STOMP Short Course

June 19-20, 2003

Delft University

<u>Problem 3:</u> Solute transport in a saturated porous medium

Abstract: *This test case illustrates transport of a solute within a steady state, uniform flow field. An initial square pulse of solute mass is instantaneously introduced into the flow field and transported downstream. The pulse undergoes advection, dispersion and molecular diffusion. The user is introduced to solute transport input file cards, standard and higher order transport options, and the importance of controlling Peclet and Courant numbers.*

Problem Description and Input Parameters

The input file for this problem is presented in Appendix A. The governing equation for advection-dispersion in a saturated porous media is

$$\frac{\partial}{\partial t}(RC) + \frac{\partial}{\partial x_j}(q_j C) - \frac{\partial}{\partial x_i}\left(D_{ij}\frac{\partial C}{\partial x_j}\right) = Q \qquad \text{for } i,j = 1,2,3 \qquad 3.1$$

where C is the time (t) and space dependent (x) solute concentration, R is the retardation factor, q is the Darcy velocity, D is the dispersion tensor, and Q is a sink/source term. In the STOMP simulator, the solute transport equation is solved after the flow field has been computed.

The accuracy of the results obtained from numerical simulation of transport is usually affected by the values of the grid Courant, Cr, and Peclet, Pe, numbers. The Courant number controls the oscillations in the solution arising from the discretization of time derivative, and is defined as

$$Cr = \frac{v \Delta t}{\Delta x} \qquad 3.2$$

where Δt is the size of the time-step and Δx is the grid spacing.
The Peclet number is a measure of the ratio between the advective and the dispersive components of transport, and controls the oscillations in the solution due to the spatial discretization of the domain. The Peclet number is defined as

$$Pe = \frac{v \Delta x}{D} \qquad 3.3$$

The initial value problem discussed here was recommended by the Convection-Diffusion Forum during the VII International Conference on Computational Methods in Water Resources (Baptista et al., 1988), with the purpose of having a common comparison. The following numerical values for the problem dimensions and parameters are those suggested by the Forum. The one-dimensional domain extends from $0 < x < 20000$ m, the pore water velocity is 0.5 m/day, and the initial pulse is located at 1400 m $< x <$ 2600 m. Grid spacing is specified as 200 m, time-steps are 96 days, and total simulation time is 9600 days. An effective dispersion coefficient of 50 m^2/day is used by specifying a dispersivity of 100 m. When solute transport is considered the Solute/Fluid Interaction Card and the Solute/Porous Medium Interaction Card have to included. For this problem, the cards are

```
#-------------------------------------------------------------
~Solute/Fluid Interaction Card
#-------------------------------------------------------------
1,
Tracer,conventional,0.0,m^2/d,continuous,1.0e+12,d,
0,

#-------------------------------------------------------------
~Solute/Porous Media Interaction Card
#-------------------------------------------------------------
Porous Medium,100,m,,m,
Tracer,0.,,
```

Initial and boundary conditions for the solute have to be provided in the Initial Conditions and Boundary Conditions Card, respectively.

An analytical solution given by van Genuchten and Alves (1982) is available for comparison with the simulated results. The analytical solution is modified to account for a translation of the initial pulse in the positive x-axis direction. Assuming the solute to be conservative, and given the initial and boundary conditions

$$
\begin{aligned}
&C(x,0) = 0 && \text{for} && 0 \le x \le 1400 \text{ and } 2600 \le x \\
&C(x,0) = 1 && \text{for} && 1400 \le x \le 2600 \\
&C(0,t) = 0 && \text{for} && t > 0 \\
&\frac{\partial C}{\partial x}(\ \ ,t) = 0 && \text{for} && t > 0
\end{aligned}
\tag{3.4}
$$

the solution to the advection-dispersion equation is

$$
\begin{aligned}
C(x,t) = {} & \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x - x_2 - vt}{(4Dt)^{1/2}}\right) - \operatorname{erfc}\left(\frac{x - x_1 - vt}{(4Dt)^{1/2}}\right)\right] \\
& + \frac{1}{2}\exp\left(\frac{vx}{D}\right)\left[\operatorname{erfc}\left(\frac{x + x_2 + vt}{(4Dt)^{1/2}}\right) - \operatorname{erfc}\left(\frac{x + x_1 + vt}{(4Dt)^{1/2}}\right)\right]
\end{aligned}
\tag{3.5}
$$

As an example, spatial solute concentration distributions for a Peclet number of 20 and various Courant numbers are shown in Fig. 3.1 for the standard Patankar solute transport option and in Fig. 3.2 for the higher order TVD option. The STOMP results are compared with the analytical solution.

