TOUGH
Training Courses

Problem 2DVZ:
Infiltration Test in the
Vadose Zone

Earth Sciences Division
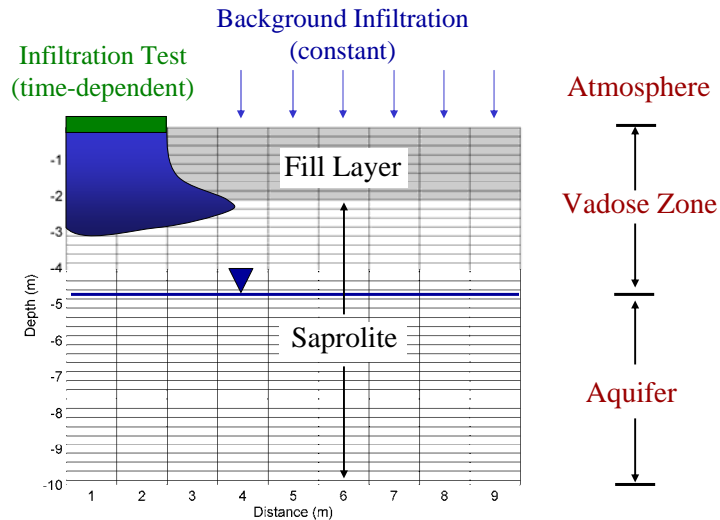Lawrence Berkeley National Laboratory
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Outline Problem 2DVZ

- Problem Description
- Part A: Mesh Generation
- Part B: Material Properties
- Part C: Boundary Conditions
- Part D: Background Infiltration
- Part E: Initial Conditions
- Part F: Steady-State Infiltration
- Part G: Infiltration Test
- Problem Variations (EOS3)

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Problem Description

Infiltration Test (time-dependent)

Background Infiltration (constant)

Atmosphere

Fill Layer

Vadose Zone

Saprolite

Aquifer

Depth (m)

Distance (m)

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Goals of Sample Problem

- Model the flow of water in the vadose zone (using EOS9)
- Create a 2-D mesh using MESHMAKER (ELEME and CONNE blocks)
- Assign rock properties in ELEME block to specify geological layers
- Assign boundary conditions (modifying ELEME block by hand and using free software available for TOUGH2)
- Add constant background infiltration (using GENER block)
- Get steady-state initial conditions (obtaining INCON block)
- Simulate infiltration test (using INCON and GENER blocks)
- Become familiarized with time-stepping and output parameters (PARAM block)
- Consider problem variations including extension to nonisothermal flow (using EOS3)

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Part A: Mesh Generation

Part A involves generating the MESH file that contains the ELEME and CONNE blocks. The MESHMaker block is used for this purpose.

A.1 MESHMaker block (p. 160, 177-183 in manual)

➢ Open *PartA.txt*. Note that the first line is reserved for the title. See Figure 1. Textpad, WordPad and Notepad can be used for editing the text files. Caution: do not insert "tabs" into the files.

➢ First generate a 1-D Cartesian mesh in the Z-direction. Enter "XYZ" for the variable WORD (p. 160), and consult manual (p. 180). Specify a total of 42 elements, with a grid spacing of 1.0E-3, 0.25, 0.25, …., 0.25, 1.0E-3 m.

➢ (Hint: fill in values for the blank spaces marked by "?")

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```
Input file for Part A of sample problem 2DVZ
MESHMAKER ----*----2----*----3----*----4----*----5----*----6----*----7----*----8
???                     Select XYZ for cartesian grid


NX     1 1.0000         Select dX and dY to yield cross section of column
NY     1 1.0000
NZ     1 ?              Add (dummy) top boundary element
NZ    ?? 0.2500         Create uniform grid for 10 m long column
NZ     ? 1.0E-3         Add (dummy) bottom boundary element
                        Needs one empty line to terminate XYZ block
                        Needs another empty line to terminate MESHMAKER
ENDFI
```

Figure 1. MESHM block for *PartA.txt* of Sample problem 2DVZ.

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A.2 Run TOUGH2 with *PartA.txt* as input file

➤ Open a DOS command prompt window:

START→Programs→Accessories→Command Prompt

(or double-click on *cmd.exe* in C:\TOUGH2)

➤ Change directory to location of input files, for example:

cd C:\TOUGH2\...\PartA

(or copy input files into directory C:\TOUGH2 and run code there)

➤ Run TOUGH2 with EOS9 by typing:

t2_eos9 < *PartA.txt* > *PartA.out*

➤ Open the following output files:

PartA.out, MESH

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SIDE NOTE (Block `ELEME`)

- Element name (format: `AAAII`, e.g., `ELE99`)
- Material type (5 character name or number of order in `ROCKS` block)
- Volume [m³]
- Optional:
    - Interface area to heat-conducting, confining layer
    - X-, Y- and Z-coordinates

```
E L EME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
EL NE NSEQ NADD MAT MA2   VOLX      AHTX       PMX        X         Y         Z
```

```
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1         SOIL  0.100E-09 0.100E+01         0.500E+00 0.500E+00 -.500E-10
A21 1         FRACT 0.500E-01                   0.500E+00 0.500E+00 -.250E-01
A31 1             7 0.500E-01                   0.500E+00 0.500E+00 -.750E-01
.....
Name        Material   Volume    AHTX   (Perm Mod.)  X         Y         Z
```

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SIDE NOTE (Block `CONNE`)

- A connection connects two elements
- Each element can have multiple connections
- Names of two elements (`AAAII AAAII`)
- Anisotropy index
- Nodal distances to common interface [m]
- Interface area [m²]
- Cosine of angle between gravity and connection line

```
CONNE---------1------*------2------*------3------*------4------*------5------*------6------*------7------*------8
EL1 NE1 EL2 NE2 NSEQ  NAD1  NAD2   ISOT     D1            D2           AREAX         BETAX         SIGX
```

