5 EXAMPLES

5.1 General

MOUSER is accompanied by a set of sample files of input/output that correspond to the example problems described in this Chapter. The sample files can be downloaded from: http://www.groundwater.buffalo.edu. Several types of files are provided:

- files with the ".txt" extension are input files
- files with the ".out" extension are "summary" output files that include a listing of the input parameters, various comments, selected calculations.
- files with the ".dat" extension include numerical concentration/flux/mass output only.

The data file prefixes are named according to the following convention: all files begin with "t" (test), followed by a 1- or 2-digit problem number, followed by a letter indicating the simulation model (a = analytical, f = finite layer, n = numerical). For example, *t12a.txt* is the input file for test problem 12, intended for use with the analytical model. All test problems can be solved using the numerical algorithm, and most can also be solved with the finite layer or analytical models. Comparison of output from multiple models is a useful means of verifying accuracy, although minor differences are observed for most test problems due to the different computational approaches.

Descriptions of the specific test problems follow.

5.2 Diffusion dominated application: slurry wall

Five test simulations were performed to generate 100-year temporal profiles for a 1-meter thick slurry wall (input files *t1 – t5*). The basic parameters were assembled according to the general guidance provided in Chapter 4. A summary of the input parameters is contained in Table 5.1 and plots of the model output are shown in Figures 5.1 through 5.3. A concentration profile is shown only for the *t1* case (Figure 5.3) because simulations *t*2 -- *t*4 incorporate the zero concentration exit BC, while simulation *t*5 has a negligible exit concentration due to the influence of decay/dilution in the mixing zones. Other distinguishing features are summarized as follows:

- The data set *t1* represents a generic vertical barrier scenario for a solute that does not sorb or decay. A constant concentration entrance BC and semi-infinite exit BC were specified. The flux across the barrier exit reaches a peak at approximately year 20, while the concentration and cumulative mass increase over the entire time period.
- For *t2*, the exit BC was changed to a zero concentration condition, which leads to a different shape for the flux profile. A steady-state flux is reached after approximately 20 years.
- For *t3*, the zero concentration exit BC was retained and solute decay was included. The specification of a nonzero decay rate results in a significantly reduced steady-state flux.
- For *t4*, the zero concentration exit BC was retained, decay was eliminated, and significant sorption capacity was added to the barrier. The flux profile gradually

approaches the steady-state of the *t2* case, but does not reach this threshold during the simulation period due to sorption.

- For *t5*, sorption and decay were set to zero, the entrance boundary was changed to the finite mass condition, and the semi-infinite exit was specified. A "mixing zone" width of 1.0 was specified for the entrance. The resulting flux profile somewhat resembles the *t1* case at early times, but eventually approaches zero because of depletion of the finite source.

Each of the above test problems was modeled using all three methods, with visually indistinguishable output. Output from the finite layer model was used to construct Figures 5.1-5.3. For the numerical model, two minor changes in discretization were necessary: i) for problems involving a semi-infinite boundary (t1, t5), the number of spatial nodes was increased from 51 to 251 and the number of time steps was increased from 51 to 751, and ii) for t3, the number of time steps was increased from 51 to 251 for improved accuracy in the calculated numerical mass balance (necessary because of the interaction between diffusion and decay in the computed entrance boundary flux).

