TOUGH Short Course

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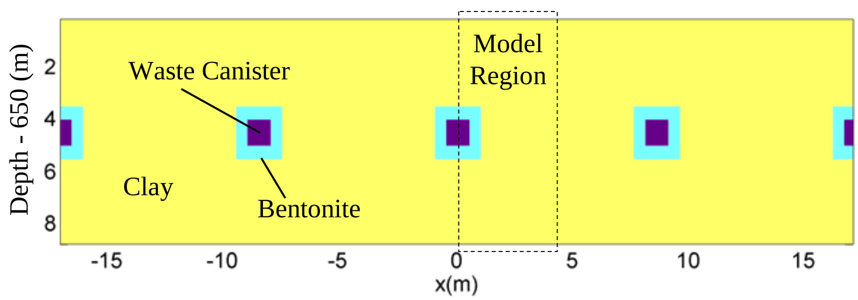
EOS7R Sample Problem

- Problem description
- Part A: Material properties
- Part B: Mesh generation
- Part C: Initial conditions
- Part D: Radionuclide Case 1
- Part E: Radionuclide Case 2

Problem Description



- Case 1: Release of ^{241}Am and decay into ^{237}Np
  - Aqueous phase, isothermal
- Case 2: Generation of ^{14}C and decay into nitrogen gas
  - Two-phase, nonisothermal

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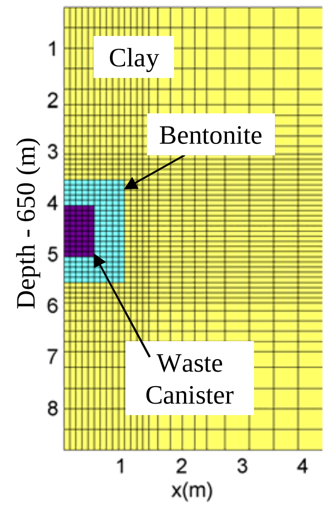
Model

- Two-dimensional model takes advantage of symmetry
  - Irregular grid spacing
- Initial Conditions
  - Single-phase aqueous
  - Flow in vertical direction (downward)
- Boundary conditions
  - Constant conditions at top
  - Constant conditions at bottom (zero flux during static equilibration)
  - Zero flux at the sides



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Part A: Material Properties

```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
CLAY     2     2650.       .12  1.00E-17  1.00E-17  1.00E-17       2.5     905.5
   1.83e-9   3.47e-5               1.             1.00e-00  1.00E-03
    7            0.4       0.5      1.0       0.05
    7            0.4       0.5    5.6e-7                   1.0
CONTA    2     2650.       .17  1.00E-17  1.00E-17  1.00E-17      52.0     905.5
   1.83e-9   3.47e-5               1.             1.00e-00  1.00E-03
    7            0.4       0.3       1.       0.05
    7            0.4       0.3    1.E-5                    1.0
BENTO    2     2650.       .40  1.00E-20  1.00E-20  1.00E-20      1.35     964.0
   3.58e-9    1.5e-5               1.             1.00e-00  1.00E-03
    7            0.4       0.3       1.       0.05
    7            0.4       0.3    5.6e-9                   1.0
TOPBC    2     2650.       .12  1.00E-17  1.00E-17  1.00E-17       2.5     905.5
   1.83e-9   3.47e-5               1.             1.00e-00  1.00E-03
    7            0.4       0.5       1.       0.05
    7            0.4       0.5    5.6e-7                   1.0
BOTBC    2     2650.       .12  1.00E-17  1.00E-17  1.00E-17       2.5     905.5
   1.83e-9   3.47e-5               1.             1.00e-00  1.00E-03
    7            0.4       0.5       1.       0.05
    7            0.4       0.5    5.6e-7                   1.0
```

Figure 3. Portion of input file *MatDist.txt* containing entries in ROCKS block for three materials: Clay (CLAY), Bentonite (BENTO) and the waste container (CONTA). Two additional materials (TOPBC, BOTBC; with same properties as clay) can be used to facilitate equilibration.

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Q-A.1: (a) Which material has the lowest permeability, and (b) is the permeability modeled as isotropic or anisotropic?

Q-A.2: What functions are being used to model the relative permeability and capillary pressure?

Q-A.3: How does the capillary pressure behavior for the bentonite buffer differ from that for the waste canister and clay materials? (Hint: look at CP(3) and definition on p. 189)

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Part B: Mesh Generation

B.1 Generate 1-D mesh in x-direction

- Open *MakeMesh.txt* (see Figure 4)
- Fill in correct number of grid increments in the x-direction
- Open Command Prompt, and type: cd C:\TOUGH2\ProbRN
- Run code by typing: t2_7r < *MakeMesh.txt* > *MakeMesh.out*
- Open output file *MESH*

Q-B.1.1: What are the minimum and maximum x, y and z values?

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Q-B.1.2: Calculate the minimum and maximum element volumes from the input file and compare with those generated in the MESH file. Do they agree?

Q-B.1.3: In any single connection, the distances from the element centers to the nodes (D1 and D2) may be different. Explain why.

