Example Problem W-3
Solute Transport in Saturated Porous Media

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

The governing equation for advection-dispersion in saturated porous media is

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

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

$$Cr = \frac{v\Delta t}{\Delta x} \tag{2}$$

where Δt is the size of the time-step and Dx 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, *Pe*, is defined as

$$Pe = \frac{v \Delta x}{D} \tag{3}$$

where *D* is the hydrodynamic dispersion coefficient.

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 be 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

$$
\begin{aligned}
&C(x,0) = 0 && \text{for} \quad 0 \le x \le 1400 \text{ and } 2600 \le x \\
&C(x,0) = 1 && \text{for} \quad 1400 \le x \le 2600 \\
&C(0,t) = 0 && \text{for} \quad t > 0 \\
&\frac{\partial C}{\partial x}(\infty, t) = 0 && \text{for} \quad t > 0
\end{aligned}
\tag{4}
$$

the solution to the advection-dispersion equation is

$$
\begin{aligned}
C(x,t) = {} & \frac{1}{2}\left\{ \operatorname{erfc}\left[\frac{x - x_2 - vt}{(4Dt)^{1/2}}\right] - \operatorname{erfc}\left[\frac{x - x_1 - vt}{(4Dt)^{1/2}}\right]\right\} \\
& + \frac{1}{2}\exp\left(\frac{vx}{D}\right)\left\{ \operatorname{erfc}\left[\frac{x + x_2 + vt}{(4Dt)^{1/2}}\right] - \operatorname{erfc}\left[\frac{x + x_1 + vt}{(4Dt)^{1/2}}\right]\right\}
\end{aligned}
\tag{5}
$$

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.

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.
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.

Input File

```
#-------------------------------------------------------
~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 (STOMP-W) 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,
0,s,0.25,m/d,0.0,1/m^3,
east,dirichlet,outflow,
100,100,1,1,1,1,
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,
```

Solutions to Selected Exercises

Exercise 1

This problem considers an unretarded (unsorbed) solute, therefore, the migration of the center of mass is governed by the pore-water velocity. Initially, the center of mass of the solute is located at an x-direction distance of 2,000 m. A horizontal Darcy velocity of 0.25 m/d with a porosity of 0.5 converts to a pore-water velocity of 0.50 m/d; therefore, after a period of 9,600 d the solute center of mass will have moved 4,800 m and be located at an x-direction distance of 6,800 m.

Exercise 2

The Peclet number is a function of the pore-water velocity, grid dimension, and effective diffusion-dispersion coefficient, according to Eqn. (3)

$$Pe = (0.5\ m/day)(200\ m)/(50\ m^2/day) = 2.0$$

The Courant number is a function of the pore-water velocity, time step, and grid dimension, according to the following expression

$$Cr = (0.5\ m/d)(96\ d)/(200\ m) = 0.24$$

Exercise 3

The pressure at the east boundary surface is specified as atmospheric (101325 Pa). The centroid of node (1,1,1) is located 99.5 node dimensions away from the east boundary surface. Therefore, with a uniform x-direction grid spacing of 200 m, the initial pressure at node (1,1,1) is calculated as

$$(99.5\ nodes)(200\ m/nodes)(1\ Pa/m) + 101325\ Pa = 121225\ Pa$$

Exercise 4

The resulting plot is shown in Figure 1.

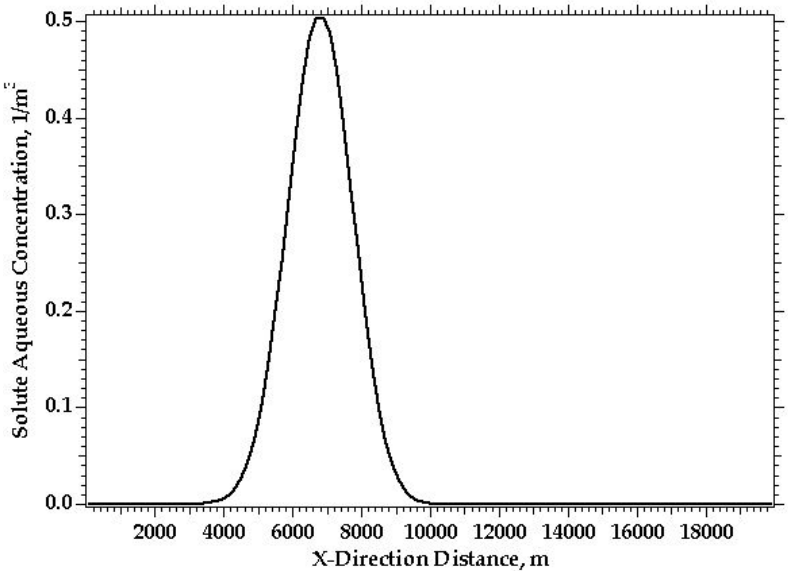

Figure 1. Solute aqueous concentration profile at 9600 days

Exercise 5

Peclet numbers of 20 and 50 are created by using a solute longitudinal dispersivity of 10 and 4 m, respectively on the *Solute/Porous Media Interaction Card*. The results for all Peclet numbers are shown in Figure 2. The higher Peclet numbers yield lower solute dispersion.

