Example Problem 6
NAPL infiltration and redistribution in a 2-D aquifer system

Abstract: *The first objective of this two-part example is to investigate the effects of fluid density and viscosity on the movement of NAPLs after a spill in a partly saturated, hypothetical, aquifer. The user will investigate the effects of NAPL fluid properties on infiltration and redistribution. The objective of the second part is to compute steady-state initial conditions through a separate simulation. The Restart file generated by this simulation is used to define the initial conditions for the actual infiltration event. The Water-Oil mode (STOMP-WO) is used for this application.*

6.1 Problem Description

Part 1.

A known amount of LNAPL, with a density of 800 kg/m^3 and a viscosity of 0.002 Pa s, is injected into a hypothetical two-dimensional aquifer. The input file of this problem is shown in section 6.3.1. The simulation domain is 50-m long and 10-m high. A total of 25 and 20 uniform nodes are used in the x- and z-direction, respectively. The water table is at approximately 6 m from the surface. The NAPL is injected with a rate of 0.25 m/day at the top of node (13,1,20) for a period of 10 days. After the infiltration period, the NAPL is allowed to redistribute for 190 days. The total simulation time is 200 days.

Part 2

This problem differs from the problem in Part 1 in that the steady-state initial conditions prior to the NAPL infiltration can not be specified in the Initial Conditions Card because precipitation (100 ml/year) is included. When more complex initial conditions are required, a separate run has to be completed that yields a *restart* file that contains the proper initial conditions. The input file for the simulation computing the steady-state initial conditions is shown in section

6.3.2. The input file shown in 6.3.3 uses the restart file created with the input file shown in section 6.3.2.

6.2 Exercises

Part 1.

1. Run the problem outlined in section 6.3.1. Make a plot of the LNAPL saturation distribution at t = 10 and t = 200 days. Check the surface file and see if the proper amount of NAPL has entered the system.
2. Increase the density of the NAPL to 1200 kg/m^3 and run the simulation. Make plots at t = 10 and 200 days and compare results with plots made in Exercise 1
3. Increase the viscosity of the NAPL to 0.02 Pa s, while keeping the NAPL density at 1200 kg/m^3. Run the simulation and make plots at t = 10 and 200 days. Compare results with plots made in Exercises 1 and 2. Change the viscosity and the density back to the original values.
4. Instead of using a Neumann boundary condition to allow NAPL into the domain, use an equivalent source at node (13,1,20). Run the simulation and compare results.

Part 2.

5. Run the problem outlined in section 6.3.2. This simulation yields a *restart.x* file. Rename the *restart.x* file to *restart*. Check the output file or the screen and verify that the vertical aqueous flux is approximately 100 mm/year throughout the unsaturated domain. Compare the initial and steady-state aqueous saturations.

6. Run the problem in section 6.3.3. Comment on the differences between this input file and the file shown in section 6.3.1. Run the simulation and make plots at t = 10 and 200 days. Compare results with plots made in Exercise 1.

7. Change the horizontal gradient on the water table from -40 Pa/m to -70 Pa/m. Make sure to change the necessary boundary conditions and initial conditions on both of the input files used in this simulation! Run the simulation and make plots at t = 10 and 200 days. Compare results with the plots made in Exercise 6.
8. In this problem, the Neumann boundary is used for the aqueous phase at the top boundary. A hydraulic gradient boundary conditions is used at the west and east boundary. Explain why these two boundaries are, in principle, not compatible. Provide two methods that correct the compatibility problem.