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```
*RADIONUCLIDE TRANSPORT PROBLEM*
MESHM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
        0.
NX      ??
       0.1       0.1       0.1       0.1       0.1       0.1       0.1       0.1
       0.1       0.1       0.1       0.1       0.1       0.1       0.1       0.2
       0.2       0.2       0.2       0.2       0.4       0.4       0.4       0.4
       0.4
NY       1       1.0
NZ       1       1.0


ENDFI


********************************************************************************
Use this distribution of z-direction grid increments to generate 2-D mesh
********************************************************************************
NZ       5       0.4
NZ       5       0.2
NZ      15       0.1
NZ      15       0.1
NZ       5       0.2
NZ       5       0.4
```

Figure 4. Input file *MakeMesh.txt*

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B.2 Generate 2-D mesh

- A distribution of z-direction grid increments is given at the bottom of *MakeMesh.txt*. Copy the corresponding lines of text and paste them in the appropriate place in the MESHM block (i.e., replace the line containing "`NZ          1            1.`" with those lines.)
- Note the alternative way to specify grid increments in the z-direction (compared to that used for the x-direction)
- Run code and open output file *MESH*

Q-B.2.1: Now what are the minimum and maximum x, y and z values?

Q-B.2.2: Examine the naming convention for the element names. In this case, how are the five-character element names related to the element coordinates? For example, how can you tell in what column an element is found simply by looking at the element name?

B.3 Assigning material properties to mesh (ELEM block)

- Open *MESH_MatNum*. This file is similar to the mesh generated in the previous step except that the material distribution specific to this sample problem has already been generated (material numbers have been inserted in the spaces for parameter MA2 in columns 19-20).

Q-B.3.1: Given the material properties specified in *MatDist.txt*, what are the (a) names and (b) depths corresponding to the elements at the top and bottom of the waste container?
(Hint: `CONTA` is material number three so look for MA2 = 3)

Q-B.3.2: What is the maximum x-coordinate corresponding to the presence of bentonite?

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Part C: Simulating Initial Conditions

Before simulating radionuclide transport, steady-state conditions under single-phase aqueous flow must be calculated (and then used as initial conditions).

- Open *MatDist.txt* and rename it *SimInit.txt.*
- Copy and paste contents of file *MESH_MatNum* into *SimInit.txt.* Place the contents under the empty `INCON` block (leaving one blank line in between). Close `CONNE` block with blank line. Now the input file contains the generated mesh information.
- To obtain steady-state distribution most efficiently, parameters of the `MULTI` block can be specified to exclude gas from the simulation (NK=4) and to run the code under isothermal conditions (NEQ=4). Make these changes in *SimInit.txt.*

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Q-C.1: What are the primary variables for this case (see p. 45)?

Q-C.2: Given their positions in the input file (PARAM.4 and PARAM.5), what are the current initial values of the primary variables?

