Solute transport dispersion test

by Xiang Huang at EES16, Los Alamos National Lab

1. Governing Equations

The governing equation for conservative solute transport is:

$$\frac{\partial(nC)}{\partial t} + \rho_b \frac{\partial C_R}{\partial t} = \nabla \cdot (nD_l \cdot \nabla C) - \nabla \cdot (qC) \tag{1}$$

where n is the porosity, C is solute concentration, ρ_b is bulk density, and C_R is the concentration of solutes adsorbed on the solids. The hydrodynamic dispersion is expressed as, $D_l = D^* + \alpha v = D^* + \alpha \frac{q}{n}$, where D^* is the molecular dispersion coefficient, α is mechanical dispersivity, and q is the Darcy velocity computed from $q = -\frac{k}{\mu} \cdot (\nabla p + \rho g)$. When the local equilibrium assumption is invoked for the sorption process, Eq. (1) can be written as

$$R \frac{\partial(nC)}{\partial t} = \nabla \cdot (nD_l \cdot \nabla C) - \nabla \cdot (qC) \tag{2}$$

where R is referred to as the dimensionless retardation factor and defined as $R = 1 + \frac{\rho_b}{n} \frac{\partial C_R}{\partial C}$. For the linear sorption isotherm sorption process, it assumes that the adsorbed concentration is directly proportional to the dissolved concentration. The retardation factor is thus given by $R = 1 + \frac{\rho_b}{n} K_d$, where K_d is the distribution coefficient.

2. Model description and setup

We used FEHM to simulate the 1D advection-dispersion transport of solutes in groundwater with a uniform Darcy flux and linear equilibrium sorption. Figure 1 shows the schematic diagram of the simulation domain with the initial and boundary conditions. The time step is 0.1 day, and the total simulation time is 10 days. The 5-meter simulation domain is discretized into 500 cells. Table 1 lists the key parameters.
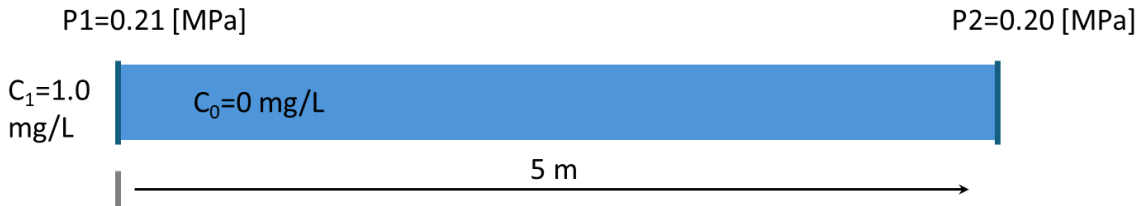
P1=0.21 [MPa]   P2=0.20 [MPa]

C_1=1.0 mg/L C_0=0 mg/L

5 m

Figure 1. 1D column model with constant solute concentration at the left injection side.

Table 1 The key parameters used in the numerical model

Parameter	Description	Values
P1	Fluid pressure inlet	0.21 [MPa]
P2	Fluid pressure outlet	0.20 [MPa]
C0	Initial solute concentration	0.0 [mg/L]
C1	Solute influent constant concentration	1.0 [mg/L]
k	Permeability	1.0×10^{-14} [m^2]
μ	Viscosity	1.0×10^{-3} [Pa·s]
q	Calculated Darcy velocity	2.0×10^{-8} [m/s]
v	Calculated linear pore water velocity	2.0×10^{-6} [m/s]
n	Porosity	0.01 [-]
ρ	Water density	1000 [kg/m^3]
ρ_b	Rock bulk density	1400 [kg/m^3]
α	Longitudinal dispersivity	0, 0.1 [m]
D^*	Molecular dispersion coefficient	0, 2.0×10^{-7} [m^2/s]
Kd	Linear sorption distribution coefficient	0, 1.0×10^{-2} [L/mg]

To examine whether the dispersion coefficient is defined correctly as described in textbook, we completed a series of parametric tests. Table 2 lists the scenarios of the model runs. The simulated concentration profiles and breakthrough curves were compared with the analytical solutions.