6.3 Input Files

6.3.1 Input File for Part 1

```
#---------------------------------------------------------
~Simulation Title Card
#---------------------------------------------------------
1,
STOMP Tutorial Problem 6a,
Mart Oostrom/Mark White,
PNNL,
June 03,
15:00,
1,
Simulation of NAPL spills in 2D domain,

#---------------------------------------------------------
~Solution Control Card
#---------------------------------------------------------
Normal,
Water-Oil,
2,
0,s,10,d,1,s,1,d,1.25,8,1.e-6,
10,d,200,d,1,s,10,d,1.25,8,1.e-6,
10000,
Variable Aqueous Diffusion,
,

#---------------------------------------------------------
~Grid Card
#---------------------------------------------------------
Uniform Cartesian,
25,1,20,
2,m,
1,m,
0.5,m,

#---------------------------------------------------------
```

```
~Rock/Soil Zonation Card
#----------------------------------------------------------
1,
Sand,1,25,1,1,1,20,

#----------------------------------------------------------
~Mechanical Properties Card
#----------------------------------------------------------
Sand,2650,kg/m^3,0.43,0.43,,,Millington and Quirk,

#----------------------------------------------------------
~Hydraulic Properties Card
#----------------------------------------------------------
Sand,10,hc m/day,,,10,hc m/day,

#----------------------------------------------------------
~Saturation Function Card
#----------------------------------------------------------
72.0,dynes/cm,,,32,dynes/cm,
Sand,Van Genuchten,0.1,1/cm,2.0,0.10,72.0,dynes/cm,,

#----------------------------------------------------------
~Aqueous Relative Permeability Card
#----------------------------------------------------------
Sand,Mualem,,

#----------------------------------------------------------
~NAPL Relative Permeability Card
#----------------------------------------------------------
Sand,Mualem,,

#----------------------------------------------------------
~Oil Properties Card
#----------------------------------------------------------
NAPL,
165.834,g/mol,251.,K,394.4,K,620.2,K,
47.6,bar,289.6,cm^3/mol,0.2758,0.2515,0.0,debyes,
-1.431e+1,5.506e-1,-4.513e-4,1.429e-7,
Equation 1,-7.36067,1.82732,-3.47735,-1.00033,
Constant,800.0,kg/m^3,
Constant,0.002,Pa s,
1.0e8,Pa,

#----------------------------------------------------------
~Initial Conditions Card
#----------------------------------------------------------
2,
Aqueous Pressure,140000,Pa,0.0,1/m,,,-9793.5192,1/m,1,25,1,1,1,20,
NAPL Pressure,-1.e9,Pa,,,,,,,1,25,1,1,1,20,

#----------------------------------------------------------
~Boundary Conditions Card
#----------------------------------------------------------
3,
top,zero flux,neumann,
13,13,1,1,20,20,2,
0,d,-1.e9,Pa,0.0,-0.25,m/day,
10.0,d,-1.e9,Pa,0.0,-0.25,m/day,
```

```
west,hydraulic gradient,dirichlet,
1,1,1,1,1,20,1,
0,d,140000,Pa,0.0,-1.e9,Pa,
east,hydraulic gradient,dirichlet,
25,25,1,1,1,20,1,
0,d,140000,Pa,0.0,-1.e9,Pa,

#-----------------------------------------------------------
~Output Options Card
#-----------------------------------------------------------
9,
13,1,20,
13,1,15,
13,1,10,
13,1,8,
13,1,6,
13,1,4,
1,1,7,
1,1,6,
1,1,4,
1,1,day,m,6,6,6,
2,
napl saturation,,
aqueous saturation,,
2,
10,d,
100,d,
3,
no restart,,
napl saturation,,
aqueous saturation,,

#-----------------------------------------------------------
~Surface Flux Card
#-----------------------------------------------------------
3,
NAPL volumetric flux,m^3/day,m^3,top,13,13,1,1,20,20,
NAPL volumetric flux,m^3/day,m^3,west,1,1,1,1,1,20,
NAPL volumetric flux,m^3/day,m^3,east,25,25,1,1,1,20,
```