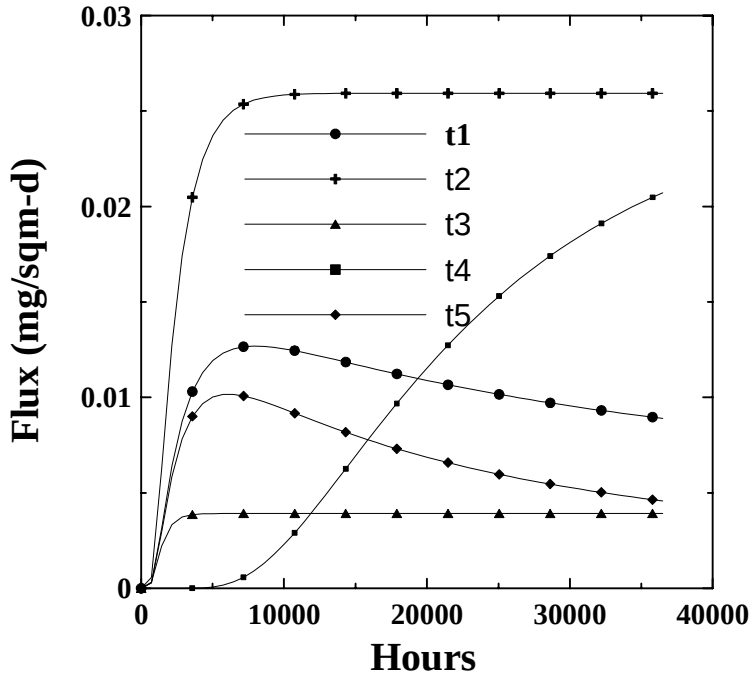

Figure 5.1 Simulated flux profiles for slurry wall

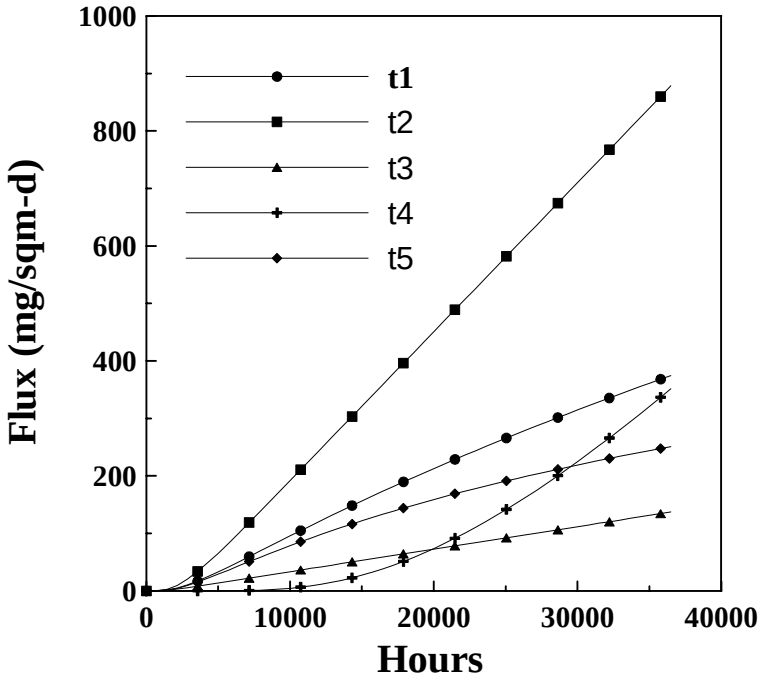

Figure 5.2 Simulated cumulative mass profiles for slurry wall

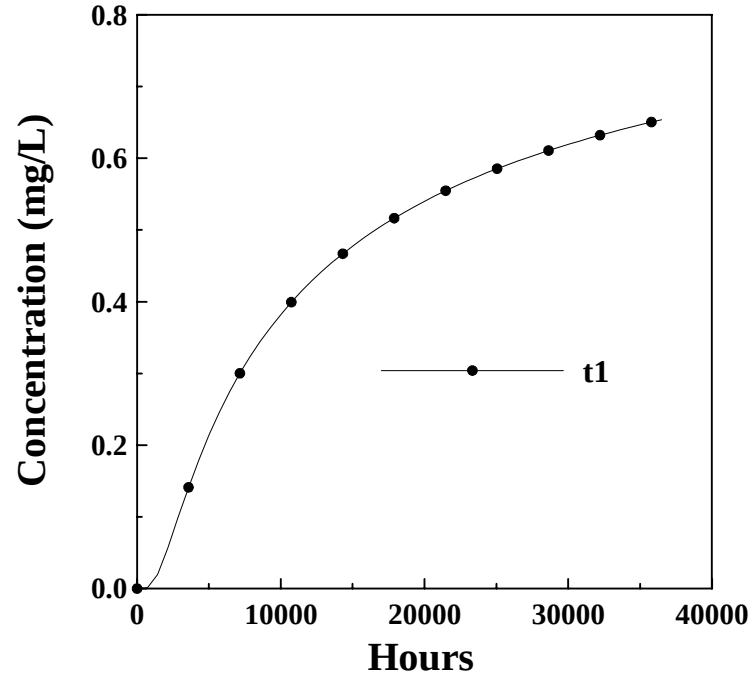

Figure 5.3 Simulated concentration profile for slurry wall

5.3 Single-solute permeable reactive barrier

Eight test simulations were performed to generate 20-day temporal and spatial profiles for a 1-meter permeable reactive barrier (PRB) for a single solute. The basic parameters were assembled according to the general guidance provided in Chapter 4. Summaries of the input parameters are contained in Table 5.2 and plots of the concentration output are shown in Figures 5.4 and 5.5. All three of the single solute algorithms produce identical results for *t6* - *t9* (except for *t10*, which cannot be solved with the analytical model); output from the finite layer model was used to construct the plots. Distinguishing features are summarized as follows:

- The data set *t6* represents a generic scenario for a solute that does not sorb or decay. A constant concentration entrance BC and semi-infinite exit BC were specified. The concentration profile follows a sigmoid shape, and steady state is reached relatively early in the simulation.
- For *t7*, the dispersivity was increased by a factor of two, resulting in slightly greater spreading in the early time profile, but no change in the steady-state condition.
- For *t8*, significant sorption capacity was added to the PRB. The shape of the concentration profile remains sigmoid, but steady state is not reached during the simulation period.
- For *t9*, sorption was modeled as a nonequilibrium process, with other conditions as specified in *t8*. Higher concentrations are noted at early times due to the delay in achieving sorption equilibrium, and the breakthrough exhibits a skewed shape.
- For *t10*, the conditions of *t9* were repeated, but decay was included, resulting in decrease in the concentration profile while maintaining a similar shape.
- The conditions of *t6* were modified to incorporate three decay rates in the range noted for iron-based PRBs (*t11*- *t13*). Decay of this magnitude results in negligible contaminant concentrations at the exit; the 20-day spatial profiles of contaminant within the barrier are shown in Figure 5.5.

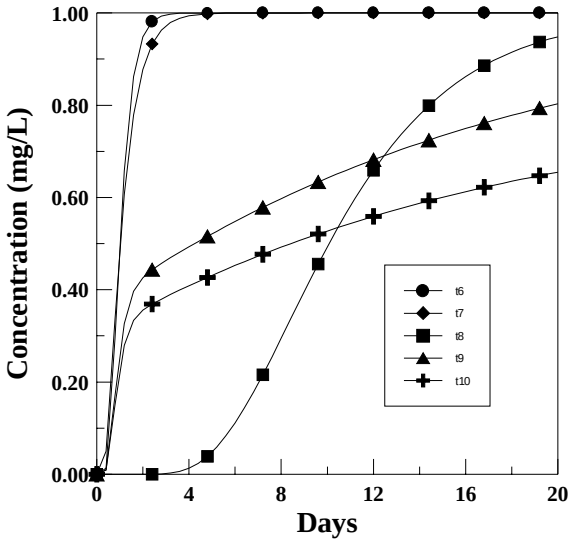

Figure 5.4 Simulated PRB effluent concentration profiles

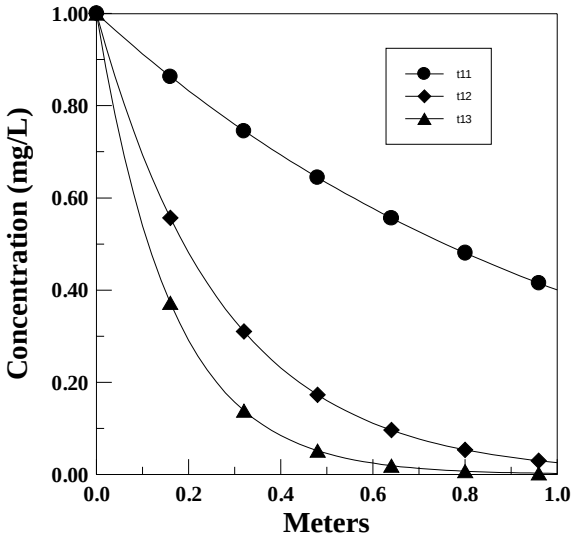

Figure 5.5 Simulated PRB spatial concentration profiles

5.4 Multi-solute permeable reactive barrier

Several test simulations were performed to illustrate the performance of the multi-solute decay model. The scenario under consideration was a 1-meter PRB constructed of iron filings, with the parent contaminant trichloroethylene (TCE) decaying to two daughter products: cis 12-dichloroethylene (DCE) and vinyl chloride (VC). The basic parameters were assembled according to the general guidance provided in Chapter 4. A summary of the input parameters is contained in Table 5.3 and plots of the model output are shown in Figures 5.6 through 5.5. Other distinguishing features are summarized as follows:

- Reaction parameters were selected according to the guidance provided by Tratnyek et al. (1997).
- For both plots, the time variable was expressed in terms of *pore volumes* (one pore volume = tv/L = 1 day for these problems).
- The effect of the exit BC is illustrated by comparison of *t14* and *t15*. As shown in Figure 5.6, the recommended zero-gradient BC (*t15*) leads to higher predicted effluent concentrations than the semi-infinite condition (*t14*), and is therefore recommended for design.
- The effect of nonequilibrium sorption was addressed in *t16* through *t20*, which are identical except for the sorption rate parameter. In the figure captions, the sorption rate constant was expressed in terms of the dimensionless *Damkohler number* ($Da = \alpha L/v$). As the sorption rate constant (α) is increased, the predictions converge on the equilibrium scenario represented by *t15*. The large rate constant used in *t20* (Da = 100) yields output identical to the equilibrium scenario of *t15* and the results are therefore not shown in the plot.

The results for test problems were generated using the multi-solute finite layer model and the numerical model. Because long simulation times (hours) are possible, the use of the numerical model for this class of multi-solute problems is recommended only for the case of nonlinear isotherms, which cannot be handled by the linear finite layer algorithm.

A more detailed discussion of the multi-solute test problems is presented in Khandelwal and Rabideau (1999).

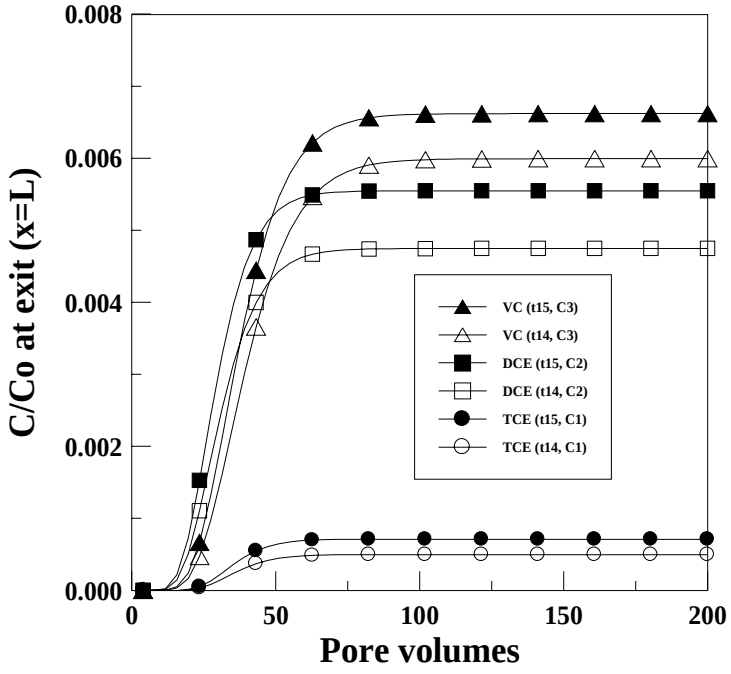

Figure 5.6 Simulated PRB effluent for equilibrium sorption (t14, t15)

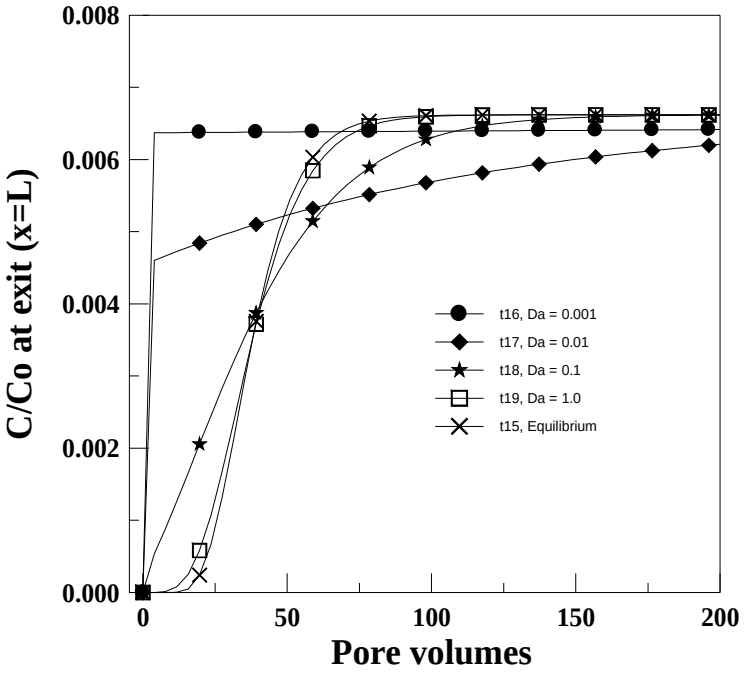

Figure 5.7 Simulated VC effluent for nonequilibrium sorption (t20 is identical to t15 and not shown)