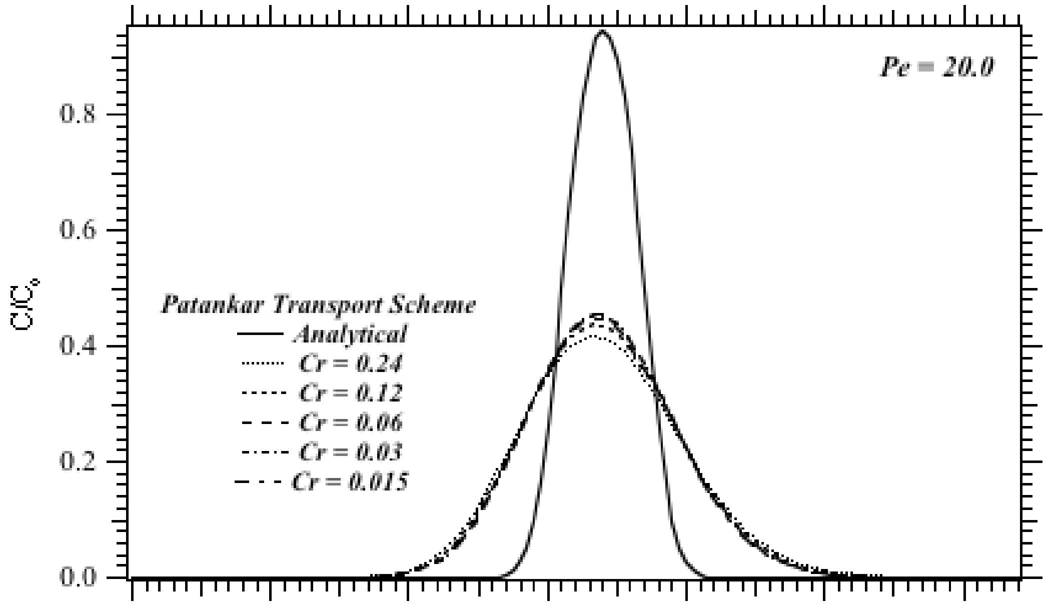

Figure 3.1. Concentration profiles for the analytical and Patankar solution scheme.

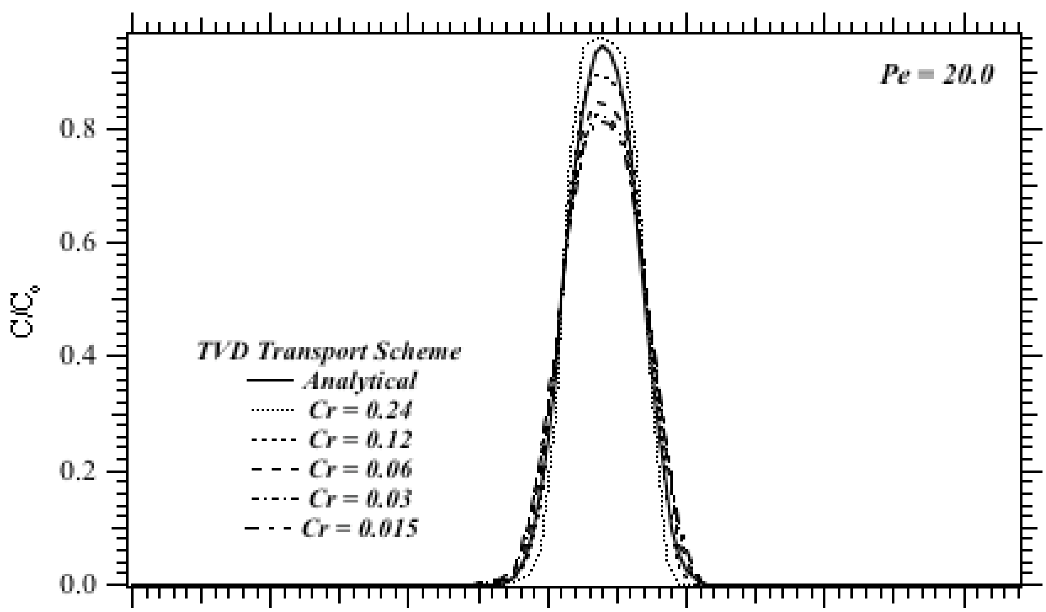

Figure 3.2. Concentration profiles for the analytical and TVD solution scheme.