```
CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A11 1A21 1                   3 0.500E-10 0.250E-01 0.100E+01 0.100E+01
A21 1A31 1                   3 0.250E-01 0.250E-01 0.100E+01 0.100E+01
A31 1A41 1                   3 0.250E-01 0.250E-01 0.100E+01 0.100E+01
...
Element 1 and 2              ISOT    D1        D2        AREAX        BETAX
```

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Q-A.1.1: Open *PartA.out* and scroll down to "PARAMETERS FOR FLEXIBLE DIMENSIONING". Are the maximum number of elements (`MNEL`) and maximum number of connections (`MNCON`) sufficiently large?

Q-A.1.2: Scroll down. Do the grid increments appear as you expected?

Q-A.1.3: Open MESH file. What are the minimum and maximum Z values?

Q-A.1.4: What are the nodal distances for the first connection (between elements "A11 1" and "A21 1")? Why are they different?

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➢ Now modify the `MESHMaker` block to create 10 grid blocks in the X-direction with 1.0 m spacing (in addition to the 42 elements already being created in the Z-direction. Make sure the alignment in the input file is correct.

Q-A.1.5: Open the `MESH` file and examine the naming sequence of the elements in the new 2-D mesh. Note that the elements have a certain naming convention with sequentially increasing letters and numbers. In this case, which elements correspond to the first column in the model (i.e., with X-coordinates equal to minimum value, and Z-coordinates spanning over total range)?

➢ Rename the output file `MESH` as *MESH_PartA* to be used later.

SIDE NOTE (Block `ROCKS`)

- Material name (5 characters, case sensitive)
- Hydrological properties
  - Porosity
  - Absolute permeability [m^2] in three (arbitrary) directions
  - Parameters of relative permeability and capillary pressure functions (overwrite defaults given in block `RPCAP`)
- Thermal properties
  - Rock grain density [kg/m^3]
  - Formation heat conductivity (wet) [W/m°C]
  - Rock grain specific heat [J/kg ° C]

```
Name    NAD    DROK      PORO    PER(1)     PER(2)     PER(3)     CWET    SPHT
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND     0     2650.     .4000 1.000E-12 1.000E-12 1.000E-13    2.51     920.
GRAVE    0     2650.     .3000 1.000E-11 1.000E-11 1.000E-11    2.51     920.
BOUND    2     2650.     .9900 1.000E-12 1.000E-12 1.000E-12    2.51  100000.
            (additional parameters on this line, see Manual p. 161)
    3              0.3       0.1
    1              0.0       0.0       1.0
```

SIDE NOTE (Additional Properties)

- Additional, EOS-specific fluid properties and other parameters are given in blocks `SELEC` and `DIFFU` (see Manual)

- For EOS9 (Richards equation):
  - Special "domain" **REFCO** contains **reference water properties**.
  - If omitted, default values are assumed.

```
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND          2650.     .4000 1.000E-12 1.000E-12 1.000E-13      2.51      920.
REFCO      1.013E05      15.0   999.213 1.135E-03 4.594E-10

              Press.     Temp.   Density Viscosity Compressibility
```

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Part B: Material Properties

In Part B of this problem we specify 4 material properties in the model domain. Materials are created in the ROCKS block, and then assigned to the desired elements in the ELEME block.

B.1 ROCKS block

➤ Open *PartB.txt*. Note two materials called SAPRO and ATMOS.

Q-B.1.1: What are the porosity and permeability values of these materials? Is the permeability of SAPRO isotropic or anisotropic? What is the reason for material ATMOS?

➤ Create a third material called FILLI with a porosity of 0.3 and isotropic permeability of 5.0E-12. Use the same RELP and PCAP data as for SAPRO (see Figure 2).

➤ Create a fourth material called BOUND with all properties (all 4 lines) the same as material SAPRO (see Figure 2). Leave a blank line after to close the block!

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```
Input file for Part B of sample problem 2DVZ
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAPRO    2    2500.0      .2000 1.000E-12 1.000E-12 1.000E-12      2.0    1000.

   7             0.30      0.20      1.0      0.05
   7             0.30      0.19    1.0e-3     5000.      1.00
ATMOS    2    2500.0       0.99 1.000E-12 1.000E-12 1.000E-12      2.0    1000.

   7             0.30      0.20      1.0      0.05
   8
FILLI    2    2500.0      .3000 5.000E-12 5.000E-12 5.000E-12      2.0    1000.

   7             0.30      0.20      1.0      0.05
   7             0.30      0.19    1.0e-3     5000.      1.00
BOUND    2    2500.0      .2000 1.000E-12 1.000E-12 1.000E-12      2.0    1000.

   7             0.30      0.20      1.0      0.05
   7             0.30      0.19    1.0e-3     5000.      1.00
(blank line)
```

Figure 2. ROCKS block in *PartB.txt* of Sample problem 2DVZ.
SAPRO and ATMOS represent saprolite and the atmosphere, while
FILLI is a 2 m-thick layer of fill material and BOUND is the lower
boundary of the model.

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SIDE NOTE (Free software available for TOUGH2)

TOUGH+ > Licensing & Download > Free Software

TOUGH+

Licensing & Download

TOUGH+ Home
News, Updates & Events
About TOUGH+
Documentation
Licensing & Download
Training & User Support
FAQ
Additional Resources
Contacts