```
...
MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    ?    ?    2    8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   39999    99991             4    5
                        1.0e-1                           9.8
    1.E-05     1.E+0
              6.37E6              1.0e-3                 0.0                 0.0
                25.0
...
```

Figure 5. Portion of input file *MatDist.txt*

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C.1 Creating hydrostatic profile

In order to create a hydrostatic profile, a constant pressure is specified at the upper layer of the model, and a no flow boundary is specified at the bottom of the model.

- The elements at the bottom of the `ELEM` block correspond to the upper layer of the model (since the MESH was modified). Make this layer inactive by adding a line with "`INA    `" above element "`A11  1`". All elements below will become inactive.
- Use the `INDOM` block to specify the pressure at the upper layer of the model. Copy `INDOM` block at bottom of file and paste below `GENER` block (leaving blank line before and after `INDOM` block).
- Specify the correct material name in `INDOM` block (i.e., replace `?????` with appropriate material name).
- Specify P = 6.37 MPa (approximate pressure at 650 meters) and salt mass fraction X_b = 1.0e-3 in the `INDOM` block.

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Steady-state conditions are approximated when the primary variables stop changing with increasingly large time steps. For this to occur, the maximum number of time steps to be calculated (`MCYC`) and the maximum time step (`DELTMX`) must be large (so that the code does not terminate before reaching steady state). These parameters are modified for time step control and are given in the `PARAM` block (see Figure 5).

Q-C.1.1: What are the values of `MCYC`, `DELTMX` and `DELTEN`?

- ➢ Make sure `MCYC` is a large number (e.g., 9999)
- ➢ Save input file as *SimInit.txt* and run code

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Q-C.1.2: What was the maximum simulation time reached? Does this indicate that steady-state conditions? (Open the output file and scroll down to the first occurrence of "`OUTPUT DATA`") Confirm your answer by examining *SAVE* file and determining whether the pressure profile changes with depth.

- ➢ If steady-state conditions were not reached, the initial time step was probably too small in this case. Change `DELTEN` to 1.0e+3
- ➢ Re-run the code and rename *SAVE* file as *SAVE_SimInit.*

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Q-C.1.3: Open the main output file (e.g., *SimInit.out*) and examine the results. (a) Is the maximum simulation time indicative of steady-state conditions? (b) How many iterations were completed?

Q-C.1.4: Does the pressure at the bottom of the model match the expected hydrostatic pressure (given the depth of water)?

Q-C.1.5: Determine whether the amounts of water and brine in the system are the same before and after the simulation. Explain why or why not.

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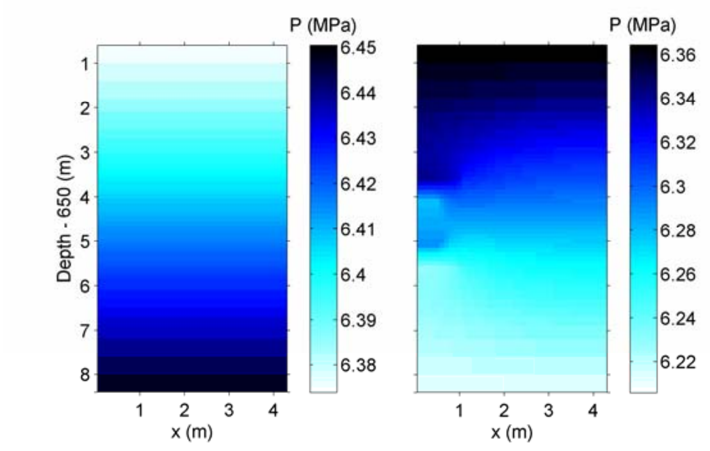

Figure 6. Initial pressure with no vertical flow (left) and with vertical flow (right).

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C.2 Creating steady-state profile with vertical flow

In order to induce vertical flow constant pressures are specified at the upper and bottom layers of the model. For this case, the elements on the top AND bottom of the model must be made inactive.

- Save *SimInit.txt* as *SimInit_Flow.txt*
- Move the line in the ELEM block with "`INA `" to the location right above the element "`BF1  1`" in order to make the upper and lower layers of the model inactive.
- Make the pressure in the lower layer equal to 6.2 MPa. To do this, another modification of the `INDOM` block is needed. In addition to the entry for `TOPBC`, add an entry for the elements at the bottom of the model (`BOTBC`). Be sure to specify the correct material name.
- Save file and run code. Rename resulting *SAVE* file as *SAVE_SimInit_Flow* (It will be used in Part D).

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Part D: Radionuclide Case 1

In this problem, the release of ^{241}Am and its subsequent decay into ^{237}Np are simulated using the model developed in the previous parts of the problem. The goal is to examine the following:

- Radionuclide release in center of waste container
- Distribution of radionuclides after 2000 years

- Americium 241 (^{241}Am)
  - Among isotopes resulting from weapons production
  - The half life is $t_{1/2}$ = 458 years (or 1.44e+10 sec)
  - Strongly sorbing, Kd value ~ 1.0 (m^3/kg)
- Neptunium 237 (^{237}Np) is the daughter radionuclide
  - Long-lived decay product of ^{241}Am
  - The half life is $t_{1/2}$ = 2.14e+6 years (or ~6.0e+13 sec)
  - Weakly sorbing, Kd value ~ 1.0e-3 (m^3/kg)

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➢ Save *SimInit_Flow.txt* and rename it *SimRad1.txt*.

➢ The file *SAVE_SimInit_Flow* contains the initial conditions that will be used in this simulation. Copy and paste the contents of this file into the main input file (*SimRad1.txt*) in the location of the empty `INCON` block. Only one line with the "`INCON`" keyword should remain. Close the `INCON` block with a blank line. Now the input file contains the needed initial conditions.

➢ Remove the `INDOM` block

➢ This case will not involve the evolution of gas, so keep the `MULTI` block the same as the previous one (NK=4 and NEQ=4).

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D.1 Radionuclide properties

In order to simulate an instantaneous release of ^{241}Am, the parent and daughter radionuclide properties must be specified in the input file as well as the distribution coefficients for each material.

➢ Add the given half-lives for the parent and daughter radionuclides (Rn1 and Rn2) and the molecular weights.

```
...
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    1   24    2
     -1.e5

     0.e-0     0.e-1
     0.e-6     0.e-6    0.e-6  1.162e-7     0.e-6     0.e-6
     1.0e1       1.0    0.e-6  1.162e-9                        1.e+30
     1.0e1       1.0    0.e-6  1.162e-9                        1.e+30
...
```

Figure 7. Example of SELEC block from input file.

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Q-D.1.1: What number is used for the inverse Henry's constant and what does it imply for the assumption of NK = 4 (Hint: is gas formation likely to occur)?

- Check that the correct Kd values are used in the `ROCKS` blocks (specify `XKD3` and `XKD4` for each material on lines `ROCKS.1.1`).
- Enter maximum simulation time is 2000 years (parameter `TIMAX` on line `PARAM.2`). Units must be seconds (6.3072e+10).
- If a line with a "`+++     `" remains in your `INCON` block, remove it and the following line (but keep blank line after it). This is information from the previous simulation used to track time (e.g., absolute time reached and total number of time steps). Here the previous run was performed to establish steady-state conditions ending at t=0, so the continuation info is not needed.

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D.2 Radionuclide Source

- The third and fourth primary variables (X3 and X4) are the mass fractions of Rn1 and Rn2. Simulate an instantaneous release of ^{241}Am by specifying X3 = 1.0e-3

Q-D.2.1: How could this be made a constant source rather than instantaneous? (Hint: a change in the `ELEM` block would be required)