Table 5.1 Input for slurry wall simulations

Line	Parameter	t1	t2	t3	t4	t5
1	Remark (remark)	NS	NS	NS	NS	NS
2	Sorption model flag	0	0	0	0	0
	Isotherm model flag	0	0	0	0	0
	Decay model flag	0	0	0	0	0
3	Output profile flag	0	0	0	0	0
	Output format flag	0	0	0	0	0
	Calibration flag	0	0	0	0	0
4	Method flag	0,1,2	0,1,2	0,1,2	0,1,2	0,1,2
	Flow calculation flag	0	0	0	0	0
	Transport numerical flag	0	0	0	0	0
	Reaction numerical flag	0	0	0	0	0
5*	Summary output file	t1x.out	t2x.out	t3x.out	t4x.out	t5x.out
6*	Data output file	t1x.dat	t2x.dat	t3x.dat	t4x.dat	t5x.dat
7	Number of solutes	1	1	1	1	1
**	Number of spatial nodes	2,2,251	2,2,51	2,2,51	2,2,51	2,2,251
**	Number of time steps	51,51,751	51,51,51	51,51,751	51,51,51	51,51,751
	Temporal output increment	1	1	1	1	1
8	Entrance BC flag	0	0	0	0	5
	Exit BC flag	1	2	2	2	1
9	Initial simulation time	0.0	0.0	0.0	0.0	0.0
	Final simulation time	36500	36500	36500	36500	36500
	Initial output location	1.0	1.0	1.0	1.0	1.0
	Final output location	1.0	1.0	1.0	1.0	1.0
10**	Domain length (L)	1, 1, 4.0	1.0	1.0	1.0	1,1,4.0
	Porosity (n)	0.4	0.4	0.4	0.4	0.4
	Bulk density (ρ_b)	1.59	1.59	1.59	1.59	1.59
11	Hydraulic conductivity (K)	8.64e-5	8.64e-5	8.64e-5	8.64e-5	8.64e-5
	Hydraulic gradient (i)	0.01	0.01	0.01	0.01	0.01
12	Dispersivity (a_L)	0.1	0.1	0.1	0.1	0.1
	Hindrance (H_p)	1.36	1.36	1.36	1.36	1.36
13	Solute name	Badstuff	Badstuff	Badstuff	Badstuff	Badstuff
14	Initial entrance BC (C_0)	1.0	1.0	1.0	1.0	1.0
	Entr. fin. mass thick. (h_f)	NA	NA	NA	NA	1.0
15	Exit BC conc. or gradient	0.0	0.0	0.0	0.0	0.0
16	Initial concentration (C_{in})	0.0	0.0	0.0	0.0	0.0
17	Diffusion coeffic. (D_d)	8.64e-5	8.64e-5	8.64e-5	8.64e-5	8.64e-5
	Aqueous decay const. (λ_a)	0.0	0.0	0.001	0.0	0.0
	Sorbed decay constant (λ_s)	0.0	0.0	0.0	0.0	0.0
	Sorption equil. const. (K_d)	0.0	0.0	0.0	2.264	0.0

NS = not shown; NA = not applicable; * x is replaced by a, f, or n depending on method
** input depends on solution method

