TOUGH Short Course

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Sample Problem 2

- Description of Problem
- Problem 2a: Steady-State Conditions
- Problem 2b: Injection of DNAPL
- Problem 2c: Redistribution of DNAPL

Model Description for Problem 2

- Cylindrical model (simplified version of full-scale model)
- Isothermal
- PCE injected at 1.0E-4 kg/s for 1 day
- Initial Conditions
  - Single-phase aqueous
- Boundary conditions
  - Water saturated at top
  - No flow at sides and bottom
  - PCE outlet closed
- Simulation requires three steps
  - Steady-state profile calculated (Prob. 2a)
  - PCE injection (Prob. 2b)
  - Redistribution (Prob. 2c)

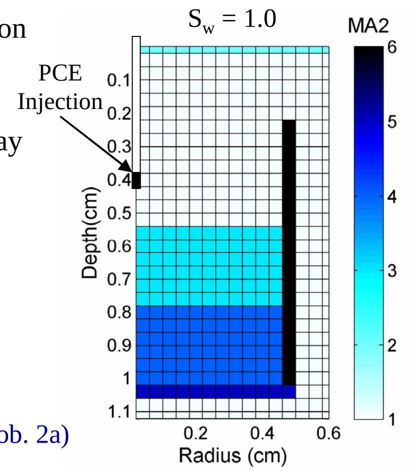

Figure 1. Material distribution

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Problem 2A: Steady-State Conditions

A.1 Primary Variables

Part A of this problem requires calculation of steady-state conditions for single-phase aqueous conditions. This can be accomplished most efficiently by reducing the number of possible components and phases in block MULTI.

Q-A.1.1: Open file P2a_0.txt and examine block MULTI. Which equations are being omitted?

Q-A.1.2: Is this simulation isothermal or non-isothermal?

Q-A.1.3: What are the primary variables for this case (see Table 3 on p. 20 of Manual)?

A.2 Mesh

The 2D cylindrical mesh used for this example is provided. The five character element names are composed as follows: ZZZRR, where ZZZ is the depth increment going from 1 to 30, and RR is the radial increment going from 1 to 16. The first space of RR is blank for radial increments 1 to 9. Similarly, the first two spaces of ZZZ are blank for increment numbers 1 to 9 and the first space is blank for increment numbers 10 to 30.

Q-A.2.1: What are the minimum and maximum (a) radii and (b) depths?

Q-A.2.2: Which elements comprise the upper layer of the model?

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Q-A.2.3: The material types are being specified using parameter MA2 in block ELEM. What material type are the elements in the upper layer?

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A.3 Boundary Conditions

There are several ways in which boundary conditions can be implemented in T2VOC (Section 5 in T2VOC manual).

> **Q-A.3.1**: What types of boundaries are specified in the (a) upper layer of the model and (b) at the side and bottom of the model, and (c) how were they specified?

Dirichlet boundary conditions can also be specified using the concept of inactive elements (Section 5 of manual), which reduces the number of unknowns by removing the elements whose properties should not change from the mass/heat balance equations. Each element occurring after a one line entry with the word INA is assumed to be inactive, while each occurring before it is assumed active.

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- Open Command Prompt, and type: cd C:\TOUGH2\Prob2
- Run problem by typing: T2_v < P2a_0.txt > P2a_0.out
- Examine output file P2a_0.out

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Output parameters given by T2VOC (first list) are defined as:

notation	meaning
P	gas phase pressure, Pa.
T	temperature, ° C .
SO	NAPL phase saturation.
SW	aqueous phase saturation.
SG	gas phase saturation.
PVOC	VOC vapor pressure, Pa.
PAIR	air partial pressure, Pa.
PSATO	VOC saturated vapor pressure, Pa.
PSATW	water saturated vapor pressure, Pa.
PCO	gas-NAPL capillary pressure, Pa.
PCW	gas-water capillary pressure, Pa.