```
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
...
AO1 1           0.17001265E+00
 0.641066843096E+07 0.999999999942E-03 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
AP1 1           0.17001296E+00
 0.641164840218E+07 0.100000000028E-02 1.000000000000E-03 0.000000000000E+00
 0.250000000000E+02
AQ1 1           0.17001326E+00
 0.641262837383E+07 0.100000000024E-02 0.000000000000E+00 0.000000000000E+00
 0.250000000000E+02
...
```

Figure 8. Specifying release of Rn1 in INCON block.

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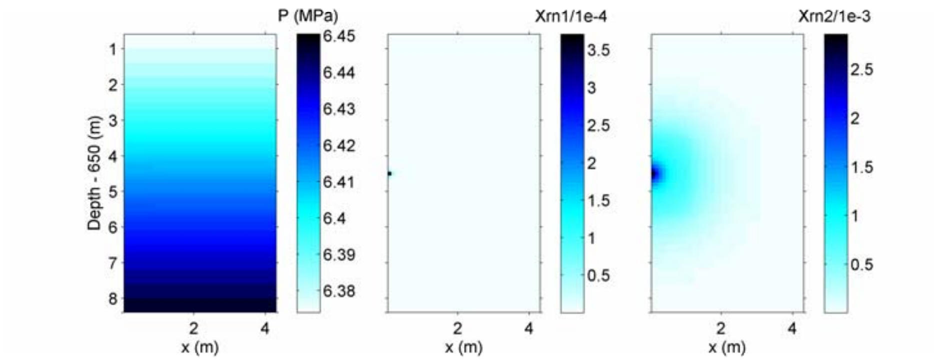

Figure 8. Distribution of pressure and mass fractions of Rn1 and Rn2, respectively, at t = 500 years without vertical flow.

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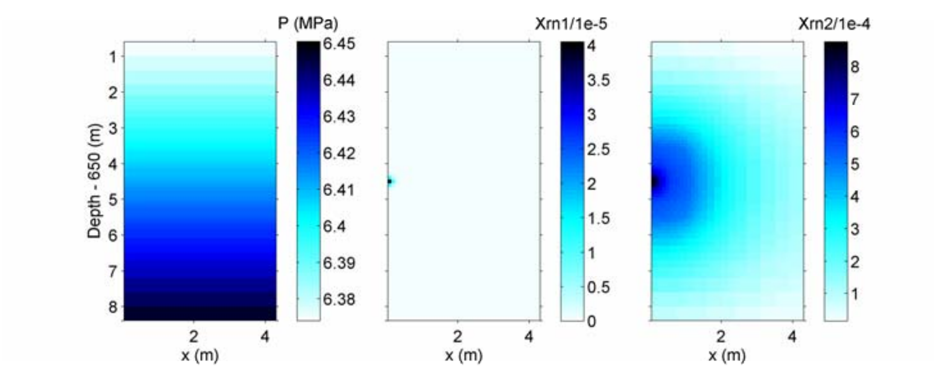

Figure 9. Distribution of pressure and mass fractions of Rn1 and Rn2, respectively, at t = 2000 years without vertical flow.

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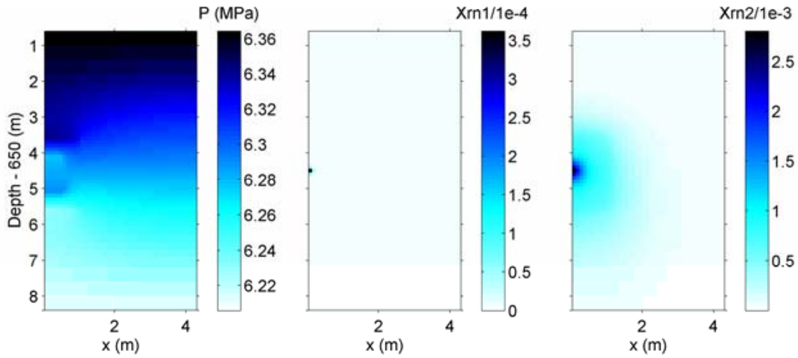

Figure 10. Distribution of pressure and mass fractions of Rn1 and Rn2, respectively, at t = 500 years for case of vertical flow.

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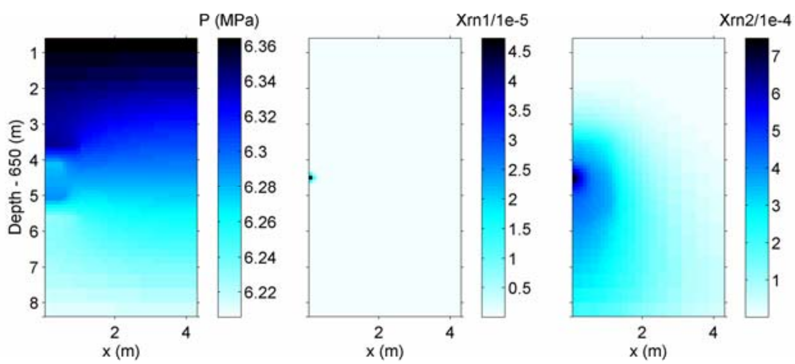

Figure 11. Distribution of pressure and mass fractions of Rn1 and Rn2, respectively, at t = 2000 years for case of vertical flow.

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Part E: Radionuclide Case 2

A corrosion process is considered in this problem in which gas containing carbon 14 (^{14}C) is generated from the waste packet along with heat, and subsequent decay into nitrogen gas occurs. Pressure build-up within the waste package is examined, along with potential effects on transport of a fracture in the bentonite.

- Carbon 14 (^{14}C)
  - Unstable isotope of carbon ($t_{1/2}$ = 5730 years or 1.8e11 sec)
  - Contained in activated metals from nuclear reactor components that corrode in the subsurface (slowly releasing ^{14}C)