Module	Version	Description	Manual	Source
		Free Software (no support)		
EXT	1.0	Extracts data from TOUGH2 output file for visualization with TECPLOT	Instructions	Ex
AMESH	1.0	Generates irregular TOUGH+ mesh	AMESH User's Guide	AME
T2CHK	1.0	Calculates equilibrium saturations and data for plotting characteristic curves.	Instructions	
MoveMesh	1.0	Moves coordinates of TOUGH2 mesh.	See source code	Move
StratMesh	1.0	Mesh generator for 3D grids with multiple hydrostratigraphic units of variable thickness.	See source code and sample input file	Strat StratM
AddBound	1.0	Deletes elements on a specified domain or replaces them with a single boundary element.	See source code	AddB
Perm2Mesh	1.0	Reads coordinates and log(permeability modifier) from a file and assigns them to TOUGH2 elements.	See source code	Perm
AssignRock	1.0	Assigns rock type name to all elements within a specified box.	See source code	AssignRock.f AssignRock.exe
DelMatrix	1.0	Deletes all elements with a permeability smaller than a cut-off value.	See source code	DelMatrix.f —
CutCavity	1.0	Cuts cavities of various shapes into 2D and 3D models.	See source code	CutCylinder.f CutRect.f CutEllipsoid.f —
EOS9EOS3	1.0	Converts EOS9-SAVE file to EOS3-INCON file.	See source code	EOS9EOS3.f Eos9Eos3.exe
DeleteElements	1.0	Deletes elements and connections in specified domain.	See source code	DeleteElements.f DeleteElements.exe

• *AssignRock* is a program that allows you to assign a rock type to all elements that fall within a user-specified coordinate range.
• Easier than modifying ELEME block by hand!
• Some people use their own scripts (e.g., in Matlab)

• http://www.esd.lbl.gov/TOUGHPLUS/software-free.html

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B.2 `ELEME` and `CONNE` blocks

- ➤ *AssignRock.exe* is run by typing, "AssignRock", and then follow the prompt to enter: input mesh file name, output file name, X_{min}, X_{max}, Y_{min}, Y_{max}, Z_{min}, Z_{max}.

- ➤ Add three layers by running *AssignRock.exe* three times   (first use input mesh file *MESH_PartA* with output file name *MESH_PartB1*, then use input mesh file *MESH_PartB1* with output file name *MESH_PartB2*, etc.)

  FILLI layer: $[Z_{min}, Z_{max}] = [-2, 0]$

  SAPRO layer: $[Z_{min}, Z_{max}] = [-9.95, -2]$

  BOUND layer: $[Z_{min}, Z_{max}] = [-10.01, -9.95]$

  For each use $[X_{min}, X_{max}] = [0, 10.1]$, and $[Y_{min}, Y_{max}] = [0, 1]$

- ➤ Check the final output file (e.g., *MESH_PartB3*) to ensure that the distribution of materials is correct (see Figure 3).

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```
ELEME
A11 1          FILLI0.1000E-020.1000E+01          0.5000E+000.5000E+00-.5000E-03
A21 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1260E+00
A31 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.3760E+00
A41 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.6260E+00
A51 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.8760E+00
A61 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1126E+01
A71 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1376E+01
A81 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1626E+01
A91 1          FILLI0.2500E+00                    0.5000E+000.5000E+00-.1876E+01
AA1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.2126E+01
AB1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.2376E+01
AC1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.2626E+01
AD1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.2876E+01
AE1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.3126E+01
AF1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.3376E+01
AG1 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.3626E+01
…
B51 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.9626E+01
B61 1          SAPRO0.2500E+00                    0.5000E+000.5000E+00-.9876E+01
B71 1          BOUND0.1000E-020.1000E+01          0.5000E+000.5000E+00-.1000E+02
A11 2          FILLI0.1000E-020.1000E+01          0.1500E+010.5000E+00-.5000E-03
A21 2          FILLI0.2500E+00                    0.1500E+010.5000E+00-.1260E+00
…
B7110          BOUND0.1000E-020.1000E+01          0.9500E+010.5000E+00-.1000E+02
```

Figure 3. Preliminary `ELEME` block in *PartB.txt* of Sample problem 2DVZ. Atmosphere has not been added yet.

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SIDE NOTE (Free software available for TOUGH2)

- *AddBound* allows you to replace a row or column of elements with a single element.
- Useful for connecting top of model to atmosphere or distributed source.

• http://www-esd.lbl.gov/TOUGHPLUS/software-free.html

➢ Use *AddBound.exe* to create an atmospheric layer and connect it to the top of the fill layer. Run the program by typing "AddBound", and then following the prompt to enter:

- Input mesh file: *MESH_PartB3*
- Output mesh file: *MESH_PartB4*
- Boundary element name: 99999
- Boundary rock type: ATMOS
- Boundary element volume: 9 x 1 m x 0.25 m = 2.25 m^3
- Nodal distance to boundary element: 1.0E-3
- Domain shape: cube (=1)
- [X_{min} ,X_{max}] = [0, 10.1]
- [Y_{min} ,Y_{max}] = [0, 1]
- [Z_{min} ,Z_{max}] = [-0.1, 0]

```
ELEME
A21 1          FILLI0.2500E+00                0.5000E+000.5000E+00-.1260E+00
A31 1          FILLI0.2500E+00                0.5000E+000.5000E+00-.3760E+00
A41 1          FILLI0.2500E+00                0.5000E+000.5000E+00-.6260E+00
A51 1          FILLI0.2500E+00                0.5000E+000.5000E+00-.8760E+00
A61 1          FILLI0.2500E+00                0.5000E+000.5000E+00-.1126E+01
A71 1          FILLI0.2500E+00                0.5000E+000.5000E+00-.1376E+01
A81 1          FILLI0.2500E+00                0.5000E+000.5000E+00-.1626E+01
A91 1          FILLI0.2500E+00                0.5000E+000.5000E+00-.1876E+01
AA1 1          SAPRO0.2500E+00                0.5000E+000.5000E+00-.2126E+01
AB1 1          SAPRO0.2500E+00                0.5000E+000.5000E+00-.2376E+01
AC1 1
AD1 1
AE1 1
AF1 1
AG1 1
…
B51 1          SAPRO0.2500E+00                0.5000E+000.5000E+00-.9626E+01
B61 1          SAPRO0.2500E+00                0.5000E+000.5000E+00-.9876E+01
B71 1          BOUND0.1000E-020.1000E+01      0.5000E+000.5000E+00-.1000E+02
A21 2          FILLI0.2500E+00                0.1500E+010.5000E+00-.1260E+00
…
B7110          BOUND0.1000E-020.1000E+01      0.9500E+010.5000E+00-.1000E+02
99999          ATMOS0.2250E+01                0.5425E+010.5000E+00-.5000E-01
```

Top row of elements ("A11 1", "A11 2", …, "A11 10") has been removed and replaced with a single element "99999" (see CONNE block in Fig. 4).

Figure 4. Final ELEME block in *PartB.txt* of Sample problem 2DVZ. The Atmosphere has been added.

Element "99999" is connected to "A21 1", "A21 2", …, "A21 10"

