STOMP Short Course

June 19-20, 2003

Delft University

<u>Problem 6:</u> NAPL infiltration and redistribution in a 2D 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 (STOMP4) is used for this application.*

Problem Description and Input Parameters

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 Appendix A. 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. 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. The final NAPL distribution is shown in Fig. 6.1.

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 Appendix B. The input file shown in Appendix C uses the restart file created with the input file show in Appendix B.

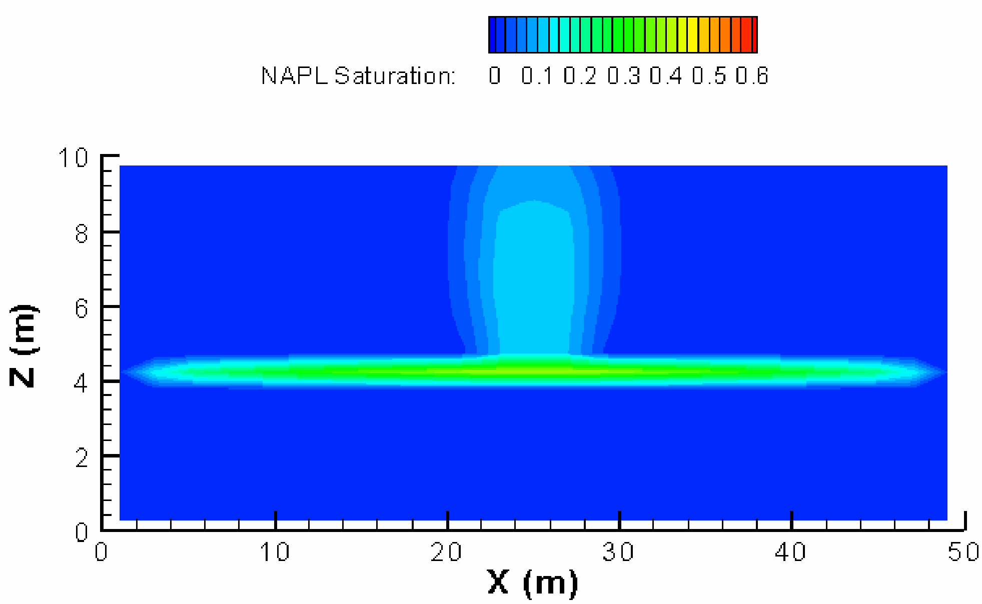

Figure 6.1. LNAPL distribution after 200 days.

Exercises

Part 1.

1. Run the problem outlined in Appendix A using the stomp4_bd.x executable. Make 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 Exer. 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 Exer. 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.

1. Run the problem outlined in Appendix B using stomp4_bd.x. 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.

2. Run the problem in Appendix C using stomp4_bd.x. Comment on the differences between this input file and the file shown in Appendix A. Run the simulation and make plots at t = 10 and 200 days. Compare results with plots made in Part 1, Exer. 1.

3. Change the horizontal gradient on the water table from -40 Pa/m to -70 Pa/m. Be 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 Exer. 6.

Appendix A

```
#-------------------------------------------------------
~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,
```

Appendix B

```
#-------------------------------------------------------------------
~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,
```

Appendix C

```
#---------------------------------------------------
~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,
```