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Output parameters given by T2VOC (second list) are defined as:

notation	meaning
CVOCGAS	VOC concentration in the gas phase, kg/m^3.
CVOCAQ.	VOC concentration in the aqueous phase, kg/m^3.
DGAS	gas phase density, kg/m^3.
DNAPL	NAPL density, kg/m^3.
VISGAS	gas phase viscosity, kg/m s.
VISNAPL	NAPL viscosity, kg/m s.
DIFFO	VOC vapor diffusivity, m^2/s.
DIFFW	water vapor diffusivity, m^2/s.
KRGAS	gas phase relative permeability.
KRAQ.	aqueous phase relative permeability.
KRNAPL	NAPL relative permeability.

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➢ Save input file from previous step (P2a_0.txt) as P2a_1.txt

➢ Find the first entry in the ELEM block for the bottom layer of elements. Above this entry, insert a blank line with the word INA in columns 1-3 (meaning inactive).

➢ Move the upper layer elements to bottom of ELEM block.

➢ The elements of the upper and lower layers should be below the INA entry, making them inactive elements.

➢ Close block ELEM with a blank line.

➢ Save and run code with the P2a_1.txt input file.

Q-A.3.2: What effect did rearranging the ELEM file have on the order printed data in the SAVE file and in the main output file?

An element named "INA 0" will appear in the output. It can be ignored.

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A.4 Initial Conditions

Domain- (or material-) specific conditions are given in the INDOM block. For this problem, the INDOM block is used to give the initial conditions in the upper layer of the model, while the initial conditions in the remaining elements are given by the default values set in the PARAM block.

Q-A.4.1: What are the default initial conditions?

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A.5 Obtaining Steady-State Conditions

The parameters that need to be modified for time step control are given in the PARAM block. Steady-state conditions are achieved (approximately) when the primary variable values no longer change with increasingly large time step values. 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).

- Save the previously modified input file (P2a_1.txt) as P2a_2.txt
- Change MCYC and MCYPR from 1 to 1000.
- Check that DELTMX = 1.0e10.
- Save and run code using the P2a_2.txt input file.

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Q-A.5.1: What was the maximum simulation time reached and the time step at the last iteration? (Open the output file and scroll down to the first occurrence of “OUTPUT DATA”)

Q-A.5.2: What message in the output file indicated that steady state was reached?

Q-A.5.3: Open the SAVE file and examine the output. Does the pressure in the sand at the bottom of the tank match the hydrostatic pressure (given the depth of water inferred from question **Q-A.2.1**)?

- Rename the SAVE file as SAVE_P2a.

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Problem 2B: Injection of DNAPL

- Save the last input file from Part A (P2a_2.txt) as P2b_0.txt

B.1 Primary Variables (with VOC)

Q-B.1.1: How should the MULTI block be changed in order to (a) allow for the presence of water, air, and VOC components and (b) omit the heat balance equation.

Q-B.1.2: List the expected primary variable combinations for this part of the simulation (see Table 3 on p. 20 of manual)?

- Change the MULTI block accordingly.

B.1 Implementing Steady-State Distribution as Initial Conditions

The SAVE file generated at the end of the previous simulation (renamed SAVE_P2a) contains the output at the last time step of the simulation corresponding to the steady-state distribution. These data will serve as the initial conditions for Part B.

- Change MOP(19) to 1 so that the primary variables can be initialized for a three-component simulation (NK = 3) using the initial conditions obtained from the two-component simulation run (NK = 2). See p. 51 in T2VOC manual.
- Replace the INCON line in the current input file (file P2b_0.txt) with the contents from the file SAVE_P2a.
- At the bottom of the new INCON block, remove the +++ and the following line (it contains information from the previous run and cross-referencing information not needed for our purposes.)

B.3 Injecting PCE

Next we use the GENER block (p. 57 of Manual) to inject PCE at a depth of 42 cm at a constant rate of 1.0E-4 kg/s for 24 hours.