Table 2 The simulation cases

No.	Description	α [m]	D^* [m^2/s]	Kd [L/mg]	Upwind [-]	Element size [m]
Case1	Zero molecular dispersion	0.1	0.0	0.0	1.0	0.01
Case2	Zero mechanical dispersion	0.0	2.0×10^{-7}	0.0	1.0	0.01
Case3	Zero molecular dispersion Zero mechanical dispersion	0.0	0.0	0.0	1.0	0.01
Case4	Zero molecular dispersion Zero mechanical dispersion Smaller upwind weighting factor	0.0	0.0	0.0	0.5	0.01
Case5	Zero molecular dispersion Zero mechanical dispersion Finer mesh	0.0	0.0	0.0	1.0	0.0025
Case6	Zero molecular dispersion Zero mechanical dispersion Smaller upwind weighting factor Finer mesh	0.0	0.0	0.0	0.5	0.0025
Case7	molecular dispersion mechanical dispersion	0.1	2.0×10^{-7}	0.0	1.0	0.01
Case8	molecular dispersion mechanical dispersion Linear sorption	0.1	2.0×10^{-7}	1.0×10^{-2}	1.0	0.01

3. Simulation results and comparison with analytical solutions

Figures 2 and 3 show an excellent match between the numerical solutions and analytical solutions. Case1a and Case2a have identical concentration profiles along the flow distance at the selected days; Case1b and Case2b have identical breakthrough curves at the selected observation points. This means they have identical hydrodynamic dispersion coefficients.
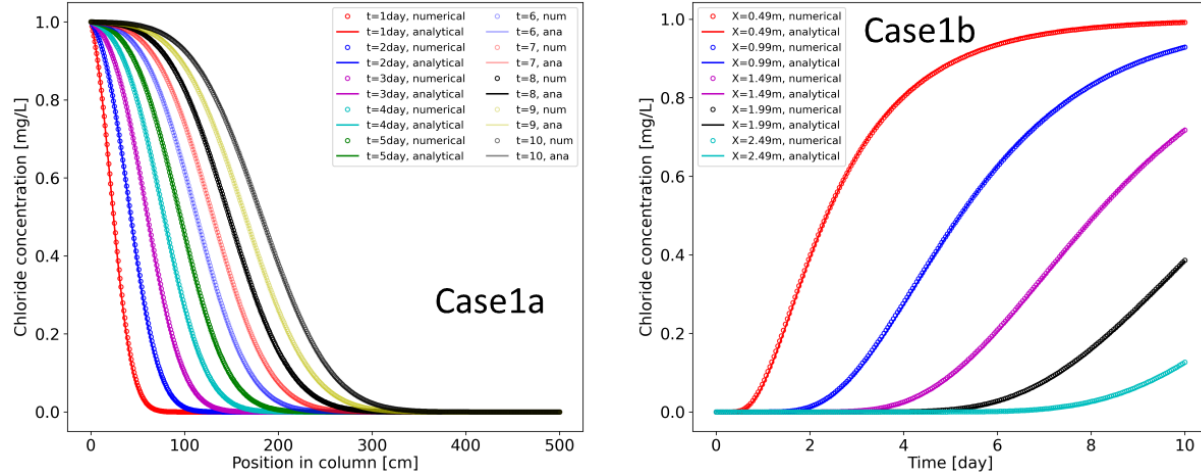