Exercises

1. Based on the initial location of the solute, the flow rate and the duration of the simulation, determine the location of the peak concentration at the end of the simulation.
2. Compute the Peclet and Courant numbers of the simulation described in the *input* file shown in Appendix A.
3. Show through a calculation why the imposed pressure of 121225 Pa at node 1,1,1,1,1,1, in the Initial Conditions Card is consistent with the -1.0 Pa/m gradient and the Dirichlet boundary condition of 101325 Pa at the east side of the domain.
4. Run the simulation and post process the *plot* file. Make a graph of the solute concentration vs. distance.
5. Repeat the simulation for Peclet numbers of 20 and 50 by manipulating the horizontal dispersivity. Make graphs of the spatial solute concentration distribution.
6. Repeat the simulation for Courant numbers of 0.12 and 0.015 by manipulating the time stepping. Make graphs of the spatial solute concentration distribution.
7. Repeat the simulation for Pe = 20 and Cr = 0.24 using standard Patankar transport. Compare the results with the results obtained with TVD transport. Reset the time step and dispersivity values after completion of the simulation.
8. The retardation coefficient, *R*, for linear retardation is given as

   $R = 1 + \frac{K_d (1 - n_D) \rho_s}{s_l n_D}$ where K_d is the partitioning coefficient (L^3/M), n_d the diffusive porosity, s_l the aqueous saturation and ρ_s the particle density. In the Solute/Porous Media Interaction Card, enter a value for K_d such that *R* equals 2. Run the simulation and compare the results with the base simulation.

9. Edit the Initial Conditions and Boundary Conditions Cards to reflect the following: The Peclet number is 20. Initially, there is no solute present in the entire domain. From t = 0 to t =2400 days, solute is injected with the aqueous phase from the west boundary using a Aqueous Concentration boundary condition for the solute with a concentration of 1.0 $1/m^3$. From t = 2400 to t = 9600 days, the Aqueous Concentration is 0.0 $1/m^3$. Add a plot time at t = 2400 days. Make graphs of the solute distribution at 2400 and 9600 days.

References

Baptista A, P Gresho, and E Adams. 1988. Reference Problems for the Convection-Diffusion Forum. *VII International Conference on Computational Methods in Water Resources*, Cambridge, Massachusetts.

van Genuchten MT, and WJ Alves. 1982. *Analytical Solutions of the One-Dimensional Convective-Dispersive Solute Transport Equation*. ARS Technical Bulletin 1661, USDA.

Appendix A

```
#-------------------------------------------------------------
~Simulation Title Card
#-------------------------------------------------------------
1,
STOMP Tutorial Problem 3,
Mart Oostrom/Mark White,
PNNL,
June 03,
15:00,
2,
Classic test problem for 1D Transport problem,
Water mode (STOMP1) with transport,


#-------------------------------------------------------------
~Solution Control Card
#-------------------------------------------------------------
Normal,
Water w/TVD transport,
1,
0,s,9600,d,96,d,96,d,1.0,8,1.e-6,
10000,
,


#-------------------------------------------------------------
~Grid Card
#-------------------------------------------------------------
Uniform Cartesian,
100,1,1,
200,m,
1,m,
1,m,


#-------------------------------------------------------------
~Rock/Soil Zonation Card
#-------------------------------------------------------------
1,
Porous Medium,1,100,1,1,1,1,


#-------------------------------------------------------------
~Mechanical Properties Card
#-------------------------------------------------------------
Porous Medium,,,0.5,0.5,,,Millington and Quirk,


#-------------------------------------------------------------
~Hydraulic Properties Card
#-------------------------------------------------------------
Porous Medium,2448.3743,hc m/day,,,,,
```

```
#-------------------------------------------------------------
~Saturation Function Card
#-------------------------------------------------------------
Porous Medium,van Genuchten,0.015,1/cm,2.0,0.05,,


#-------------------------------------------------------------
~Aqueous Relative Permeability Card
#-------------------------------------------------------------
Porous Medium,Mualem,,


#-------------------------------------------------------------
~Solute/Fluid Interaction Card
#-------------------------------------------------------------
1,
Tracer,conventional,0.0,m^2/d,continuous,1.0e+12,d,
0,


#-------------------------------------------------------------
~Solute/Porous Media Interaction Card
#-------------------------------------------------------------
Porous Medium,100,m,,m,
Tracer,0.,,


#-------------------------------------------------------------
~Initial Conditions Card
#-------------------------------------------------------------
Gas Pressure,Aqueous Pressure,
2,
Aqueous Pressure,121225,Pa,-1.0,1/m,,,,,1,100,1,1,1,1,
Solute Aqueous Volumetric,Tracer,1.0,1/m^3,,,,,,,8,13,1,1,1,1,


#-------------------------------------------------------------
~Boundary Conditions Card
#-------------------------------------------------------------
2,
west,neumann,aqueous conc,
1,1,1,1,1,1,1,
0,s,0.25,m/d,0.0,1/m^3,
east,dirichlet,outflow,
100,100,1,1,1,1,1,
0,s,101325,Pa,,,


#-------------------------------------------------------------
~Output Options Card
#-------------------------------------------------------------
7,
8,1,1,
13,1,1,
33,1,1,
34,1,1,
```

```
35,1,1,
36,1,1,
37,1,1,
1,1,d,m,6,6,6,
3,
solute aqueous concentration,tracer,1/m^3,
x aqueous volumetric flux,m/day,
aqueous courant number,,
0,
3,
no restart,,
solute aqueous concentration,tracer,1/m^3,
x aqueous volumetric flux,m/day,
```