

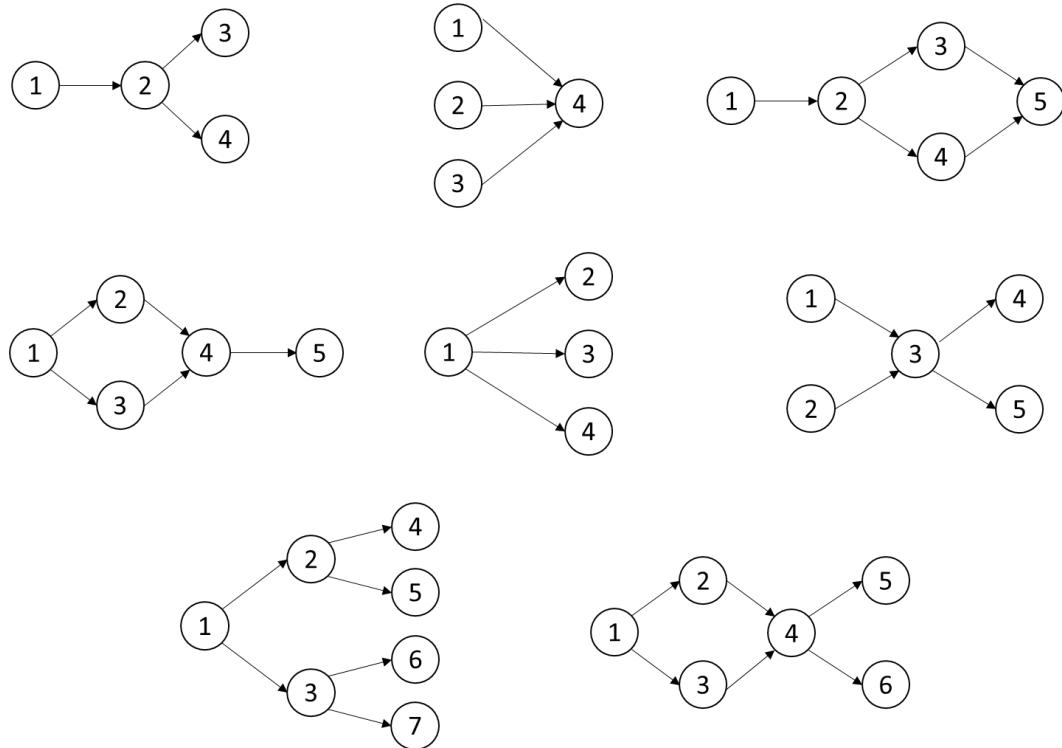
User's guide for DECA^Y

Analytical solution for one-dimensional solute transport
with multispecies subject to first-order decay reactions



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Introduction

An analytical solution has been derived and implemented for one-dimensional transport of multiple species along a decay chain with branching. The new solution, designated DECAY, extends existing solutions to consider more than three species with branching reactions. The treatment of branching accommodates species potentially having more than one parent and species having more than one daughter product. The DECAY solution is currently limited to handling three levels of reactions.

The DECAY solution considers advection, dispersion, equilibrium sorption, and first-order straight-chain and branching decay reactions. The species may have different dispersion and sorption coefficients. The solution accommodates the specification of different decay rates for the dissolved and sorbed phases for each species. Yield coefficients can be specified so that the calculations can be conducted in terms of concentrations expressed in units of either mass or moles per unit volume of water. The DECAY solution accommodates Dirichlet and Cauchy inflow boundary conditions with Bateman-type source histories.

This user's guide is divided into three main section: notation, input and output instructions, and an overview of the extensive testing that has been conducted and the results of the testing.