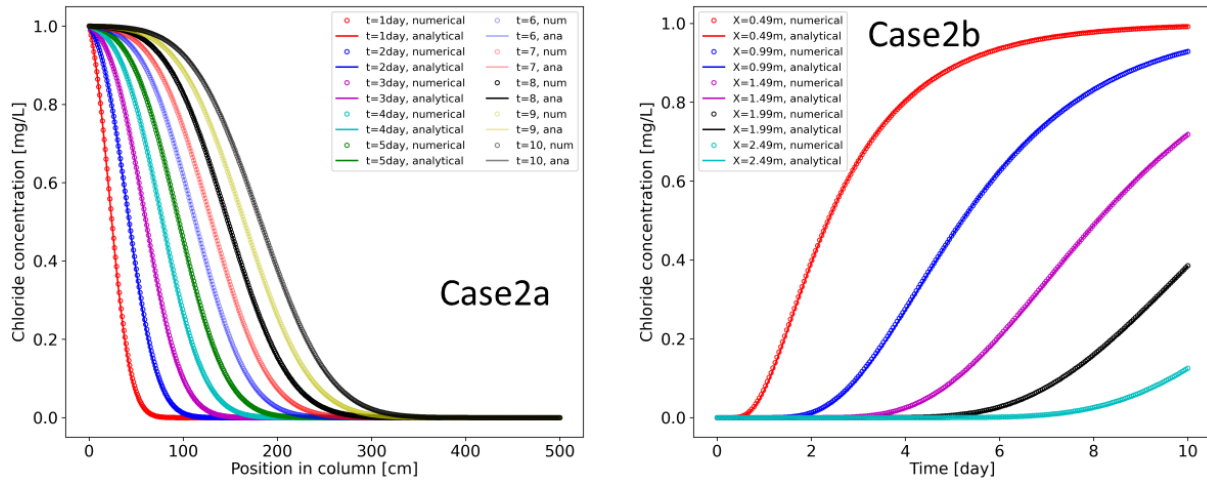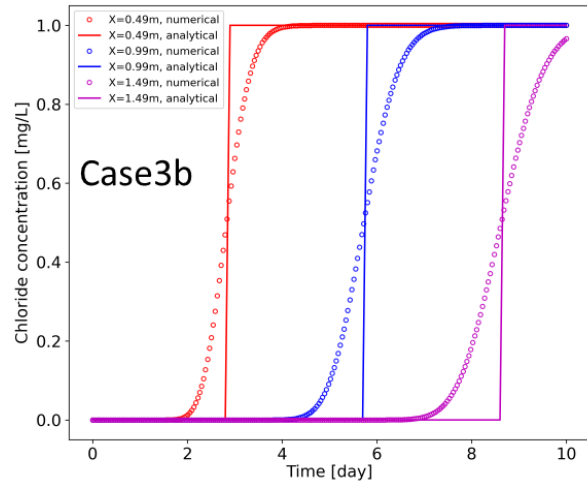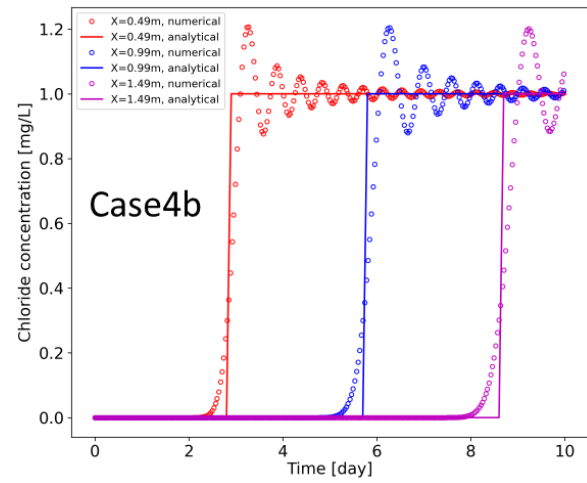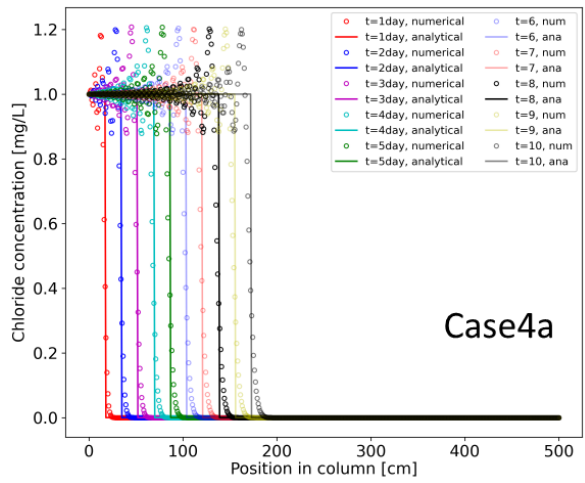Figure 2. FEHM simulation results vs. analytical solutions for the Case1