6.3.2 Input File Part 2 (steady-state run).

```
#-------------------------------------------------------------------
~Simulation Title Card
#-------------------------------------------------------------------
1,
STOMP Tutorial Problem 6b (steady-state calculations),
Mart Oostrom/Mark White,
PNNL,
June 03,
15:00,
2,
Steady state calculations to set up flow field,
Restart file will be used for subsequential NAPL infiltration simulation,

#-------------------------------------------------------------------
~Solution Control Card
#-------------------------------------------------------------------
Normal,
Water-Oil,
1,
0,s,1000,yr,1,d,1000,yr,1.25,8,1.e-6,
10000,
Variable Aqueous Diffusion,
,

#-------------------------------------------------------------------
~Grid Card
#-------------------------------------------------------------------
Uniform Cartesian,
25,1,20,
2,m,
1,m,
0.5,m,

#-------------------------------------------------------------------
~Rock/Soil Zonation Card
#-------------------------------------------------------------------
1,
Sand,1,25,1,1,1,20,

#-------------------------------------------------------------------
~Mechanical Properties Card
#-------------------------------------------------------------------
Sand,2650,kg/m^3,0.43,0.43,,,Millington and Quirk,

#-------------------------------------------------------------------
~Hydraulic Properties Card
#-------------------------------------------------------------------
Sand,10,hc m/day,,,10,hc m/day,

#-------------------------------------------------------------------
~Saturation Function Card
#-------------------------------------------------------------------
72.0,dynes/cm,,,32,dynes/cm,
Sand,Van Genuchten,0.1,1/cm,2.0,0.10,72.0,dynes/cm,,

#-------------------------------------------------------------------
```

```
~Aqueous Relative Permeability Card
#-------------------------------------------------------------------
Sand,Mualem,,

#-------------------------------------------------------------------
~NAPL Relative Permeability Card
#-------------------------------------------------------------------
Sand,Mualem,,

#-------------------------------------------------------------------
~Oil Properties Card
#-------------------------------------------------------------------
NAPL,
165.834,g/mol,251.,K,394.4,K,620.2,K,
47.6,bar,289.6,cm^3/mol,0.2758,0.2515,0.0,debyes,
-1.431e+1,5.506e-1,-4.513e-4,1.429e-7,
Equation 1,-7.36067,1.82732,-3.47735,-1.00033,
Constant,800.0,kg/m^3,
Constant,0.002,Pa s,
1.0e8,Pa,

#-------------------------------------------------------------------
~Initial Conditions Card
#-------------------------------------------------------------------
2,
Aqueous Pressure,140000,Pa,-40.0,1/m,,,-9793.5192,1/m,1,25,1,1,1,20,
NAPL Pressure,-1.e9,Pa,,,,,,,1,25,1,1,1,20,

#-------------------------------------------------------------------
~Boundary Conditions Card
#-------------------------------------------------------------------
3,
top,neumann,zero flux,
1,25,1,1,20,20,1,
0,d,-100.0,mm/year,0.0,-1.e9,Pa,
west,hydraulic gradient,dirichlet,
1,1,1,1,1,10,1,
0,d,140040,Pa,0.0,-1.e9,Pa,
east,hydraulic gradient,dirichlet,
25,25,1,1,1,10,1,
0,d,138040,Pa,0.0,-1.e9,Pa,

#-------------------------------------------------------------------
~Output Options Card
#-------------------------------------------------------------------
9,
1,1,20,
25,1,20,
13,1,20,
13,1,18,
13,1,16,
13,1,14,
13,1,12,
13,1,10,
13,1,8,
1,1,yr,m,6,6,6,
3,
napl saturation,,
```

```
aqueous saturation,,
z aqueous volumetric flux,mm/year,
0,
2,
aqueous saturation,,
z aqueous volumetric flux,mm/year,
```