Table 5.2 Input for single solute PRB simulations

Line	Parameter	t6	t7	t8	t9	t10
1	Remark (remark)	NS	NS	NS	NS	NS
2	Sorption model flag	0	0	0	1	1
	Isotherm model flag	0	0	0	0	0
	Decay model flag	0	0	0	0	0
3	Output profile flag	0	0	0	0	0
	Output format flag	0	0	0	0	0
	Calibration flag	0	0	0	0	0
4	Method flag	0,1,2	0,1,2	0,1,2	0,1,2	1,2
	Flow calculation flag	0	0	0	0	0
	Transport numerical flag	0	0	0	0	0
	Reaction numerical flag	0	0	0	0	0
5*	Summary output file	t6x.out	t7x.out	t8x.out	t9x.out	t10x.out
6*	Data output file	t6x.dat	t7x.dat	t8x.dat	t9x.dat	t10x.dat
7	Number of solutes	1	1	1	1	1
**	Number of spatial nodes	2,2,61	2,2,61	2,2,61	2,2,61	2,61
	Number of time steps	51,51,2000	51,51,2000	51,51,2000	51,51,2000	51,2000
	Temporal output increment	1	1	1	1	1
8	Entrance BC flag	1	1	1	1	1
	Exit BC flag	1	1	1	1	1
9	Initial simulation time	0.0	0.0	0.0	0.0	0.0
	Final simulation time	20.0	20.0	20.0	20.0	20.0
	Initial output location	1.0	1.0	1.0	1.0	1.0
	Final output location	1.0	1.0	1.0	1.0	1.0
10	Domain length (L)	1.0	1.0	1.0	1.0	1.0
	Porosity (n)	0.4	0.4	0.4	0.4	0.4
	Bulk density (ρ_b)	1.59	1.59	1.59	1.59	1.59
11	Hydraulic conductivity (K)	40.0	40.0	40.0	40.0	40.0
	Hydraulic gradient (i)	0.01	0.01	0.01	0.01	0.01
12	Dispersivity (a_L)	0.1	0.2	0.1	0.1	0.1
	Hindrance (H_p)	1.36	1.36	1.36	1.36	1.36
13	Solute name	Badstuff	Badstuff	Badstuff	Badstuff	Badstuff
14	Initial entrance BC (C_0)	1.0	1.0	1.0	1.0	1.0
15	Exit BC conc. or gradient	0.0	0.0	0.0	0.0	0.0
16	Initial concentration (C_{in})	0.0	0.0	0.0	0.0	0.0
17	Diffusion coeffic. (D_d)	8.64e-5	8.64e-5	8.64e-5	8.64e-5	8.64e-5
	Aqueous decay const. (λ_a)	0.0	0.0	0.0	0.0	0.2
	Sorbed decay constant (λ_s)	0.0	0.0	0.0	0.0	0.0
	Sorption equil. const. (K_d)	0.0	0.0	2.264	2.264	2.264
18^	Sorption rate constant (α)	NA	NA	NA	0.1	0.1

NS = not shown; NA = not applicable; * x is replaced by a, f, or n depending on method
** number depends on method; *** line number depends on test problem; ^ only for t10

Table 5.2 (cont'd) Input for single solute PRB simulations

Line	Parameter	t11	t12	t13
1	Remark (remark)	NS	NS	NS
2	Sorption model flag	0	0	0
	Isotherm model flag	0	0	0
	Decay model flag	0	0	0
3	Output profile flag	1	1	1
	Output format flag	0	0	0
	Calibration flag	0	0	0
4	Method flag	0,1,2	0,1,2	0,1,2
	Flow calculation flag	0	0	0
	Transport numerical flag	0	0	0
	Reaction numerical flag	0	0	0
5*	Summary output file	t11x.out	t12x.out	t13x.out
6*	Data output file	t11x.dat	t12x.dat	t13x.dat
7	Number of solutes	1	1	1
	Number of spatial nodes	101,101,201	101,101,201	101,101,201
**	Number of time steps	1,1,2000	1,1,2000	1,1,2000
	Temporal output increment	1	1	1
8	Entrance BC flag	0	0	0
	Exit BC flag	1	1	1
9	Initial output time	20.0	20.0	20.0
	Final simulation time	20.0	20.0	20.0
	Initial output location	0.0	0.0	0.0
	Final output location	1.0	1.0	1.0
10	Domain length (L)	1.0	1.0	1.0
	Porosity (n)	0.4	0.4	0.4
	Bulk density (ρ_b)	1.59	1.59	1.59
11	Hydraulic conductivity (K)	40.0	40.0	40.0
	Hydraulic gradient (i)	0.01	0.01	0.01
12	Dispersivity (a_L)	0.1	0.2	0.1
	Hindrance (H_p)	1.36	1.36	1.36
13	Solute name	Badstuff	Badstuff	Badstuff
14	Initial entrance BC (C_0)	1.0	1.0	1.0
15	Exit BC conc. or gradient	0.0	0.0	0.0
16	Initial concentration (C_{in})	0.0	0.0	0.0
17	Diffusion coeffic. (D_d)	8.64e-5	8.64e-5	8.64e-5
	Aqueous decay const. (λ_a)	1.0	5.0	10.0
	Sorbed decay constant (λ_s)	0.0	0.0	0.0
	Sorption equil. const. (K_d)	0.0	0.0	0.0