Executing simulations with the DECA^Y program

Simulations with the DECA^Y program are conducted with the executable file DECA^Y.exe. The instructions for running DECA^Y are simple. The user can click on the executable file and type the names of input and output files in response to the program prompts. An example is shown below. Here it assumed that the DECA^Y software has been installed in the subdirectory C\decay.

```
C:\decay>decay.exe
FILENAME FOR INPUT DATA FILE:
Example.inp
FILENAME FOR OUTPUT LISTING:
Example.out
FILENAME FOR PLOTTING OUTPUT:
Example.dat
```

Alternately, the user can create a batch file and a response file and run the program from the Command Prompt. An example is shown below.

```
C:\decay>decay < decay.fil

The response file decay.fil has the following contents:
Example.inp
Example.out
Example.dat
```

The simplest way to specify the input is to start with an existing input file and modify its contents with a text editor.

Input instructions

The DECAY input file contains the information on the flow field, the structure and properties of the sequential or branching decay reactions. An example of the DECAY input file is shown in Figure 1. The variables and the description of each dataset are presented on Table 1.

The input is specified in free format, with each parameter value separated by either a blank space or a comma.

| | | | | | | |
|-------|------------|------------|------------|------------|------------|--------------------------------------|
| (1) | 1.0000E-02 | | | | | Q |
| (2) | 1.0000E-01 | | | | | POR |
| (3) | 1.0000e+00 | | | | | RHOB |
| (4) | 5 | | | | | NSPECIES |
| (5) | 2 | | | | | NLEVELS |
| (6) | 1.8000E-01 | 1.8000E-01 | 1.8000E-01 | 1.8000E-01 | 1.8000E-01 | D |
| (7) | 0.0000e-02 | 0.0000e-01 | 0.0000e+00 | 0.0000e+00 | 0.0000e+00 | KD |
| (8) | 3.0000E-03 | 2.0000E-03 | 2.0000E-03 | 1.0000E-03 | 5.0000E-04 | LAMDA1 |
| (9) | 3.0000E-03 | 2.0000E-03 | 2.0000E-03 | 1.0000E-03 | 5.0000E-04 | LAMDA2 |
| (10) | 0 | 1 | 1 | 2 | 3 | LEVEL OF DECAY |
| (11) | 0 | 1 | 1 | 2 | 1 | NUMBER OF PARENTS |
| (12) | 0 | | | | | SPECIES NO. OF PARENTS FOR SPECIES 1 |
| | 1 | | | | | SPECIES NO. OF PARENTS FOR SPECIES 2 |
| | 1 | | | | | SPECIES NO. OF PARENTS FOR SPECIES 3 |
| | 2 | 3 | | | | SPECIES NO. OF PARENTS FOR SPECIES 4 |
| | 4 | | | | | SPECIES NO. OF PARENTS FOR SPECIES 5 |
| (13) | 0.0000e+00 | | | | | Y FOR SPECIES 1 |
| | 0.7380e+00 | | | | | Y FOR SPECIES 2 |
| | 0.7380e+00 | | | | | Y FOR SPECIES 3 |
| | 0.6450e+00 | 0.6450E+00 | | | | Y FOR SPECIES 4 |
| | 0.4490e+00 | | | | | Y FOR SPECIES 5 |
| (14) | 1.0000e+00 | | | | | ETA FOR SPECIES 1 |
| | 0.2000e+00 | | | | | ETA FOR SPECIES 2 |
| | 0.8000e+00 | | | | | ETA FOR SPECIES 3 |
| | 1.0000e+00 | 1.0000e+00 | | | | ETA FOR SPECIES 4 |
| | 1.0000e+00 | | | | | ETA FOR SPECIES 5 |
| (15) | 1 | | | | | IBC |
| (16a) | 1 | | | | | NP(1) |
| (16b) | 0 | 1 | | | | TI(1),CI(1) |
| | 1 | | | | | NP(2) |
| | 0 | 0 | | | | TI(2),CI(2) |
| | 1 | | | | | NP(3) |
| | 0 | 0 | | | | TI(3),CI(3) |
| | 1 | | | | | NP(4) |
| | 0 | 0 | | | | TI(4),CI(4) |
| | 1 | | | | | NP(5) |
| | 0 | 0 | | | | TI(5),CI(5) |
| (17) | 0.0000E+00 | 5.0000e+01 | 1.0000e+00 | | | XMIN,XMAX,DX |
| (18) | | 1 | | | | NT |
| (19) | 2.0000E+02 | | | | | TIMES |