➢ Until now, the GENER block was empty (i.e., the keyword was present, but it was followed by a blank line). In file P2b_0.txt, create another line under the GENER keyword, and enter the following information (using correct input format):

- Element name at which injection will occur: " 12 1"
- 5 character name of source: "INJ 1"
- Type of source or sink: "COM3"
- Constant injection rate: 1.0E-4 kg/s
- Fixed enthalpy of injected PCE: 3.80E4 J/kg
- Make sure this block ends with a blank line.

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➢ Set initial time step (DELTEN) to a small number (10.0 seconds)

➢ Specify for the code to stop after one iteration (set MCYC to 1) and provide output at that time (set MCYPR = 1)

➢ Save and run code with input file P2b_0.txt

Q-B.3.1: Open the main output file and scroll down to just above the first occurrence of "OUTPUT DATA". In which elements has the NAPL phase evolved?

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- **Q-B.3.2**: Scroll down below the first occurrence of “OUTPUT DATA”. Look at the output for the element at which PCE was injected. Describe how the total pressure and saturations of NAPL, water and gas have changed from the initial conditions after one time step.

- **Q-B.3.3**: Open the SAVE file and examine the output of the primary variables. For an element near the top of the tank (e.g., “ 2 1” what phases are present (and what are the primary variables)?

- **Q-B.3.3**: Scroll down in the SAVE file and look at the output for the element at which PCE was injected (“ 12 1”). What phases are present and what are the primary variables in this element?

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Use block FOFT to print time-dependent data to file (called FOFT) for element “ 15 1”. See p. 169 of TOUGH2 manual.

- After adding block FOFT, save the current input file (P2b_0.txt) as P2b_1.txt.

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The injection is meant to last for 24 hours, so the maximum simulation time (TIMAX) must be set accordingly.

- Set the maximum simulation time (TIMAX) to 8.64E4 [s]
- Increase MCYC and MCYPR to 1000
- Save file and run code with P2b_1.txt input file. This will take longer to run than the previous parts of the problem.
- Rename the SAVE file as SAVE_P2b

Q-B.3.4: What is the total mass of PCE in the system at the end of the injection?

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Q-B.3.4: Open output file FOFT. The second column is the time [s], the third is the element number for which data is being printed, and the third is the pressure [Pa]. How long after the NAPL injection starts does it take for the pressure in element " 15 1" to deviate from its steady-state value?

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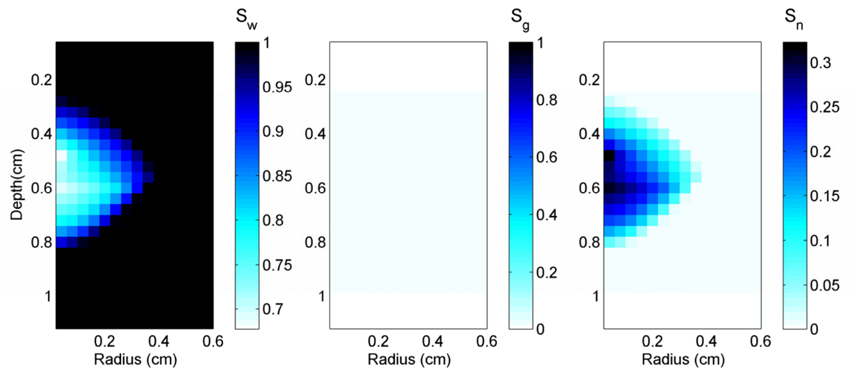

Figure 2. Distribution of Water, Gas, and NAPL saturations after constant injection of PCE for 1 day (Part 2b).

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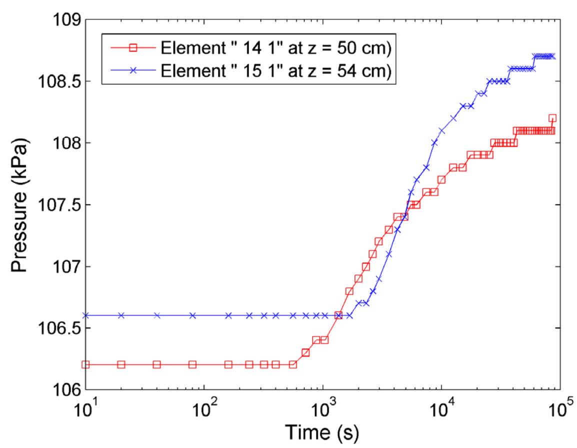

Figure 3. Pressure response with time after onset of PCE injection (shown for elements above and below interface between the sand and the sand/clay layers) (Part 2b).