6.3.3 Input File Part 2 (NAPL Infiltration).

```
#---------------------------------------------------
~Simulation Title Card
#---------------------------------------------------
1,
STOMP Tutorial Problem 6b (NAPL Infiltration),
Mart Oostrom/Mark White,
PNNL,
June 03,
15:00,
2,
Simulation of NAPL spill in 2D domain,
Simulation starts with Restart file,

#---------------------------------------------------
~Solution Control Card
#---------------------------------------------------
Restart,
Water-Oil,
2,
0,s,10,d,1,s,1,d,1.25,8,1.e-6,
10,d,200,d,1,s,10,d,1.25,8,1.e-6,
10000,
Variable Aqueous Diffusion,
,

#---------------------------------------------------
~Grid Card
#---------------------------------------------------
Uniform Cartesian,
25,1,20,
2,m,
1,m,
0.5,m,

#---------------------------------------------------
~Rock/Soil Zonation Card
#---------------------------------------------------
1,
Sand,1,25,1,1,1,20,

#---------------------------------------------------
~Mechanical Properties Card
#---------------------------------------------------
Sand,2650,kg/m^3,0.43,0.43,,,Millington and Quirk,

#---------------------------------------------------
~Hydraulic Properties Card
#---------------------------------------------------
```

```
Sand,10,hc m/day,,,10,hc m/day,

#--------------------------------------------------
~Saturation Function Card
#--------------------------------------------------
72.0,dynes/cm,,,32,dynes/cm,
Sand,Van Genuchten,0.1,1/cm,2.0,0.10,72.0,dynes/cm,,

#--------------------------------------------------
~Aqueous Relative Permeability Card
#--------------------------------------------------
Sand,Mualem,,

#--------------------------------------------------
~NAPL Relative Permeability Card
#--------------------------------------------------
Sand,Mualem,,

#--------------------------------------------------
~Oil Properties Card
#--------------------------------------------------
NAPL,
165.834,g/mol,251.,K,394.4,K,620.2,K,
47.6,bar,289.6,cm^3/mol,0.2758,0.2515,0.0,debyes,
-1.431e+1,5.506e-1,-4.513e-4,1.429e-7,
Equation 1,-7.36067,1.82732,-3.47735,-1.00033,
Constant,800.0,kg/m^3,
Constant,0.002,Pa s,
1.0e8,Pa,

#--------------------------------------------------
~Initial Conditions Card
#--------------------------------------------------
0,

#--------------------------------------------------
~Boundary Conditions Card
#--------------------------------------------------
5,
top,neumann,neumann,
13,13,1,1,20,20,4,
0,d,-100,mm/year,0.0,-0.25,m/day,
10.0,d,-100,mm/year,0.0,-0.25,m/day,
10.0,d,-100,mm/year,0.0,0.,m/day,
100.0,d,-100,mm/year,0.0,0.,m/day,
top,neumann,zero flux,
1,12,1,1,20,20,1,
0,d,-100.0,mm/year,0.0,-1.e9,Pa,
top,neumann,zero flux,
14,25,1,1,20,20,1,
0,d,-100.0,mm/year,0.0,-1.e9,Pa,
west,hydraulic gradient,dirichlet,
1,1,1,1,1,10,1,
0,d,140040,Pa,0.0,-1.e9,Pa,
east,hydraulic gradient,dirichlet,
25,25,1,1,1,10,1,
0,d,138040,Pa,0.0,-1.e9,Pa,
```

```
#----------------------------------------------------
~Output Options Card
#----------------------------------------------------
9,
13,1,20,
13,1,15,
13,1,10,
13,1,8,
13,1,6,
13,1,4,
1,1,20,
1,1,15,
1,1,10,
1,1,day,m,6,6,6,
3,
napl saturation,,
aqueous saturation,,
z aqueous volumetric flux,mm/year,
2,
10,d,
100,d,
3,
no restart,,
napl saturation,,
aqueous saturation,,

#----------------------------------------------------
~Surface Flux Card
#----------------------------------------------------
3,
NAPL volumetric flux,m^3/day,m^3,top,13,13,1,1,20,20,
NAPL volumetric flux,m^3/day,m^3,west,1,1,1,1,1,20,
NAPL volumetric flux,m^3/day,m^3,east,25,25,1,1,1,20,
```

6.4 Solutions to Selected Exercises

Part 1, Exercise 1

Figure 6.1 shows the NAPL distribution at the end of the 10-day infiltration period. Through capillary action, the NAPL spreads laterally in the unsaturated zone. The lower part of the NAPL bottom has reached the capillary fringe. The angular shape of the NAPL body is a direct result of the rather coarse discretization. The plots can be improved by using a smaller grid. Figure 6.2 shows the NAPL saturations at t = 200 days. At this point in time, the NAPL had 190 days for redistribution after the source injection stopped. Most of the NAPL in the vadose zone has drained. Since the NAPL is lighter than water, the NAPL tends to spread above the capillary fringe.