```
CONNE
99999A21 1                    30.1000E-020.1250E+000.1000E+010.1000E+01
A21 1A21 2                    10.5000E+000.5000E+000.2500E+000.0000E+00
…
B71 1B71 2                    10.5000E+000.5000E+000.1000E-020.0000E+00
99999A21 2                    30.1000E-020.1250E+000.1000E+010.1000E+01
A21 2A21 3                    10.5000E+000.5000E+000.2500E+000.0000E+00
…
B71 2B71 3                    10.5000E+000.5000E+000.1000E-020.0000E+00
99999A21 3                    30.1000E-020.1250E+000.1000E+010.1000E+01
A21 3A21 4                    10.5000E+000.5000E+000.2500E+000.0000E+00
…
…
B71 9B7110                    10.5000E+000.5000E+000.1000E-020.0000E+00
99999A2110                    30.1000E-020.1250E+000.1000E+010.1000E+01
A2110A3110                    30.1250E+000.1250E+000.1000E+010.1000E+01
```

Figure 5. Final CONNE block in *PartB.txt* of Sample problem 2DVZ. The Atmosphere has been added.

➢ Now we have a mesh to insert into the TOUGH2 input file. So copy contents of *MESH_PartB4* and paste into *PartB.txt* after the `INCON` block, leaving a blank line in between (Figure 6). Remove the lines of text following the "+++" at the end of the `CONNE` block that you just inserted.

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   20001    10010000010000010040000400004000
      0.0           1.000E-00                        9.81000
   1.0E-04
                0.9
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

INDOM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

ELEME
A21 1          FILLI0.2500E+00                  0.5000E+000.5000E+00-.1260E+00
A31 1          FILLI0.2500E+00                  0.5000E+000.5000E+00-.3760E+00
…
B6110          SAPRO0.2500E+00                  0.9500E010.5000E+00-.9876E+01
B7110          BOUND0.1000E-020.1000E+01        0.9500E010.5000E+00-.1000E+02
99999          ATMOS0.2250E+01                  0.5050E010.5000E+00-.5000E-01

CONNE
99999A21 1              30.1000E-020.1250E+000.1000E+010.1000E+01
A21 1A21 2              10.5000E+000.5000E+000.2500E+000.0000E+00
…
B71 1B71 2              10.5000E+000.5000E+000.1000E-020.0000E+00
99999A21 2              30.1000E-020.1250E+000.1000E+010.1000E+01
…

ENDCY
```

Figure 6. Portion of input file for *PartB.txt* after contents of `MESH` file have been added (`ELEME` and `CONNE` blocks).

Part C: Boundary Conditions

The boundary conditions (BCs) can be specified in several ways by modifying the ELEME block (and by using the GENER block).

  ➢Copy *PartB.txt* and paste/rename it *PartC.txt*. Modify this file accordingly in the following steps.
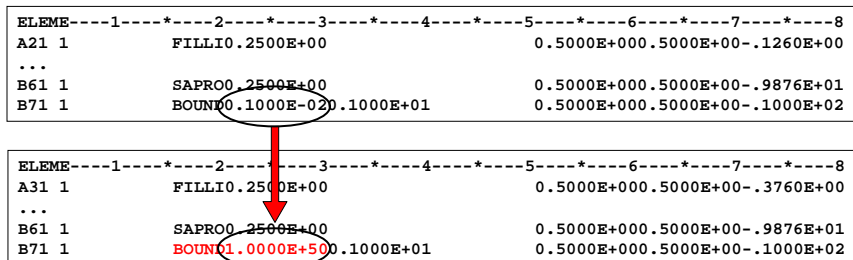
C.1 Vertical Boundaries

  ➢For the vertical (side) boundaries of the model, we wish to have zero-flux BCs (Dirichlet), which is the default condition for boundary elements in TOUGH2, so nothing more needs to be done for these boundaries.

C.2 Bottom Boundary

  ➢Specify a constant pressure (Neumann) BC at the bottom of the model by setting the element volumes to very large values (1E50); the corresponding primary variables will remain constant.

  ➢Find all elements at the bottom of the model (material BOUND) and replace their volumes by 1.0E50.

```
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A21 1         FILLI0.2500E+00                  0.5000E+000.5000E+00-.1260E+00
...
B61 1         SAPRO0.2500E+00                  0.5000E+000.5000E+00-.9876E+01
B71 1         BOUND0.1000E-020.1000E+01        0.5000E+000.5000E+00-.1000E+02
```

```
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A31 1         FILLI0.2500E+00                  0.5000E+000.5000E+00-.3760E+00
...
B61 1         SAPRO0.2500E+00                  0.5000E+000.5000E+00-.9876E+01
B71 1         BOUND1.0000E+500.1000E+01        0.5000E+000.5000E+00-.1000E+02
```

  ➢ Text editor trick: go to the "edit" menu, choose "replace". Paste BOUND0.1000E-02 into the "find" field, and type BOUND1.0000E+50 into the "replace with" field…Be careful using "replace all"!

C.3 Top Boundary

➢ In Part D, we will specify a constant flux at the top of the model by adding a water source (using GENER block) in the fill layer.

➢ Run TOUGH2 by typing "t2_eos9 < *PartC.txt* > *PartC.out*".

SIDE NOTE (Inactive element concept). Dirichlet boundaries can also be specified using inactive elements (see p. 62 of manual), which reduces the number of unknowns by removing elements from the mass/heat balance equations. All elements occurring in the ELEME block after an element with a *zero or negative volume* are assumed to be inactive, while those before are active. Alternatively, one can insert a line with a fictitious element name (e.g., with "INA" in columns 1-3); the following elements are automatically taken to be inactive.

