TOUGH Short Course

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Sample Problem 3

- Description of Problem
- Problem 3a: Steady-State Conditions
- Problem 3b: Injection of DNAPL
- Problem 3c: Redistribution of DNAPL
- Problem 3d: Remediation

Model Description for Problem 3

- Cylindrical model
- Non-Isothermal (during remediation)
- PCE injected at 1.0E-4 kg/s for 1 day
- Initial Conditions
  - Two-phase (Aqueous-Gas)
- Boundary conditions
  - S_g = 0.40 at top
  - No flow at sides and bottom
  - PCE outlet closed
- Simulation requires four steps
  - Gravity-capillary equilibrium (Prob. 3a)
  - PCE injection (Prob. 3b)
  - Redistribution (Prob. 3c)
  - Remediation (Prob. 3d) [non-isothermal]

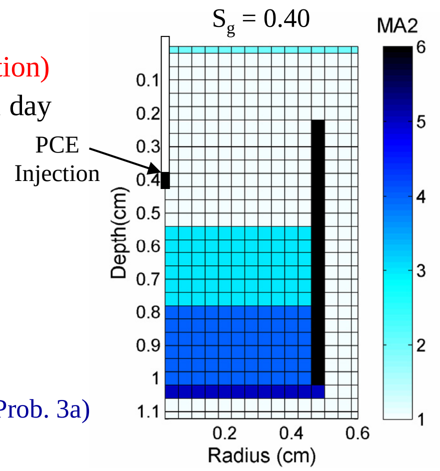

Figure 1. Material distribution

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Problem 3A: Gravity-Capillary Equilibrium

- Go back to input file P2a_0.txt and resave it as P3a.txt
- Open Command Prompt, and type cd C:\TOUGH2\Sample3

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A.1 Primary Variables

Part A of this problem requires calculation of steady-state conditions for two-phase aqueous-gas conditions. This is again accomplished by reducing the number of possible components and phases in block MULTI.

Q-A.1.1: Check that the block MULTI has the correct entries and state the possible primary variable combination(s) that should occur during this simulation (Part A).

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A.2 Boundary Conditions

Next set the boundary conditions to such so that gravity-capillary equilibrium can be obtained.

- Set initial conditions in the upper layer: $S_w = 0.40$, and $S_g = 0.60$
- For the default initial conditions, set $S_w = 1.0$
- Remember that there are currently only three primary variables
- Save and run code (P3a.txt as input file)
- Rename SAVE file as SAVE_P3a

Q-A.2.1: Examine output file and determine depth of water table.

Q-A.2.2: Name two ways to raise steady-state water table level.

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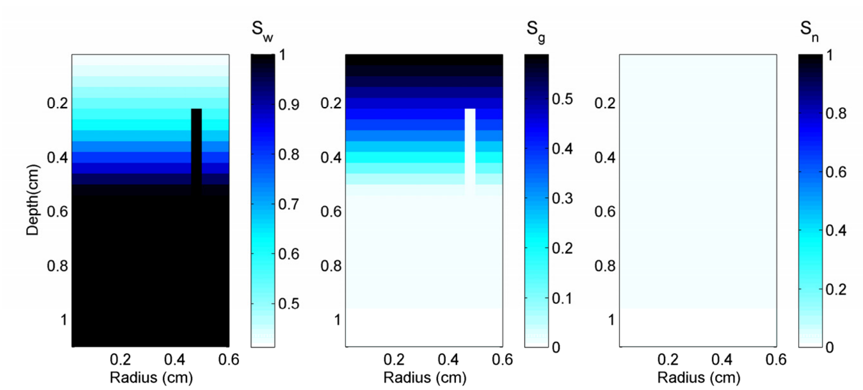

Figure 2. Distribution of phase saturations at gravity-capillary equilibrium (Part 3a).