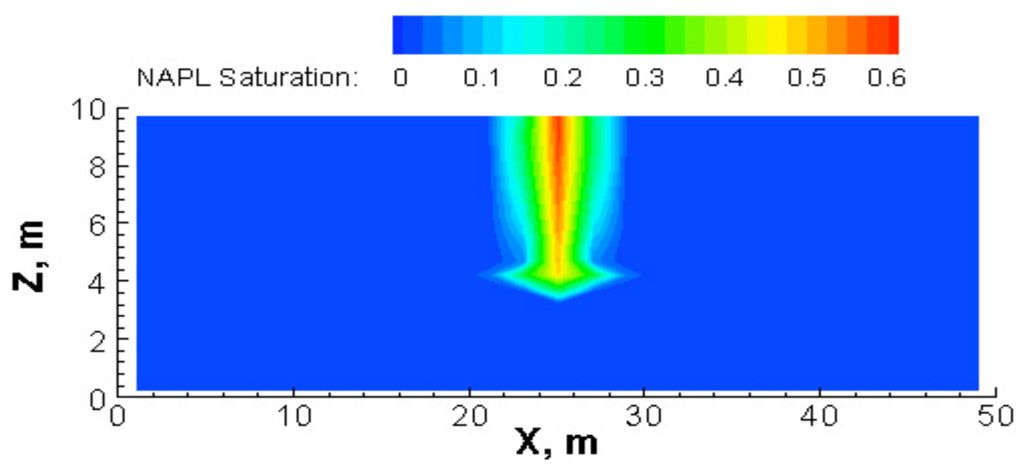

Figure 6.1 LNAPL spill distribution in 2-dimensional aquifer after 10 days.

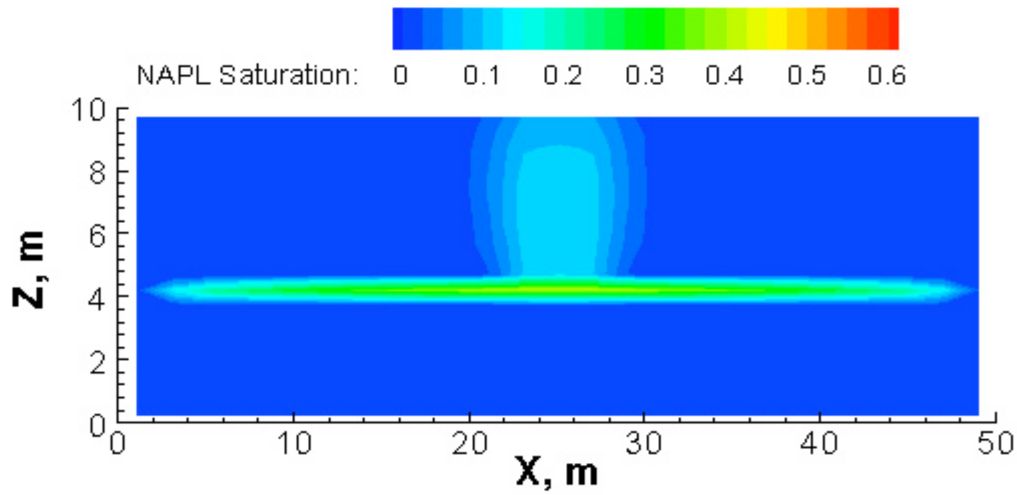

Figure 6.2 LNAPL spill distribution in 2-dimensional aquifer after 200 days.

Part 2, Exercise 2

The NAPL in this problem is a dense NAPL (DNAPL). As a result, the fluid will move below the water table, as is shown in Figures 6.3 and 6.4. After 200 days, most of the DNAPL is located on top of the bottom boundary.

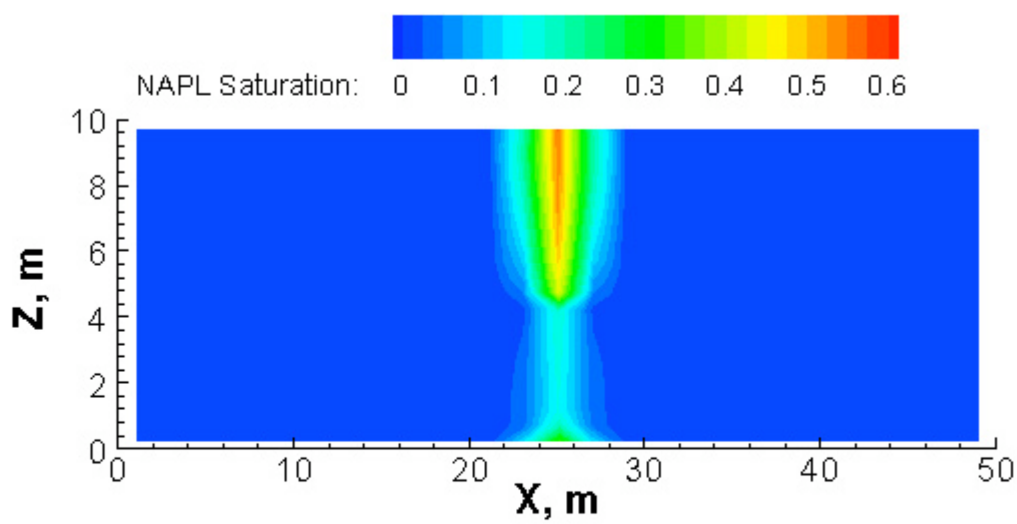

Figure 6.3 DNAPL spill distribution in 2-dimensional aquifer after 10 days.