Depending on the order—by row or by column—of the elements, this feature may require reordering the ELEME block (i.e., putting the desired inactive boundary elements after the active elements).

Part D: Background Infiltration

Background infiltration (steady-state flow in the vertical direction) is implemented by injecting water at a constant mass rate into each grid block at the top of the fill layer. The GENER block is used for this purpose (see manual starting on p. 174).

➢ Copy *PartC.txt* and paste/rename it *PartD.txt*.

➢ Next open *GENER_Info_PartD.txt* and paste contents into *PartD.txt*, after PARAM block and before ELEME block (leave blank line below).

➢ Modify the new `GENER` block in *PartD.txt* so that water is injected at a constant generation rate of 1.0E-6 kg/s.

- `TYPE` = "WATE"

- `GX` = 1.0E-6

➢ Add a source to the top row of the FILLI layer by specifying the code name of the first element [`EL`,`NE`]= "A21 1". Also enter the name of the source [`SL`,`NS`] = "INJ01".

➢ Add 9 additional sources using `NSEQ`, `NADD`, and `NADS`

- Number of additional elements with same injection rate `NSEQ` = 9

- Increment between code numbers in element names `NADD` = 1

- Increment between code numbers in source names `NADS` = 1

➢ Check that the `GENER` block is consistent with Figure 7.

➢ Run TOUGH2 by typing "t2_eos9 < *PartD.txt* > *PartD.out*"

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Figure 7. `GENER` block a) format requirements and b) portion in input file *PartD.txt* used to simulate background infiltration.

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Part E: Initial Conditions

In this step we calculate a 2-D profile for a steady-state system that contains an aquifer (water table at 5 m) and unsaturated zone above.

E.1 Primary Variables in EOS9 (p. 52 of manual)

➢ There is only one primary variable in EOS9 (see below)

Relevant
T2 Blocks
MULTI
INCON
INDOM
PARAM
SAVE

Components	# 1: water
Parameter choices	
(NK, NEQ, NPH, NB) =	(1, 1, 1, 6) water, isothermal (default; no other choices available)
Primary Variables *†	
saturated conditions	
(P_{liq}) - (water pressure: $P_{liq} \geq P_{gas}$)	
unsaturated conditions	
(S_{liq}) - (water saturation: $0 < S_{liq} < 1$)	

* The first primary variable may be initialized as X1 < 0, in which case it will be taken to denote capillary pressure, and will be converted internally to S_{liq} in the initialization phase.

† Reference gas phase pressure, flow system temperature, and (optionally) thermophysical parameters of water density, viscosity, and compressibility may be specified through a fictitious ROCKS domain 'REFCO'.

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E.2 Set Pressure at Bottom of Model using INDOM Block

➢Copy *PartD.txt* and paste/rename it *PartE.txt*.

➢The INDOM block will be used to give initial conditions for the material (BOUND) at the lower boundary of the model (it will remain fixed since it is a Dirichlet boundary).

➢Make the pressure at the bottom of the model (at 10 m depth) equal the pressure of a 5 m column of water above it by setting $P_{BOUND} = \rho gH + P_{atm} \sim 1000 \times 9.81 \times 5 + 1.013E5 = 0.1503E6$ Pa.

➢Create an INDOM block after the GENER block by typing "INDOM" on one line, the material "BOUND" on the next line, and the value of P_{bound} of the following line. Leave a blank line above and below the new block (see Figure 8).

E.3 Default initial conditions in PARAM Block

Q-E.3.1: What are the default initial conditions in *PartE.txt* for the remaining materials (PARAM.4, p. 168)?

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a)

```
INDOM (optional) 1 - - - - * - - - 2 - - - - * - - - 3 - - - * - - - 4 - - - * - - - 5 - - - - * - - - 6 - - - - * - - - 7 - - - * - - - 8
MAT
           X1                    X2                    X3                    X4
```

b)

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    20001    10010000000000200040000400
      0.0            1.000E-00                        9.81000
   1.0E-04
                    0.9    ←── Default initial conditions
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A21 1INJ01   9   1   1   0       WATE 1.0000e-04

INDOM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
BOUND
      0.150300E6


ELEME
A21 1          FILLI0.2500E+00                   0.5000E+000.5000E+00-.1260E+00
A31 1          FILLI0.2500E+00                   0.5000E+000.5000E+00-.3760E+00
```

Figure 8. a) Format requirements for INDOM block, and b) specifying
initial conditions with INDOM and PARAM.4 for *PartE.txt*.

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➢ Change MOP(7) to 0 to suppress output of input data.

➢ Run TOUGH2 by typing "t2_eos9 *<PartE.txt >PartE.out"*

➢ Examine the following output files: *PartE.out*, *SAVE*

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Figure 9. Excerpt from *PartE.out*.

Figure 10. Excerpt from *SAVE* for *PartE.txt* after 1 time step

> Figure 9 shows that the total liquid mass in place is a large number (~0.2E+54 kg) due to the large volume specified for BOUND.

> There is a special switch in TOUGH2 to remove a material from being counted in the material balance: Change `SPHT` of block `ROCKS` for BOUND to $>10^4$ for this purpose (p. 161 in manual).

> Make this change and run the code again. The new total liquid mass in place should be ~0.2E+05 kg.

```
Input file for Part E of sample problem 2DVZ
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
… (Several lines omitted)
FILLI    2    2500.0    .3000 5.000E-12 5.000E-12 5.000E-12      2.0      1000.