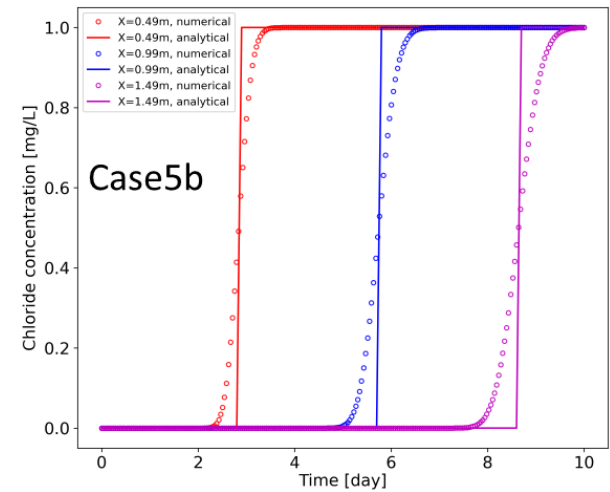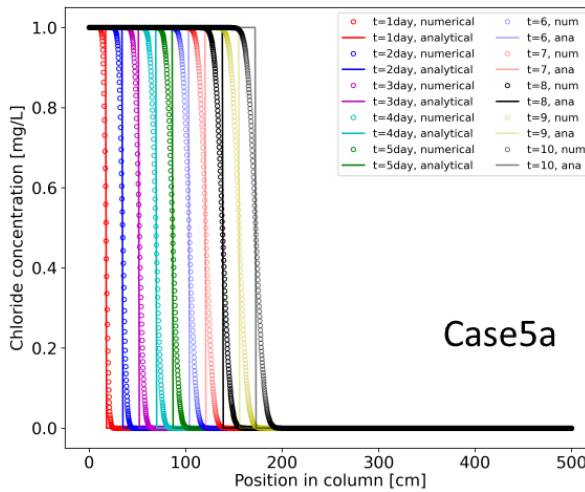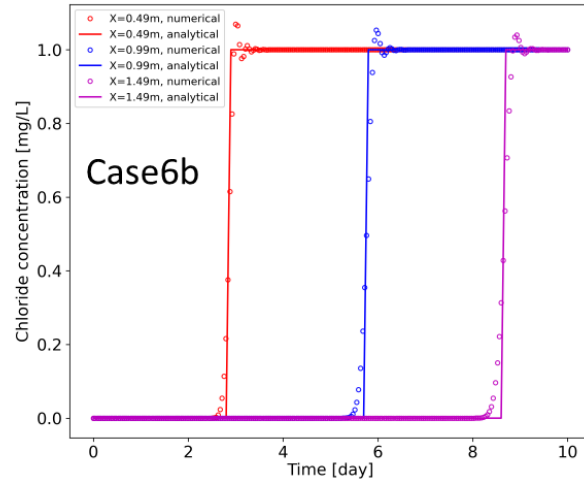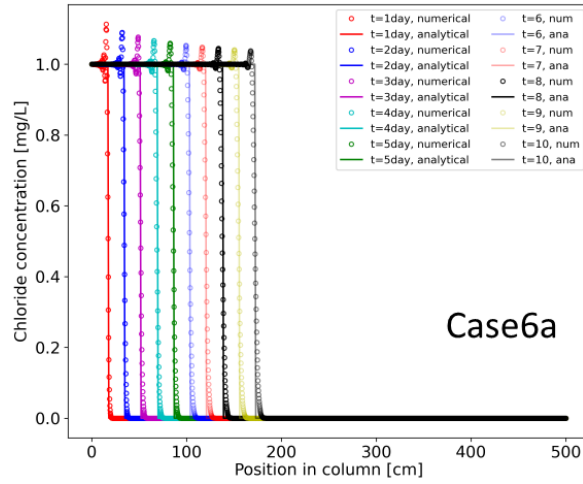Figure 3. FEHM simulation results vs. analytical solutions for the Case2

For the pure advection cases, i.e., zero hydrodynamic dispersion cases in Figures 4~7, it can generate a slightly better match by decreasing the upstream weighting factor from 1.0 to 0.5 but will cause substantial numerical oscillations (see case4a and case 4b). These oscillations can be reduced by implementing a higher numerical scheme and finer mesh to get a better match with the analytical solutions, as shown in Figure 7.
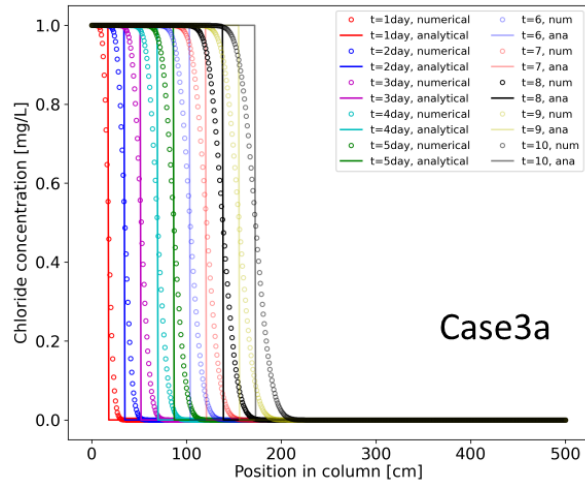
Figure 4. FEHM simulation results vs. analytical solutions for the Case3