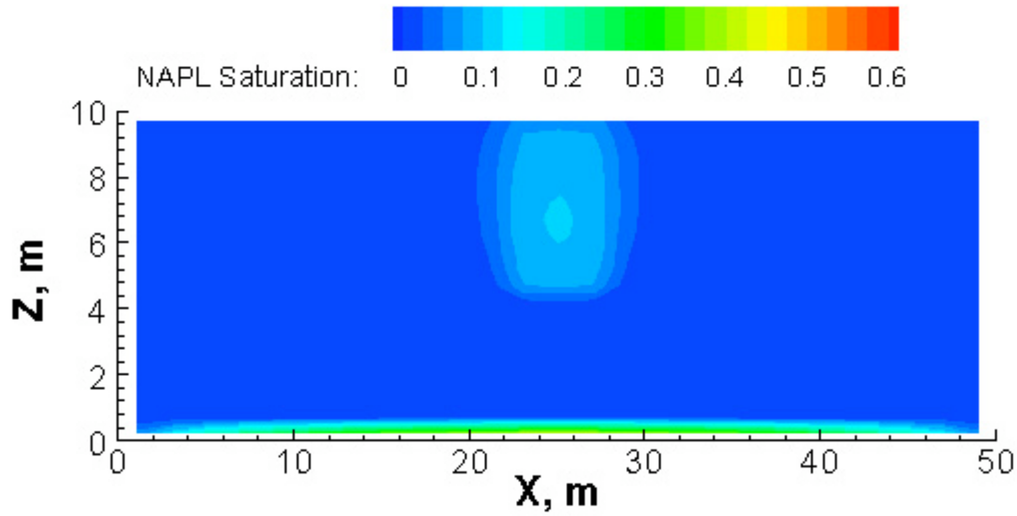

Figure 6.4 LNAPL spill distribution in 2-dimensional aquifer after 200 days.

Part 1, Exercise 3

An increase in the viscosity slows down the movement of the DNAPL. After 10 days, the DNAPL has not yet reached the water table (Figure 6.5). After 200 days, the DNAPL has migrated to the lower parts of the domain, below the water table (Figure 6.6). The lateral spreading is less than shown in Figure 6.4.

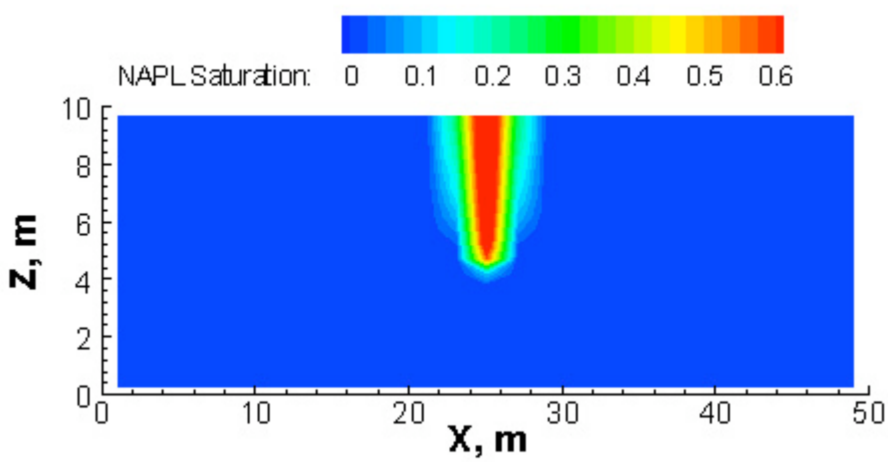

Figure 6.5 LNAPL spill distribution in 2-dimensional aquifer after 10 days.