   7           0.30      0.20      1.0      0.05
   7           0.30      0.19    1.0e-3     5000.      1.00
BOUND    2    2500.0    .2000 1.000E-12 1.000E-12 1.000E-12      2.0    (1.0E5)
   7           0.30      0.20      1.0      0.05
   7           0.30      0.19    1.0e-3     5000.      1.00    Removes BOUND
(blank line!)                                                from material balance
…
```

Part F: Steady State

In this step we run the code to steady state to obtain the initial conditions for the ponded infiltration simulation. The parameters that need to be modified for time step control are given in the `PARAM` block (see side note 2 pages below). Steady-state conditions are achieved (approximately) when the primary variables no longer change with increasingly large time steps. For this to occur, the maximum number of time steps to be calculated (`MCYC`) must be a large number and the maximum time step (`DELTMX`) must also be large so that the code does not terminate before reaching steady state.

> Copy and paste/rename *PartE.txt* as *PartF.txt*.

> Increase `MCYC` to 1000 in `PARAM.2` (p. 156) so that the code can run to steady state. Check that `DELTMX` is blank or large.

> Run TOUGH2 by typing "t2_eos9 < *PartF.txt* > *PartF.out*.

> Examine the output files *PartE.out*, *SAVE*.

SIDE NOTE (Simulation Time)

Variable	Description	Default
TSTART	Starting time of simulation	0
TIMAX	Simulated end time	∞
MCYC	Maximum number of time steps	-
DELTEN	Initial time step size	-
DELTMX	Upper limit for time step size	∞

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   2 MCYC    1001000000000002000400004000
   TSTART      TIMAX     DELTEN     DELTMX                 9.81000
   1.0E-04
            0.9
```

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   21000    1001000000000002000400004000
     0.0           1.000E-00                       9.81000
   1.0E-04
            0.9
```

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Q-F.1.1: What was the maximum simulation time and the time step at the last iteration? (Open *PartF.out* and scroll down to the last occurrence of "OUTPUT DATA")

Q-F.1.2: What message in the output file indicated that steady state was reached?

Q-F.1.3: Is the water table at the correct depth?

➢ See Figures 11 and 12.
➢ Rename the *SAVE* file as *SAVE_PartF,* and delete the line starting with "+++" and the lines below.
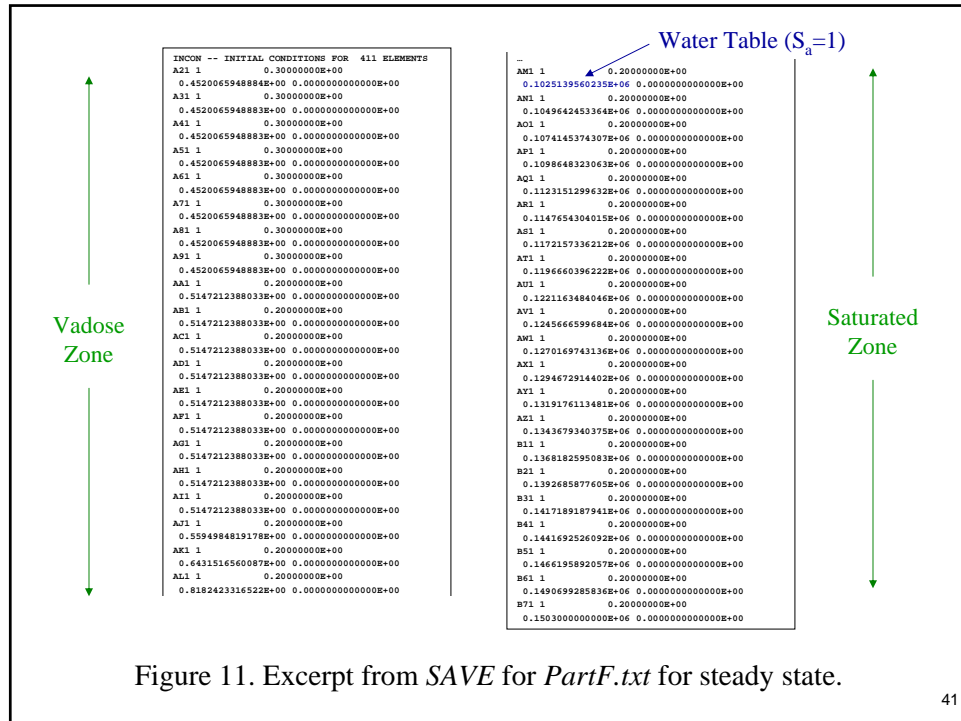
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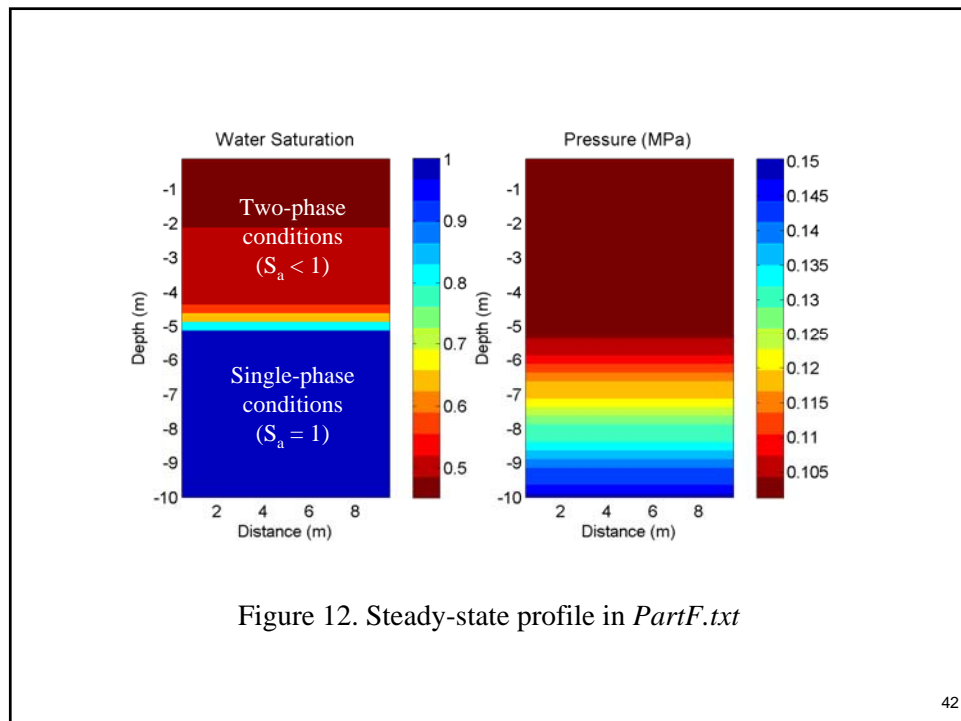Figure 11. Excerpt from *SAVE* for *PartF.txt* for steady state.

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Figure 12. Steady-state profile in *PartF.txt*

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SIDE NOTE (What makes TOUGH2 stop?)

- Reached one of the user–specified stopping criteria:
  - Maximum number of time steps
  - Maximum simulation time
- Convergence failures:
  - Wrong initialization of primary variables
  - Too many (>10) consecutive time steps converging within a single Newton-Raphson iteration →
    - Steady state is reached
    - Time step is too small (check DELTEN, DELTMX, TIMES block)
    - Newton-Raphson error criterion is too loose (reduce RE1)
  - Convergence failure followed by convergence within a single Newton-Raphson iteration →
    - May indicate steady state!
    - Serious convergence difficulty (usually phase changes)
  - More than 25 time-step reductions

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Part G: Infiltration Test

In this step we will 1) use the initial conditions simulated in Part F, and 2) add constant-rate infiltration by specifying another source in the GENER block. The *SAVE* file generated at the end of the previous step contains the output corresponding to the steady-state distribution for this problem, which will serve as the initial conditions.

  ➢ Copy *PartF.txt* and paste/rename as *PartG.txt*.

  ➢ Replace the INCON block in *PartG.txt* with the contents of the SAVE file created in the last step (*SAVE_PartF.txt*). Also remove the INDOM block (or just change keyword to xNDOM).

  ➢ Now add the new GENER block and a TIMES block from the file *GENER_TIMES_Info_PartG.txt*. The GENER block includes an additional time-dependent source for an infiltration test. The TIMES block creates output at certain times. See Figure 13.

  Q-G.1.1: Explain the time-dependent infiltration source (its strength, duration, elements to which it is applied, etc.)?

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```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A21 1INJ01    9    1    1    0       WATE 1.0000e-06
A21 1INF01    1    1    1    3       COM11
         0.0e0         8.64E4          1.0e10
    1.0000e-02            0.0             0.0
           0.0            0.0             0.0


TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
6
      0.0    21600.0    43200.0    86400.0  172800.0 5529600.0
```