  - K_d = 5.0e-4 and K_H^{-1} = 1E-8 Pa^{-1}
- Nitrogen 14 (^{14}N) is the daughter product
  - Non-radioactive ($t_{1/2}$ is infinite)
  - K_d = 5.0e-4 (assumed) and K_H^{-1} = 1E-10 Pa^{-1}

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➢ Open file *SimRad2.txt*

➢ Modify the `MULTI` block to allow for gas phase and heat to be included in the simulations (NK=5 and NEQ=6).

Q-E.1: The initial conditions were already generated for this simulation. Explain the main difference between the initial conditions in this file (look in `INCON` block) and those generated for the hydrostatic conditions in section Part C.1 (look at file *SAVE_SimInit*).

Q-E.2: Based on the `INCON` block, what is the initial gas saturation in the system?

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```
*RADIONUCLIDE TRANSPORT PROBLEM*
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
CLAY     2     2650.       .12  1.00E-17  1.00E-17  1.00E-17       2.5     905.5
   1.83e-9   3.47e-5              1.                5.00e-04  5.00E-04
    7             0.4       0.5       1.0       0.05
    7             0.4       0.5    5.6e-7                1.0
CONTA    2     2650.       .17  1.00E-17  1.00E-17  1.00E-17      52.0     905.5
   1.83e-9   3.47e-5              1.                5.00e-04  5.00E-04
…

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    ?    ?    2    8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3  10     99991              4    5
                  ??     1.0e+3                          9.8
    1.E-04     1.E+0
              6.37E6               1.0e-3                0.0                 0.0
                 0.0                 25.0
SELEC----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6    1   24    2
     -1.e5

     0.e-0     0.e-1
     0.e-9     0.e-9     1.e-5    0.0e-9     0.e-9    1.e-11
    1.8e11        ??     1.e-5    1.0e-9                          ??
    1.0e30        ??     1.e-5    1.0e-9                          ??
…
```