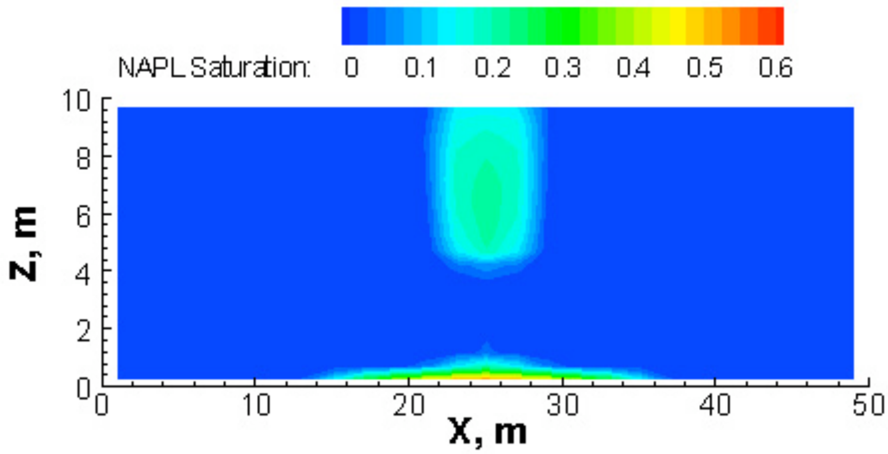

Figure 6.6 LNAPL spill distribution in 2-dimensional aquifer after 200 days.

Part1, Exercise 4

To use a source instead of a boundary condition to introduce the NAPL into the domain use the following source card

```
#-------------------------------------------------------------
~Source Card
#-------------------------------------------------------------
1,
NAPL Volumetric,13,13,1,1,20,20,2,
0,d,.5,m^3/d,
10,d,.5,m^3/d,
```

(You will also have to change the LSTM parameter in the parameters file and the boundary conditions!)

Part 2, Exercise 6

The effects of the imposed gradients on LNAPL movement are not yet visible in Figure 6.7. However, as soon as the LNAPL moves below the water table, the LNAPL body is forced to move laterally. The lateral movement in the eastern direction is clearly visible in Figure 6.8.

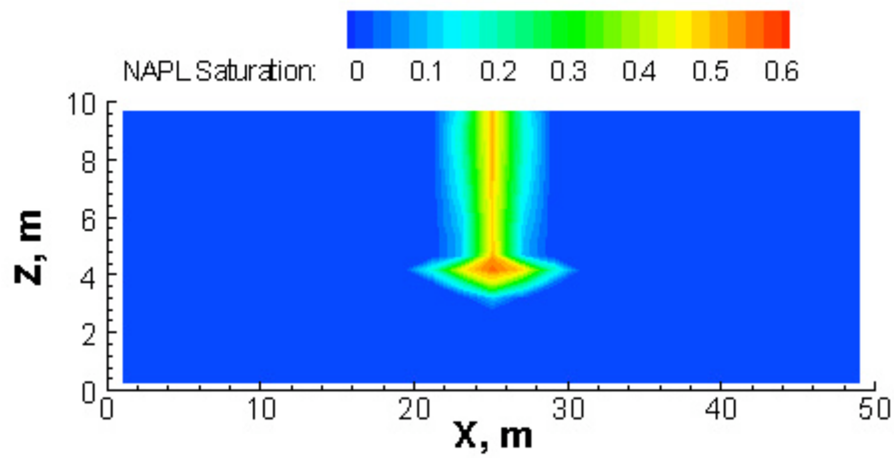

Figure 6.7 LNAPL spill distribution in 2-dimensional aquifer after 10 days. The simulation included 100ml/year precipitation and a horizontal pressure gradient of 40 Pa/m.