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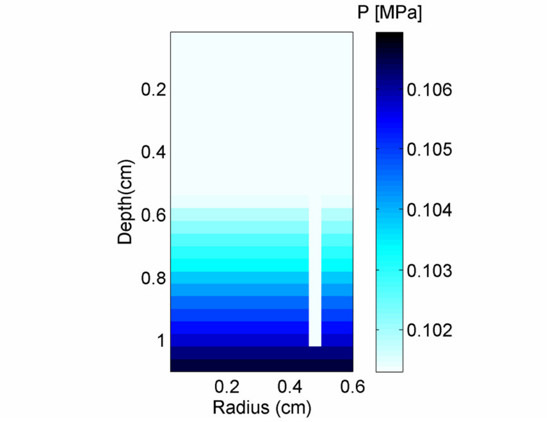

Figure 3. Pressure distribution for gravity-capillary equilibrium (Part 3a).

Problem 3B: Injection of DNAPL

- ➢ Save the last input file from Part A (P3a.txt) as P3b.txt

B.1 Primary Variables

- ➢ Change block MULTI allow for the presence of water, air, and VOC components (NK = NEQ = NPH = 3). The problem can still be modeled as isothermal since heat is not introduced until Part D.

B.2 Initial Conditions from Part A

- ➢ Copy INCON block from SAVE file (SAVE_3Pa) and paste into INCON block of current input file

- ➢ Change MOP(19) to 1 to allow initial conditions format of previous run

B.3 Injecting PCE

Next we use the GENER block to inject PCE at a depth of 42 cm at a constant rate of 1.0E-4 kg/s for 24 hours.

- Insert the GENER block that was developed in Problem 2
- Set initial time step (DELTEN) to a small number (10.0 seconds)
- Set the maximum simulation time (TIMAX) to 8.64E4 [s]
- Increase MCYC and MCYPR to 1000
- Save and run code (P3b.txt); rename SAVE file as SAVE_p3b

Q-A.3.1: After examining results, increase the injection rate to 3.0E-4 kg/s. Does PCE spill over the acrylic wall of the inner sand/clay region?

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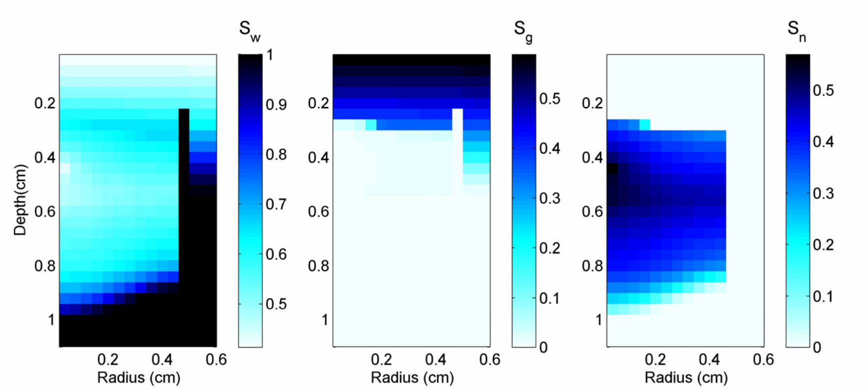

Figure 4. Distribution of phase saturations after constant injection of PCE at 1.0E-4 kg/s for 1 day (Part 3b).

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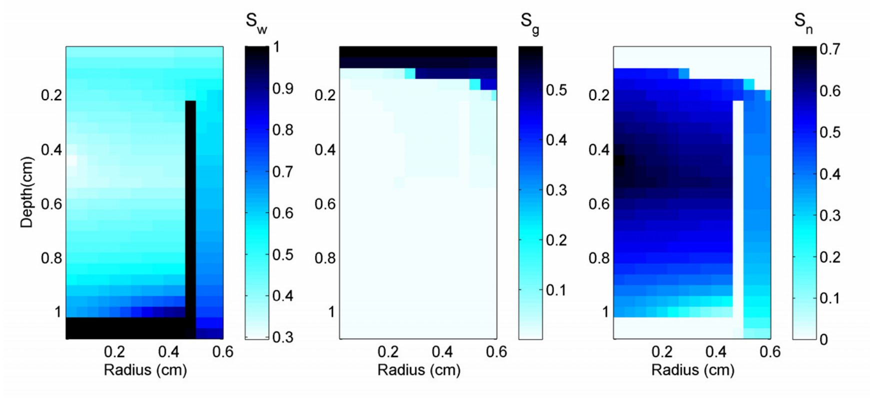

Figure 5. Distribution of phase saturations after constant injection of PCE at 3.0E-4 kg/s for 1 day. (Shown to demonstrate effect of injection rate only; not used in subsequent parts of problem.)