Figure 12. Portion of input file for *SimRad2.txt*.

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```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
AL1 1AIR 1    ?    1              ????    3.0e-10
AM1 1AIR 1    ?    1              ????    3.0e-10
AN1 1AIR 1    ?    1              ????    3.0e-10
AO1 1AIR 1    ?    1              ????    3.0e-10
AP1 1AIR 1    ?    1              ????    3.0e-10
AQ1 1AIR 1    ?    1              ????    3.0e-10
AR1 1AIR 1    ?    1              ????    3.0e-10
AS1 1AIR 1    ?    1              ????    3.0e-10
AT1 1AIR 1    ?    1              ????    3.0e-10
AU1 1AIR 1    ?    1              ????    3.0e-10


INCON -- INITIAL CONDITIONS FOR HYDROSTATIC PROFILE
A21 1           0.12000086E+00
 0.6373919816909E+07 0.9999999999992E-03 0.0000000000000E+00 0.0000000000000E+00
 0.0000000000000E+00 0.2500000000000E+02
A31 1           0.12000172E+00
 0.6377839640616E+07 0.1000000000002E-02 0.0000000000000E+00 0.0000000000000E+00
 0.0000000000000E+00 0.2500000000000E+02
A41 1           0.12000258E+00
 0.6381759471120E+07 0.9999999999907E-03 0.0000000000000E+00 0.0000000000000E+00
 0.0000000000000E+00 0.2500000000000E+02
A51 1           0.12000344E+00
 0.6385679308422E+07 0.9999999999967E-03 0.0000000000000E+00 0.0000000000000E+00
 0.0000000000000E+00 0.2500000000000E+02
A61 1           0.12000409E+00
…
```

Figure 12 (continued). Portion of input file for *SimRad2.txt*.

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E.1 Radionuclide properties

- Specify the inverse Henry's constant values and the molecular weights of the radionuclides in the `SELEC` block.
- Check that the K_d values are in the `ROCKS` block are correct.

E.2 Generation of air

To specify the total rate for a source of air or any other component (^{14}C or heat) in the waste container, the amount injected in each grid block must be calculated accordingly. Since there are 10 x 10 grid blocks making up the waster container (though only half are modeled, due to symmetry), the rate for each grid block is calculated by dividing the total rate for the waste container by 100.

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The first line of the `GENER` block begins with element "AL1 1", followed by the source name ("AIR 1") and the parameter NSEQ (currently "?"). NSEQ is the number of additional sources that will be created by adding a number (NADD) to the element name. For example, to specify additional sources for elements AL1 2, and AL1 3, then NSEQ would be 2 and NADD would be 1.

- Make NSEQ = 4 for each of the lines in the `GENER` block since there are 4 additional columns of elements that belong to the waste container material (CONTA).
- The parameter TYPE is currently given with "????". Look on p. 174-175 of the manual for a description of the different types of sources (or sinks). To inject air, make the value of TYPE equal to COM5 (air is the fifth component or primary variable).