Figure 1 Example DECAY input file

Table 1 DECAY input file instruction

| Dataset | Variable | Description |
|--|-------------------|--|
| 1 | Q | Darcy flux [L/T] |
| 2 | POR (ϕ) | Porosity [-] |
| 3 | RHOB (ρ_b) | Bulk density of porous media [M/L ³] |
| 4 | NSPECIES | Total number of species [-] |
| 5 | NLEVELS | Total number of levels [-] |
| 6 | D | Dispersion coefficient for each species [L ² /T] |
| 7 | KD | Sorption coefficient for each species [L ³ /M] |
| 8 | LAMDA1 | Decay rate in the dissolved phase [1/T] |
| 9 | LAMDA2 | Decay rate in the sorbed phase [1/T] |
| 10 | LEVEL | Level of decay for each species [-] |
| 11 | NUMP | Number of parents for each species [-] |
| Repeat datasets 12, 13 and 14 NSPECIES times | | |
| 12 | ID | Species number of parents [-] |
| 13 | Y | Yield coefficient [-] |
| 14 | ETA | Branching ratio [-] |
| 15 | IBC | Inflow boundary coefficient [-] |
| | | = 1: Type 1 inflow boundary condition |
| | | = 3: Type 3 inflow boundary condition |
| Repeat dataset 16 NSPECIES times | | |
| 16a | NP | Number of points defining inflow concentration history [-] |
| 16b | TI, CI | (Time, concentration) inflow concentration points [T, M/L ³] |
| 17 | XMIN,XMAX,DX | Minimum x-coordinate when solution is computed [L] |
| | | Maximum x-coordinate when solution is computed [L] |
| | | x-coordinate increment [L] |
| 18 | NT | Number of times when a breakthrough curve is to be computed [-] |
| 19 | TIMES | Specific times [T] |

The following parameters have been introduced to accommodate the extended capabilities of the DECAY solution.

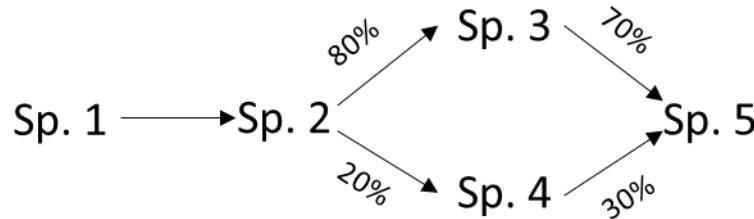
- 1) NLEVELS – the total number of LEVELs for the entire process of a chain-decay reaction (a maximum of 3 LEVELs is supported);
- 2) LEVEL – sequential order of decay reactions along a branching decay chain (for the starting species of a decay chain, its LEVEL equals to zero);
- 3) NUMP – number of parents of an individual species;
- 4) ID – species numbers of its parents (ID = 0 if NUMP = 0); and
- 5) ETA – branching ratio accounting for proportion of the transformation from its parents.

The order of species numbers starts from the left side of a decay chain to the right side and from the top to the bottom.

Three parameters are calculated internally by the program:

- 1) PATH1 – species number of parents on the decay chain;
- 2) PATH2 – species number of grandparents on the decay chain; and
- 3) PATH3 – species number of great-grandparents on the decay chain.

The specification of the input for reactions is illustrated with an example.



| | Species 1 | Species 2 | Species 3 | Species 4 | Species 5 |
|----------------|-----------|-----------|-----------|-----------|-----------|
| NLEVELS | | | 3 | | |
| LEVEL | 0 | 1 | 2 | 2 | 3 |
| NUMP | 0 | 1 | 1 | 1 | 2 |
| ID | 0 | 1 | 2 | 2 | {3,4} |
| ETA | 0 | 1.0 | 0.8 | 0.2 | {0.3,0.7} |
| PATH1 | 0 | 1 | 2 | 2 | {3,4} |
| PATH2 | 0 | 0 | 1 | 1 | 2 |
| PATH3 | 0 | 0 | 0 | 0 | 1 |