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Problem 3C: Redistribution of DNAPL

- Save p3b.txt as p3c.txt
- Copy INCON block from SAVE_p3b. Keep +++ information so as to enable next simulation to start at t = 1 day.
- Remove NAPL source from GENER block
- Change MOP(19) back to 0
- Simulate redistribution to a total simulation time of two weeks (1.2096E6 sec.).
- Run p3c.txt, rename SAVE as SAVE_p3c

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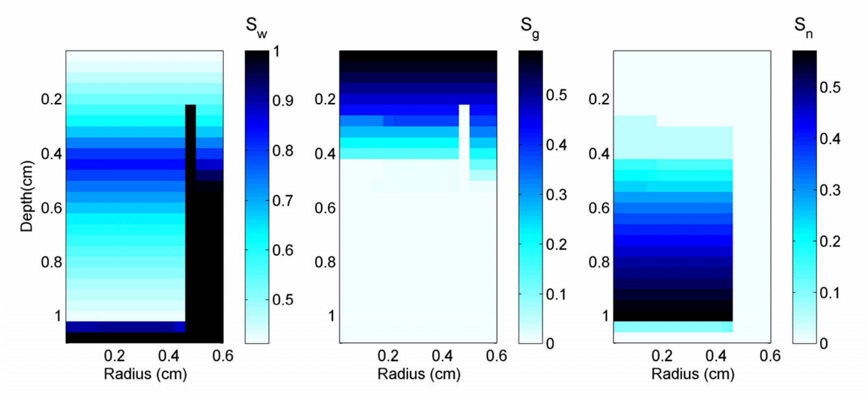

Figure 6. Distribution of phase saturations following redistribution of PCE for 14 days (Part 3c).

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Problem 3D: Remediation by Steam Injection and ???

- Save p3c.txt as p3d_0.txt
- Copy INCON block from SAVE_p3c
- Make this run non-isothermal (NEQ = 4 in block MULTI)
- Add heat injection in elements " 23 1", " 23 1", and " 23 1" in GENER block with a steam injection rate of 1.48E-4 kg/s and specific enthalpy of 2.67E6 J/kg for each.
- Run simulation for one addition 1 hour (making total simulation time equal 1.2132E6 sec.)
- Run p3d_0.txt

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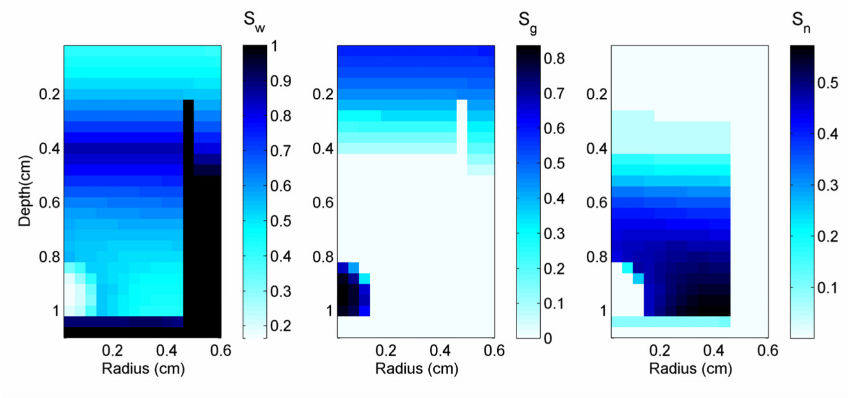

Figure 6. Distribution of phase saturations after 1 hour of steam injection (Part 3d).

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D.1 What are the next steps for remediation???

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