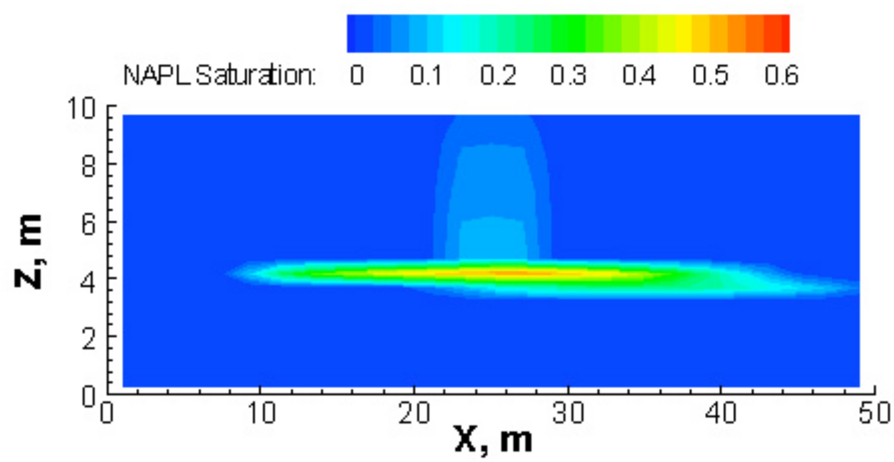

Figure 6.8 LNAPL spill distribution in 2-dimensional aquifer after 200 days. The simulation included 100ml/year precipitation and a horizontal pressure gradient of 40 Pa/m.

Part2, Exercise 7

The effects of the hydraulic gradient are clearly visible in Figures 6.9 and 6.10. The LNAPL is forced to move towards the East boundary of the domain. The movement is considerably faster than for the previous case where the gradient was 40 Pa/m.

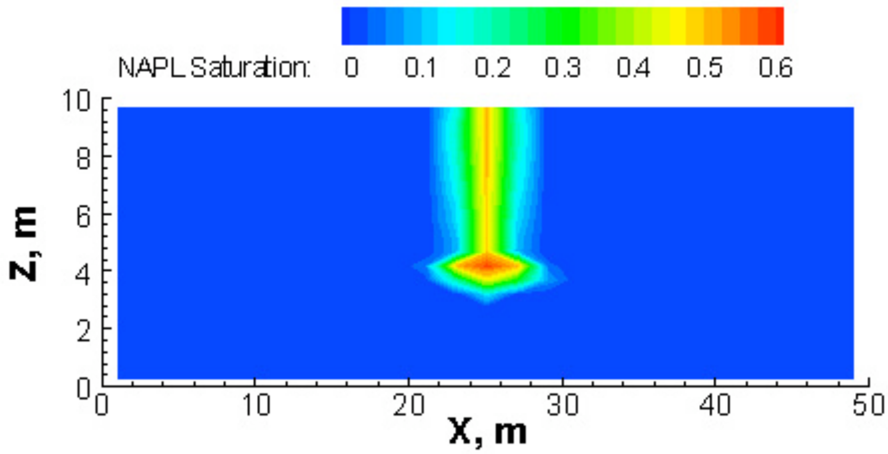

Figure 6.9 LNAPL spill distribution in 2-dimensional aquifer after 10 days. The simulation included 100ml/year precipitation and a horizontal pressure gradient of 70 Pa/m.

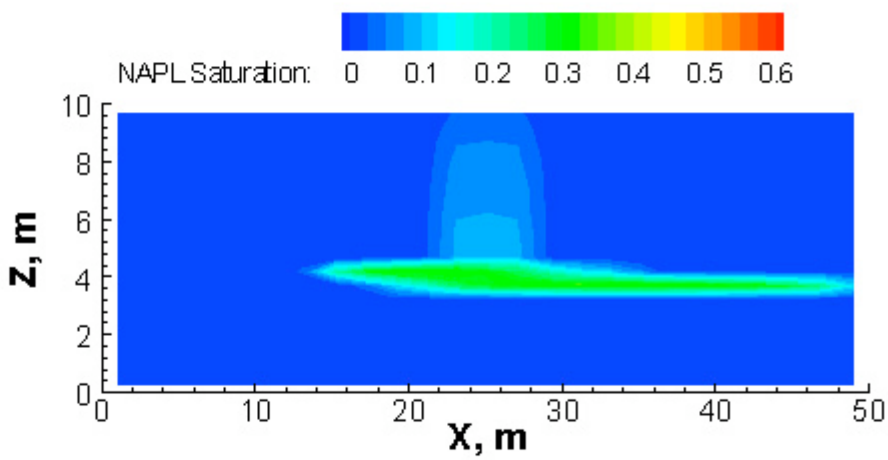

Figure 6.10 LNAPL spill distribution in 2-dimensional aquifer after 200 days. The simulation included 100ml/year precipitation and a horizontal pressure gradient of 70 Pa/m.