Figure 13. New GENER and TIMES blocks used in Part G (from *GENER_TIMES_Info_PartG.txt*) to initiate an infiltration test, and to print output at given times, respectively.

➢ Note that ITAB should be non-zero when reading data from a table, even if the problem is non-isothermal.

➢ Increase MCYC to 1000 in PARAM.2 (p. 156) to allow the code to run to steady state.

➢ Make sure MOP(12) is set to 2. This option uses the "step function" option in handling generation rates (see p. 164 of manual).

➢ Change TSTART to 0.0, and enter the total simulation time of 64 days (5529600.0 sec).

➢ Run TOUGH2 by typing "t2_eos9 < *PartG.txt* > *PartG.out*"

➢ Examine the output files *PartG.out*, and see Figures 14 and 15.

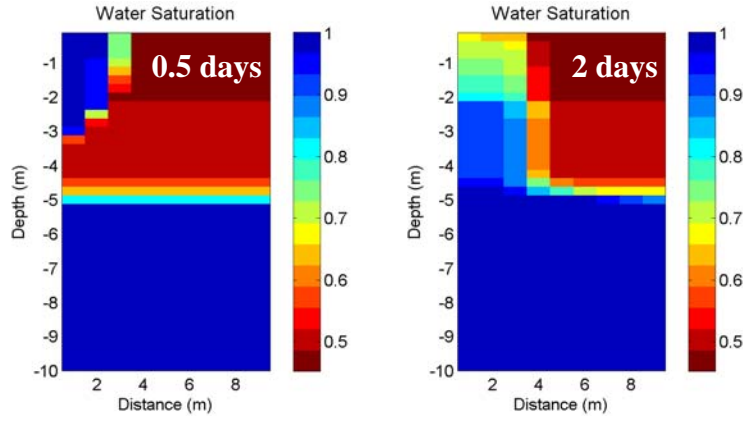Figure 14. Water saturation distribution after start of
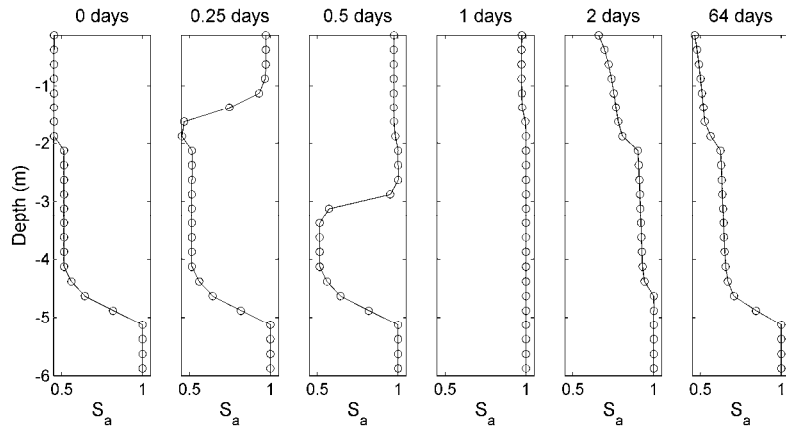infiltration test (duration of 1 day) at two times for EOS9.

Figure 15. Water saturation profile at x=0 obtained for
increasing times after start of infiltration test for EOS9.