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Problem 2C: Redistribution of DNAPL

The redistribution that occurs after PCE injection ceases will be simulated by using the SAVE file from the previous run, removing the injection source in the GENER block, and setting the total simulation time to the desired value.

- Save the previous input file (P2b_1.txt) as P2c.txt

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C.1 Using Output from Part B as Initial Conditions

The SAVE file generated at the end of the previous simulation (renamed SAVE_P2b) contains the output at the last time step of the simulation corresponding to the end of the PCE injection. These data will serve as the initial conditions for Part C.

- Change MOP(19) back to 0 so that now primary variables can be initialized in the usual manner for a three-component simulation (NK = 3).
- Replace the INCON line in the current input file (file P2c.txt) with the contents from the file SAVE_P2b.
- Remove line with +++ and following line at bottom of block INCON.
- Make sure there is a blank line following the INCON block.

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C.2 Initiate PCE redistribution

- Delete the contents of the GENER block (Leave the key word GENER followed by a blank line!).
- Change maximum simulation time to 7 days (6.048E5 seconds).
- Save and run code (with P2c.txt input file).

Q-B.3.4: Has the total amount of VOC in the system stayed the same since the end of the injection?

Q-B.3.5: Has the total amount of adsorbed VOC increased or decreased since the end of injection?

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Q-B.3.6: Has any PCE seeped through the bottom clay layer?

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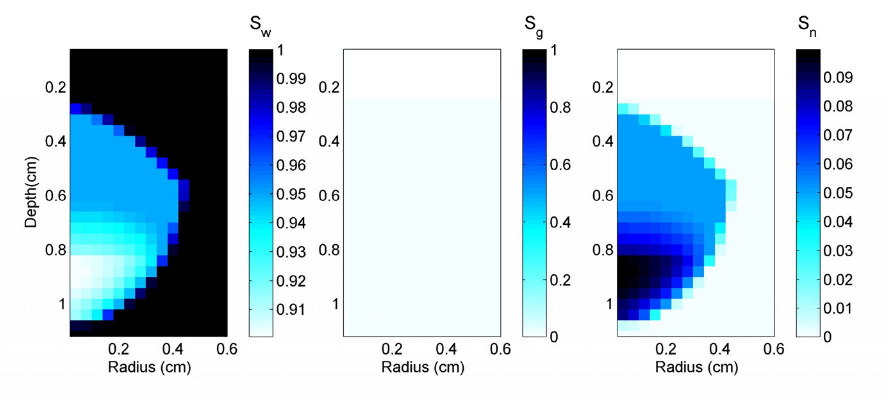

Figure 4. Distribution of Water, Gas, and NAPL saturations after redistribution for 7 days (Part 2c).

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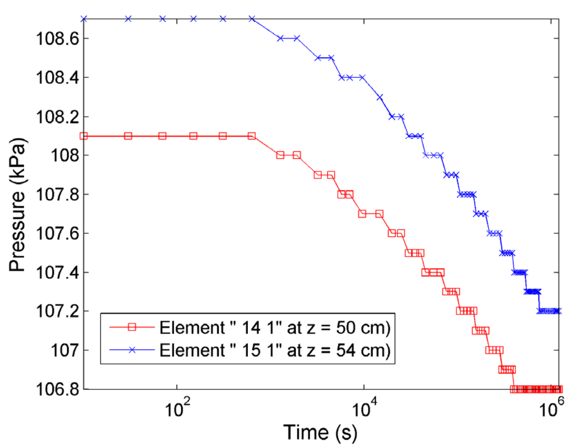

Figure 5. Pressure response with time during redistribution (shown for elements above and below interface between the sand and the sand/clay layers) (Part 2c).

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