NS = not shown; NA = not applicable; * x is replaced by a, f, or n depending on method
** number depends on method

Table 5.3a General input for multi-solute PRB simulations

Line	Parameter	t14	t15	t16-20
1	Remark (remark)	NS	NS	NS
2	Sorption model flag	0	0	1
	Isotherm model flag	0	0	0
	Decay model flag	1	1	1
3	Output profile flag	1	1	1
	Output format flag	0	0	0
	Calibration flag	0	0	0
4	Method flag	1,2	1,2	1,2
	Flow calculation flag	0	0	0
	Transport numerical flag	0	0	0
	Reaction numerical flag	0	0	0
5*	Summary output file	t14x.out	t15x.out	t--x.out
6*	Data output file	t14x.dat	t15x.dat	t--x.dat
7	Number of solutes	3	3	3
	Number of spatial nodes	2,51	2,51	2,51
	Number of time steps	101,80000	101,80000	101,8000
	Temporal output increment	1,100	1,100	1,100
8	Entrance BC flag	0	0	0
	Exit BC flag	0	1	1
9	Initial output time	0.0	0.0	0.0
	Final simulation time	200.0	200.0	200.0
	Initial output location	1.0	1.0	1.0
	Final output location	1.0	1.0	1.0
10	Domain length (L)	1.0	1.0	1.0
	Porosity (n)	0.4	0.4	0.4
	Bulk density (ρ_b)	1.59	1.59	1.59
11	Hydraulic conductivity (K)	40.0	40.0	40.0
	Hydraulic gradient (i)	0.01	0.01	0.01
12	Dispersivity (a_L)	0.1	0.2	0.1
	Hindrance (H_p)	1.36	1.36	1.36

NS = not shown; NA = not applicable

* x is replaced by f, or n depending on method

Table 5.3b Solute-specific input for multi-solute PRB simulations

Line	Parameter	t14	t15	t16-20
13	Solute #1 name	TCE	TCE	TCE
14	Initial entrance BC (C_0)	1.0	1.0	1.0
15	Exit BC conc. or gradient	0.0	0.0	0.0
16	Initial concentration (C_{in})	0.0	0.0	0.0
17	Diffusion coeffic. (D_d)	8.64e-5	8.64e-5	8.64e-5
	Aqueous decay const. (λ_a)	23.4	23.4	23.4
	Sorbed decay constant (λ_s)	0.0	0.0	0.0
	Sorption equil. const. (K_d)	10.0	10.0	10.0
18	Solute #2 name	DCE	DCE	DCE
19	Initial entrance BC (C_0)	0.0	0.0	0.0
20	Exit BC conc. or gradient	0.0	0.0	0.0
21	Initial concentration (C_{in})	0.0	0.0	0.0
22	Diffusion coeffic. (D_d)	8.64e-5	8.64e-5	8.64e-5
	Aqueous decay const. (λ_a)	2.43	2.43	2.43
	Sorbed decay constant (λ_s)	0.0	0.0	0.0
	Sorption equil. const. (K_d)	4.0	4.0	4.0
23	Solute #3 name	VC	VC	VC
24	Initial entrance BC (C_0)	0.0	0.0	0.0
25	Exit BC conc. or gradient	0.0	0.0	0.0
26	Initial concentration (C_{in})	0.0	0.0	0.0
27	Diffusion coeffic. (D_d)	8.64e-5	8.64e-5	8.64e-5
	Aqueous decay const. (λ_a)	3.0	3.0	3.0
	Sorbed decay constant (λ_s)	0.0	0.0	0.0
	Sorption equil. const. (K_d)	6.0	6.0	6.0
28	Product 1 conversion fact. (β_1)	0.03	0.03	0.03
	Product 2 conversion fact. (β_2)	1.0	1.0	1.0
29*	Sorption rate constant (α) (TCE)	NA	NA	0.001-10.0
	Sorption rate constant (α) (DCE)	NA	NA	0.001-10.0
	Sorption rate constant (α) (VC)	NA	NA	0.001-10.0

* Input line used only for t16-20, $\alpha = 10^{-3}, 10^{-2}, 10^{-1}, 10^{0}, 10^{-1}$