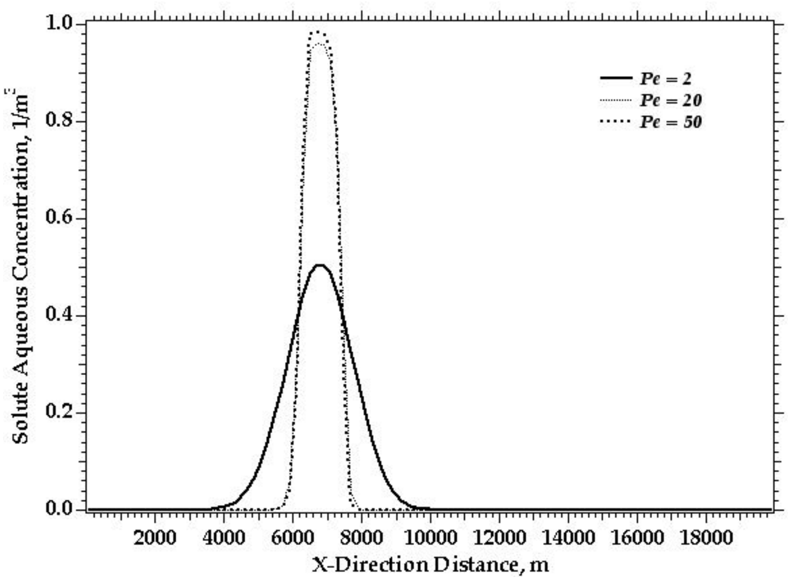

Figure 2. Solute aqueous concentration profile at 9600 days *(Pe = 2, 20, 50)*

Exercise 6

Courant numbers of 0.12 and 0.015 are created by using a time steps of 48 and 6 d, respectively on the *Solution Control Card*. The results for all Courant numbers are shown in Figure 3; where, the lower Courant numbers yield slightly higher solute dispersion.

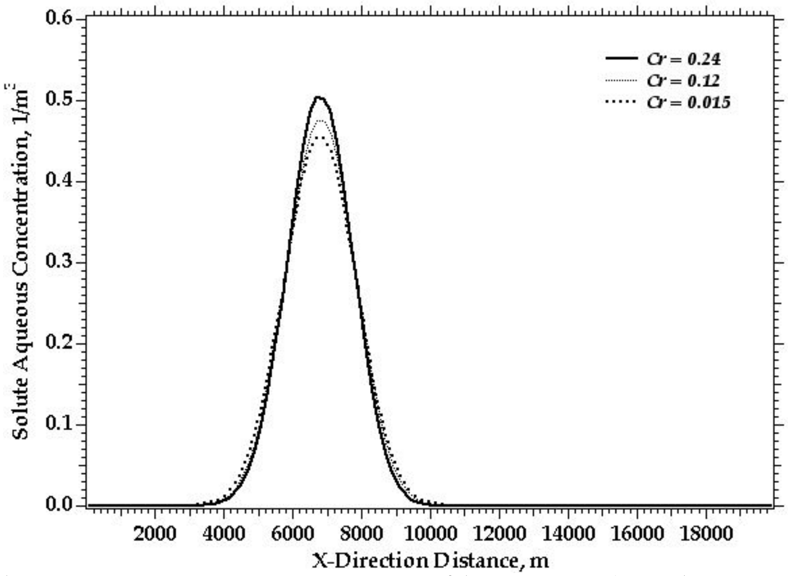

Figure 3. Solute aqueous concentration profile at 9600 days *(Cr = 0.24, 0.12, 0.015)*

Exercise 7

Whereas the Patankar transport scheme is generally more computationally efficient, it can often generate unacceptable amounts of numerical dispersion. The TVD (Total Variational Diminishing) transport method was designed to reduce the amount of numerical dispersion, but it is more computationally demanding and also requires a smaller time step. For problems with large Peclet numbers the TVD scheme must be used, as shown in Figure 4. A rule of thumb is to use Cr < .8 for Patankar and Cr < .2 for TVD.

