E+02	3.9748E-01	3.9748E-01
4.879E+02	3.9865E-01	3.9865E-01
4.845E+02	3.9940E-01	3.9940E-01
4.797E+02	3.9984E-01	3.9984E-01

4.760E+02	3.9995E-01	3.9995E-01
4.732E+02	3.9998E-01	3.9998E-01
4.711E+02	3.9999E-01	3.9999E-01
4.694E+02	3.9999E-01	3.9999E-01
4.682E+02	3.9999E-01	3.9999E-01
4.672E+02	3.9999E-01	3.9999E-01
4.665E+02	3.9999E-01	3.9999E-01
4.659E+02	3.9999E-01	3.9999E-01
4.655E+02	3.9999E-01	3.9999E-01
4.646E+02	1.0986E-01	1.0986E-01
4.635E+02	1.0986E-01	1.0986E-01
4.622E+02	1.0986E-01	1.0986E-01

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.   xxxxx condx field xxxxx

0.0000E+00

5.304E+02	3.1680E-11
5.298E+02	3.1718E-11
5.290E+02	3.1597E-11
5.282E+02	3.1920E-11
5.272E+02	3.1175E-11
5.261E+02	3.2694E-11
5.247E+02	2.9889E-11
5.232E+02	3.4632E-11
5.214E+02	2.7143E-11
5.194E+02	3.8252E-11
5.170E+02	2.2498E-11
5.136E+02	4.3277E-11
5.110E+02	1.4845E-11
5.090E+02	6.6252E-12
5.075E+02	5.1353E-12
5.064E+02	4.1306E-12
5.055E+02	3.4098E-12
5.048E+02	2.8809E-12
5.043E+02	2.4888E-12
5.039E+02	2.1963E-12
5.036E+02	1.9772E-12
5.027E+02	3.1132E-07
5.017E+02	3.2051E-07
5.004E+02	3.3022E-07
4.990E+02	3.4021E-07
4.974E+02	3.5019E-07
4.955E+02	3.5976E-07

4.934E+02	3.6850E-07
4.909E+02	3.7597E-07
4.879E+02	3.8184E-07
4.845E+02	3.8595E-07
4.797E+02	3.8874E-07
4.760E+02	3.8957E-07
4.732E+02	3.8983E-07

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.   xxxxx condz field xxxxx

	0.0000E+00	1.0000E+01
5.298E+02	3.1699E-11	3.1699E-11
5.290E+02	3.1658E-11	3.1658E-11
5.282E+02	3.1758E-11	3.1758E-11
5.272E+02	3.1547E-11	3.1547E-11
5.261E+02	3.1934E-11	3.1934E-11
5.247E+02	3.1292E-11	3.1292E-11
5.232E+02	3.2261E-11	3.2261E-11
5.214E+02	3.0888E-11	3.0888E-11
5.194E+02	3.2698E-11	3.2698E-11
5.170E+02	3.0375E-11	3.0375E-11
5.136E+02	3.2887E-11	3.2887E-11
5.110E+02	2.9061E-11	2.9061E-11
5.090E+02	1.0735E-11	1.0735E-11
5.075E+02	5.8803E-12	5.8803E-12

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.   xxxxx cap field xxxxx

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5.298E+02	9.3667E-05	9.3667E-05
5.290E+02	9.3556E-05	9.3556E-05
5.282E+02	9.3853E-05	9.3853E-05
5.272E+02	9.3163E-05	9.3163E-05
5.261E+02	9.4554E-05	9.4554E-05
5.247E+02	9.1938E-05	9.1938E-05
5.232E+02	9.6247E-05	9.6247E-05
5.214E+02	8.9149E-05	8.9149E-05

5.194E+02	9.9195E-05	9.9195E-05
5.170E+02	8.3764E-05	8.3764E-05
5.136E+02	1.0291E-04	1.0291E-04
5.110E+02	7.1729E-05	7.1729E-05
5.090E+02	6.4896E-05	6.4896E-05
5.075E+02	9.8327E-05	9.8327E-05
5.064E+02	1.2140E-04	1.2140E-04
5.055E+02	1.3750E-04	1.3750E-04
5.048E+02	1.4855E-04	1.4855E-04
5.043E+02	1.5596E-04	1.5596E-04
5.039E+02	1.6080E-04	1.6080E-04
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5.027E+02	2.8028E-03	2.8028E-03
5.017E+02	2.4862E-03	2.4862E-03
5.004E+02	2.1494E-03	2.1494E-03
4.990E+02	1.7998E-03	1.7998E-03
4.974E+02	1.4480E-03	1.4480E-03
4.955E+02	1.1077E-03	1.1077E-03
4.934E+02	7.9472E-04	7.9472E-04
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4.760E+02	2.4975E-05	2.4975E-05
4.732E+02	1.4864E-05	1.4864E-05
4.711E+02	1.1312E-05	1.1312E-05
4.694E+02	9.9503E-06	9.9503E-06
4.682E+02	9.3803E-06	9.3803E-06
4.672E+02	9.1206E-06	9.1206E-06
4.665E+02	8.9925E-06	8.9925E-06
4.659E+02	8.9247E-06	8.9247E-06

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10 Appendix D—RIB and SEPDB Databases

Information from the Reference Information Base
Used in this Report

This report contains no information from the Reference Information Base.

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for the
Reference Information Base

This report contains no candidate information for the Reference Information Base.

Candidate Information
for the
Site and Engineering Properties Data Base

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