- Inject a total of 3.0E-8 kg/s in the waster canister. That is, check that 3.0E-10 kg/s is specified for each source.

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- Save the file and run code.
- The code should have stopped after MCYC=20 iterations, but print-out should be available in multiples of MCYPR=10 (i.e., after 10 and 20 iterations). Open the main output file (*SimRad2.out*) and scroll down to the first occurrence of "OUTPUT DATA".

Q-E.2.1: Has the gas phase evolved in any elements by this time? Explain why this is the case.

Q-E.2.2: Scroll down to the next occurrence of "OUTPUT DATA" and verify that the gas phase has formed in the waste canister. Now open the SAVE file and explain how one can tell which elements contain the gas phase.

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E.3 Generation of ^{14}C and heat in waste container

In this step, the `GENER` block will be further modified to initiate injection of ^{14}C (total of 1.0E-11 kg/s) and heat (total of 100 W/m).

Q-E.3.1: What option of parameter TYPE is needed for ^{14}C and for heat? (Hint: which primary variable is ^{14}C?)

- Add two new sets of entries in the `GENER` block for ^{14}C and heat. Copy the information at the bottom of *SimRad2.txt* file and paste it into the `GENER` block under the air sources from the previous step. Fill in the remaining information (find the "?").

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E.4 Simulating pressure build-up inside of bentonite seal

- Increase (MCYC=9999) iterations, and make print-out occur at end of simulation (MCYPR=9999).
- Set maximum simulation time (TIMAX in PARAM.2) to 5.0E8 seconds (~15.8 years).
- Since graphical software is not currently available for you to visualize the output, use the FOFT block to print time-dependent data to a file (also called FOFT) for two elements, "AO1 1" and "AE1 1". These elements are located in the first column in the waste container and in the host rock, respectively.
- Save file as *SimRad2_1.txt* and run code. (May take several minutes to run.) Rename the *SAVE* file as *SAVE_SimRad2_1*.

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Q-E.4.1: Has the gas migrated through the bentonite seal? What is the pressure inside the waste container and is it likely to cause fracturing in reality? (Hint: fracturing is likely when the pressure exceeds the lithostatic pressure, which is approximately two times the hydrostatic pressure.)

Q-E.4.2: What was the total mass of ^{14}C (Rn1) and ^{14}N (Rn2) at the beginning and end of the simulation?

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E.5 Simulating pressure release following "formation" of fracture through bentonite

While the current module of TOUGH2 cannot simulate the formation of fractures, let us assume that the increased pressure observed in the previous step was enough to cause a vertical fracture through the bentonite seal.