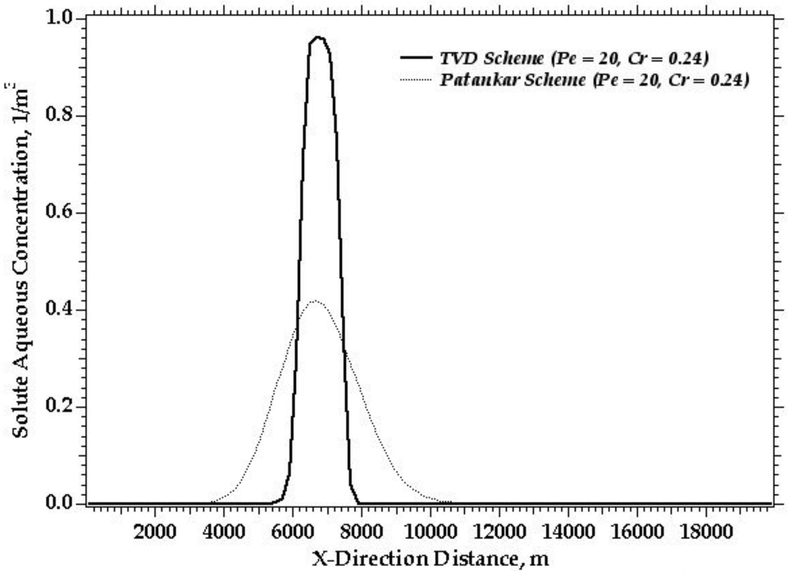

Figure 4. Solute aqueous concentration profile at 9600 days *(TVD and Patankar Schemes)*

Exercise 8

A partition coefficient of 3.7736x10^{-4} m^3/kg produces a retardation coefficient of 2.0. The base simulation used a partition coefficient of 0 m^3/kg, or a retardation coefficient of 1.0. As shown in Figure 5, doubling the retardation coefficient acts to retard the migration of the solute center of mass by a factor of 2.

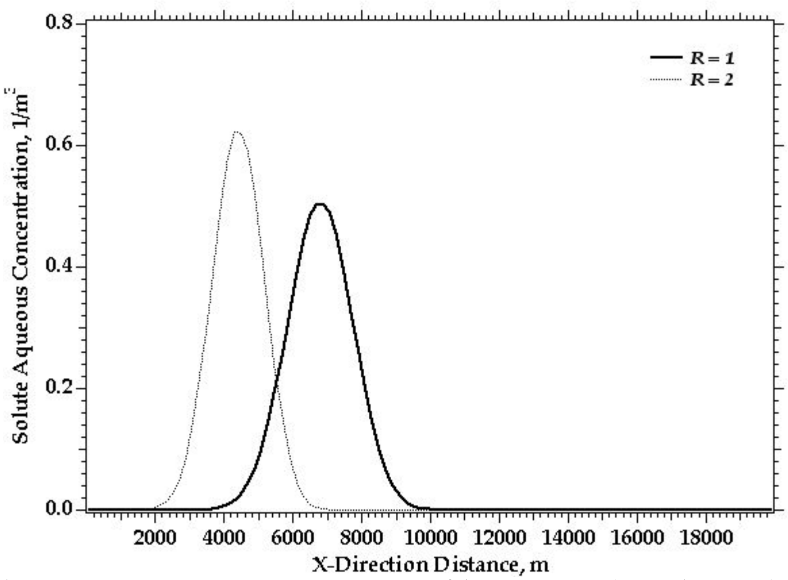

Figure 5. Solute aqueous concentration profile at 9600 days *(Retardation Coefficients = 1.0, 2.0)*

Exercise 9

The base simulation specified a slug of solute within the domain to investigate solute transport. This exercise uses a boundary condition to specify solute influent. The effect of dispersion on the influent solute slug is shown in Figure 6.

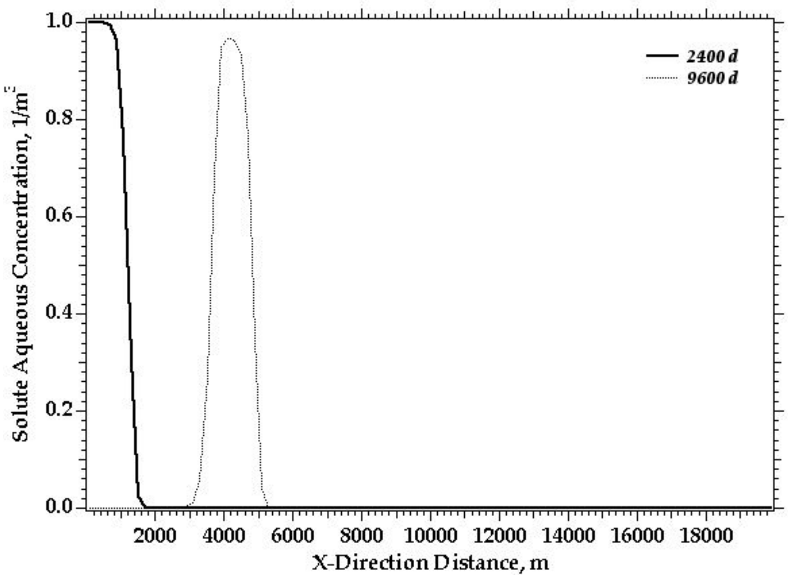

Figure 6. Solute aqueous concentration profile *(2400 and 9600 days)*