SIDE NOTE (Output Options)

Variable	Description	Default
KDATA	Specify amount of printout	-
MCYPR	Printout occurs for every multiple of MCYPR steps	1
MOP(1)	Create printout for non-convergent iterations	no
MOP(7)	Printout of input data (recommended)	no
MOP(2-6)	Additional printout from various subroutines	no
	Additional printout times to be specified in block TIMES	

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM---1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   21000     100100000100002000400004000
       0.0 5529600.0 1.000E-00                         9.81000
   1.0E-04
            0.9
```
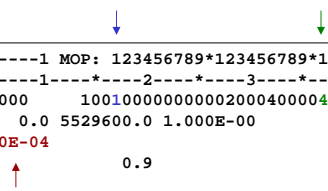
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SIDE NOTE (Newton-Raphson and Linear Eqn. Solver)

Variable	Description	Default
RE1	Relative error convergence criterion	1.0E-5
MOP(1)	Create printout for non-convergent iterations	no
MOP(21)	Select linear equation solver	3

Check block SOLVR for additional options
Check file *LINEQ* for linear equation solver data

```
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM---1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   21000     100100000000002000400004000
       0.0 5529600.0 1.000E-00                         9.81000
   1.0E-04
            0.9
```

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Problem Variation: Conversion from EOS9 to EOS3

After developing a TOUGH2 problem using EOS9, one may wish to incorporate temperature variations (i.e., make it nonisothermal) or to account for the movement of both water and gas. The TOUGH2 input file(s) can be modified accordingly to make this possible.

➤ Copy *PartG.txt* and rename it *PartH.txt*

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Primary Variables for EOS3 (p. 36 of manual)

- The primary variables for each grid block change depending on whether single- or two-phase conditions are present.
- Using values between 0 and 1 for the second primary variable implies aqueous phase conditions in a grid block (X is the primary variable). Whereas, using a value > 10 (and < 11), implies two-phase conditions (where the primary variable is $S_g + 10$).

Relevant
T2 Blocks

MULTI ◄

INCON ◄
INDOM
PARAM
SAVE

| Components | # 1: water |
| | # 2: air |

Parameter choices
(NK, NEQ, NPH, NB) = (2, 3, 2, 6) water and air, nonisothermal (default)
(2, 2, 2, 6) water and air, isothermal
molecular diffusion can be modeled by setting NB = 8

Primary Variables *
  single-phase conditions
    (P, X, T) - (pressure, air mass fraction, temperature)
  two-phase conditions
    $(P_g, S_g + 10, T)$ - (gas phase pressure, gas saturation plus 10, temperature)

* By setting MOP(19) = 1, initialization can be made with TOUGH-style variables (P, T, X) for single-phase, (P_g, S_g, T) for two-phase.

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➢ Add MULTI for isothermal case (NK=2, NEQ=2, NPH=2, NB=6)

➢ The relative permeability and capillary pressure functions for the ATMOS material should allow for transfer or air but not water.

➢ Give the atmospheric grid block "99999" a Dirichlet boundary condition with pressure equal to atmospheric and constant high gas saturation (e.g., Sa = 0.1 or Sg = 0.9).

➢ Specify initial conditions using INDOM instead of INCON (hint: delete contents of INCON block without deleting keyword); set default initial conditions in PARAM block with gas saturation equal to zero (2nd primary variable equal to X = 0).

➢ To obtain steady-state profile, remove the source was used for the infiltration test in the GENER block (INF01-INF02); leave TIMAX blank so that steady state can be reached.

➢ To simulate infiltration test, copy *SAVE* file from steady-state run to INCON block, reinsert infiltration test source, and run.
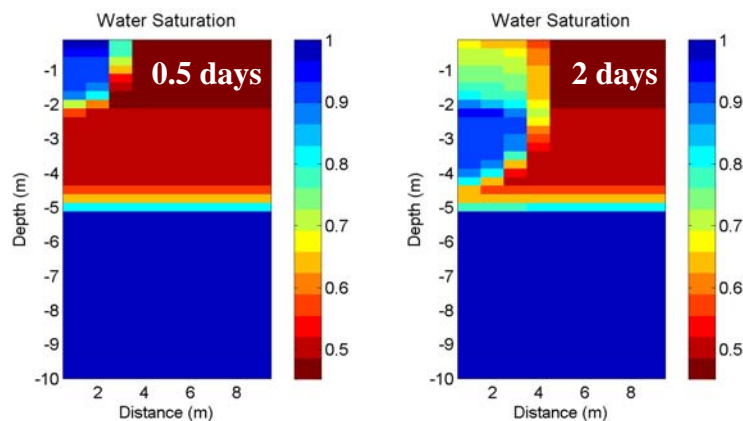
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Figure 16. Water saturation distribution after start of infiltration test (duration of 1 day) at two times for EOS 3.
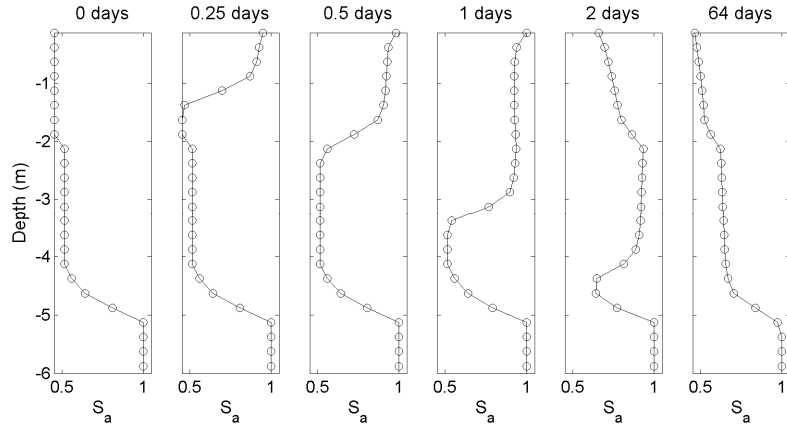
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Figure 17. Water saturation profile at x=0 for increasing times
after start of infiltration test for EOS3.