- Save the file as *SimRad2_2.txt*
- Go to the `ELEM` block and change parameter MA2, which specifies the material properties, from bentonite (BENTO) to clay (CLAY) for the first column only. This thin column of elements will serve as a fracture through the bentonite allowing a connection to the host rock.
- Copy the initial conditions from *SAVE_SimRad2_1* to the INCON block. This time keep the continuation information following the "+++"

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- Set the total simulation time to 5.01728E8 seconds (~15.8 years + 20 days).
- Save file and run code. (May take several minutes to run.)

Q-E.5.1: Has the pressure decreased inside the waste container?

Q-E.5.2: Has fracture allowed gas to migrate beyond the bentonite seal in this short simulation time?

Figures 13-18 depict distributions of pressure, gas saturation, temperature, and radionuclide mass fractions from SAVE files for various steps performed above. Figures 19-20 show the pressure and radionuclide transport response (from FOFT files) before and after the "fracture" was incorporated into the flow model.

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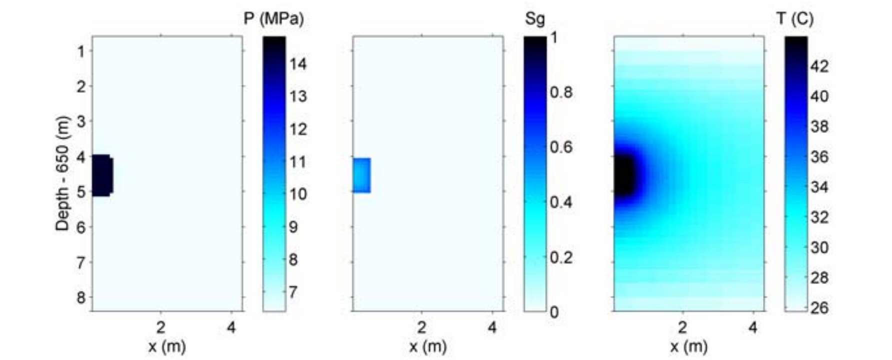

Figure 13. Distribution of pressure (P), gas saturation (Sg) and temperature (T), respectively, at 15.8 years.

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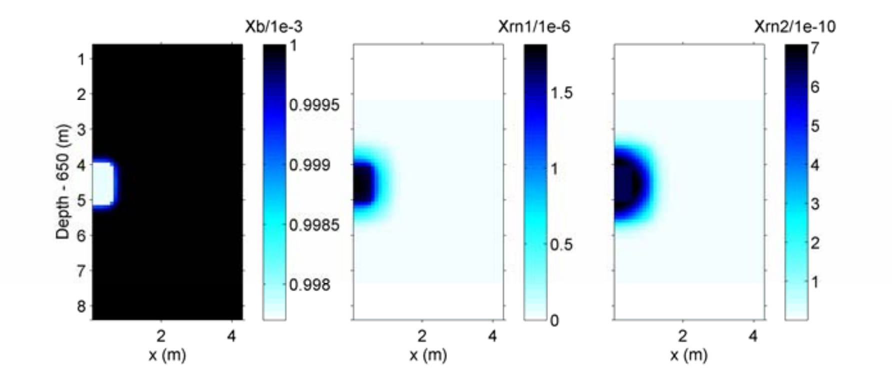

Figure 14. Mass fractions of Brine, Rn1 and Rn2, respectively, at 15.8 years.

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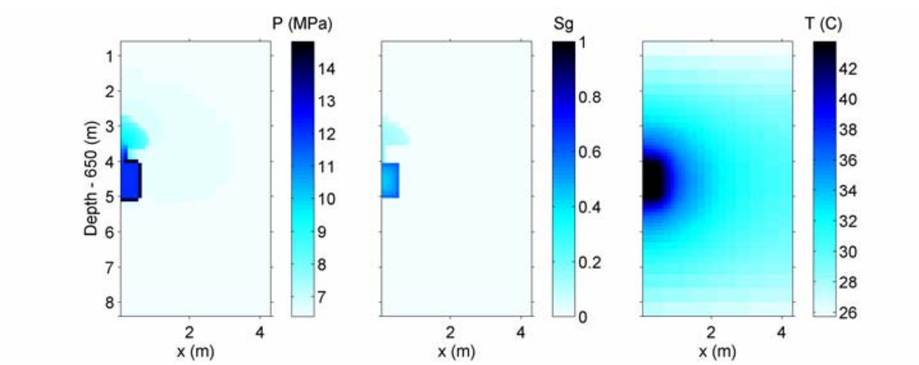

Figure 15. Distribution of pressure (P), gas saturation (Sg) and temperature (T), respectively, at 15.8 years + 20 days.

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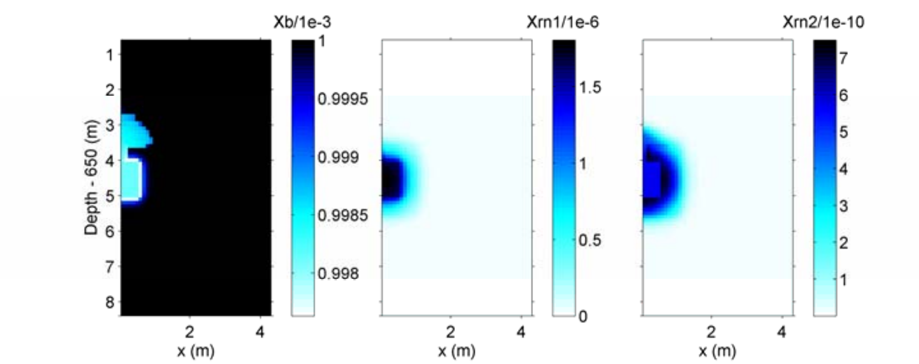

Figure 16. Mass fractions of Brine, Rn1 and Rn2, respectively, at 15.8 years + 20 days.

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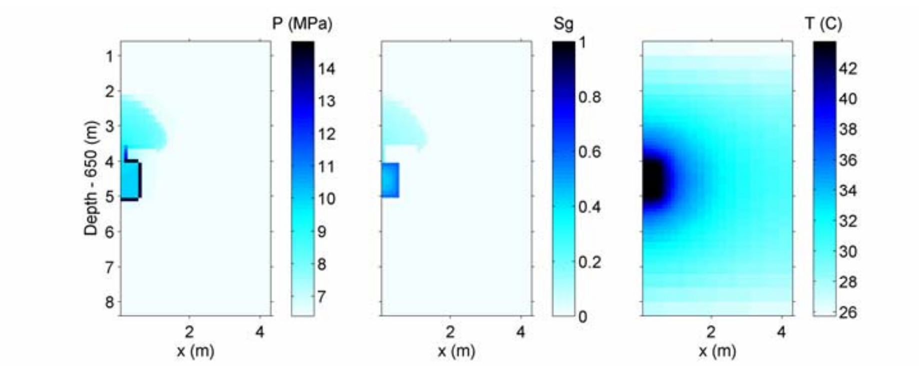

Figure 17. Distribution of pressure (P), gas saturation (Sg) and temperature (T), respectively, at 15.8 years + 50 days.

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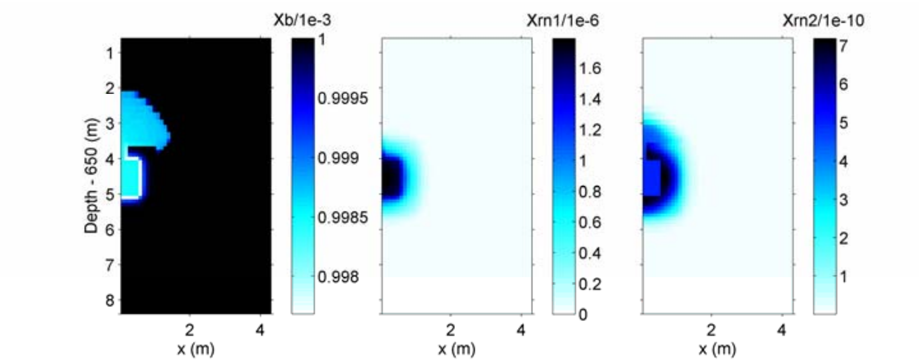

Figure 18. Mass fractions of Brine, Rn1 and Rn2, respectively, at 15.8 years + 50 days.

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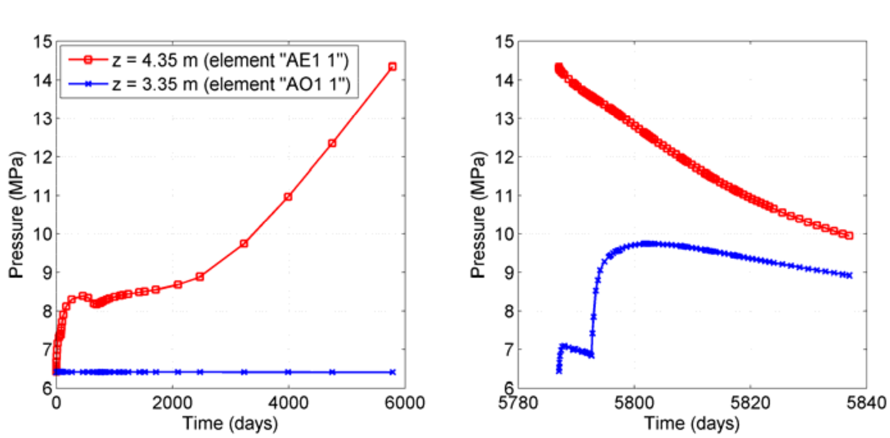

Figure 19. Pressure response before (left) and after (right) fracture is placed in bentonite seal. Element “AE1 1” is in the waste container, while element “AO1 1” is above the bentonite seal in the host rock.

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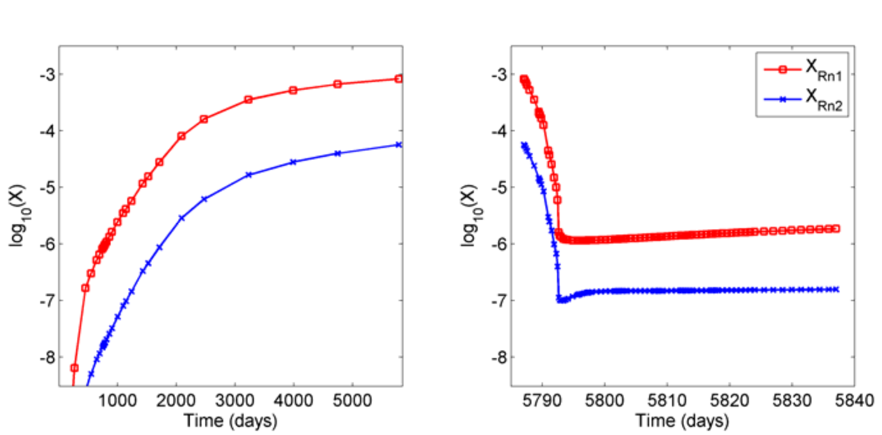

Figure 20. Mass fractions of Rn1 and Rn2 before (left) and after (right) fracture is placed in bentonite seal.

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