Figure 5. FEHM simulation results vs. analytical solutions for the Case4

Figure 6. FEHM simulation results vs. analytical solutions for the Case5

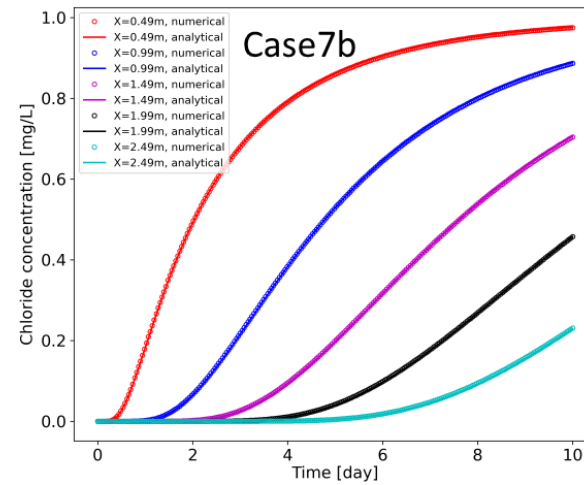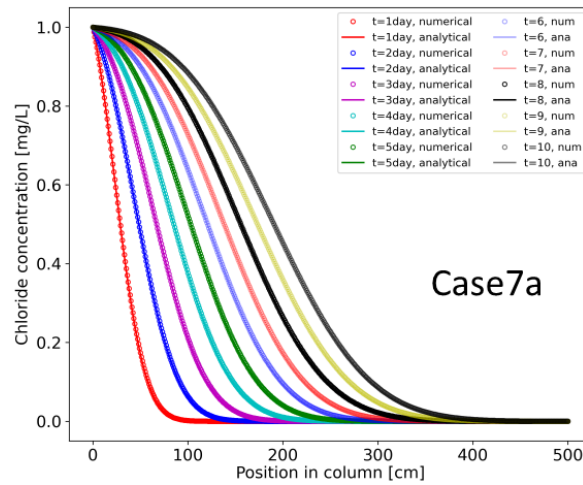Figure 7. FEHM simulation results vs. analytical solutions for the Case6

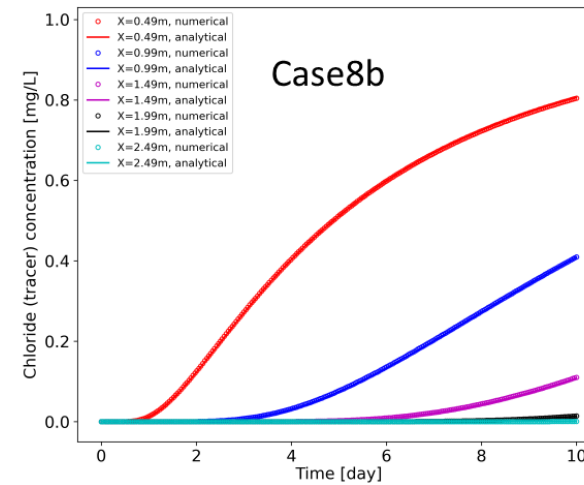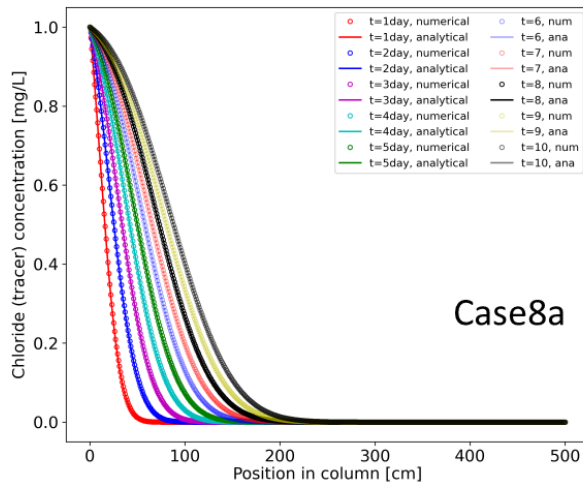Figure 8. FEHM simulation results vs. analytical solutions for the Case7

Figure 9. FEHM simulation results vs. analytical solutions for the Case8