Output files

DECAY writes two output files, an output listing file and a plot file. The listing file includes a listing of all the input parameters and the computed concentration along a given interval of the x-coordinate at specific times for each species. The plot file writes the x-coordinate and the concentration for each species at this location. If NSPECIES = 5, the plot output file will look like:

| X | C (1) | C (2) | C (3) | C (4) | C (5) |
|----------------|----------------|-----------------|----------------|-----------------|-----------------|
| 0.00000000E+00 | 1.00010001E+00 | -5.86881687E-15 | 7.83684609E-15 | -5.18273853E-14 | -1.49707865E-14 |
| 1.00000000E+00 | 9.71511936E-01 | 3.92467728E-03 | 1.56987091E-02 | 4.82229845E-04 | 5.83740655E-06 |
| 2.00000000E+00 | 9.43445282E-01 | 7.62772378E-03 | 3.05108951E-02 | 1.15287612E-03 | 1.46353337E-05 |
| 3.00000000E+00 | 9.15783899E-01 | 1.11041159E-02 | 4.44164636E-02 | 1.98749618E-03 | 2.66995276E-05 |
| 4.00000000E+00 | 8.88394410E-01 | 1.43462596E-02 | 5.73850384E-02 | 2.95976689E-03 | 4.21599889E-05 |
| 5.00000000E+00 | 8.61126952E-01 | 1.73440229E-02 | 6.93760917E-02 | 4.04140534E-03 | 6.09657212E-05 |
| 6.00000000E+00 | 8.33817402E-01 | 2.00849363E-02 | 8.03397451E-02 | 5.20222837E-03 | 8.28843349E-05 |
| 7.00000000E+00 | 8.06291309E-01 | 2.25545900E-02 | 9.02183602E-02 | 6.41037991E-03 | 1.07507832E-04 |
| 8.00000000E+00 | 7.78369634E-01 | 2.47372470E-02 | 9.89489881E-02 | 7.63274663E-03 | 1.34265637E-04 |
| 9.00000000E+00 | 7.49876265E-01 | 2.66166706E-02 | 1.06466682E-01 | 8.83556993E-03 | 1.62445509E-04 |
| 1.00000000E+01 | 7.20647053E-01 | 2.81771493E-02 | 1.12708597E-01 | 9.98524513E-03 | 1.91222398E-04 |

Figure 2 Strip of an example of the plot file

Testing of the DECA^Y solution

The DECA^Y solution and its implementation have been checked with two levels of testing:

- Part 1: Straight-chain reactions; and
- Part 2: Reactions with branching.

The test cases have been designed to test the accuracy of DECA^Y and to demonstrate its capabilities. The DECA^Y package includes the input files for each test case; the input files can serve as templates for other simulations.

Testing Part 1: Straight chain reactions

Three tests have been designed to show the ability of DECAY solving problems with straight-chain decay reactions. The results for the first two tests are compared against MT3D99 and the third test is compared against the results from van-Genuchten (1985).

1. PCE straight-chain decay reaction



A straight-chain anaerobic degradation of PCE is considered to test the DACAY solution for sequential reactions. The input parameters are tabulated on Table 2. The decay rates and the yield coefficients are obtained from Clement and Quezada (2002; Table 3.1-1) and reproduced here.

Table 2 Input parameters

| Parameters | PCE | TCE | DCE | VC |
|---|-------|-------|-------|-------|
| Darcy flux q (m/year) | 0.03 | | | |
| Porosity ϕ (-) | 0.1 | | | |
| Bulk density ρ_b (g/cm ³) | 1.0 | | | |
| Dispersion coefficient D (m ² /year) | 3 | 3 | 3 | 3 |
| Sorption coefficient K_d (cm ³ /g) | 0.1 | 0.0 | 0.0 | 0.0 |
| Dissolved phase decay rate (year ⁻¹) | 0.005 | 0.003 | 0.002 | 0.001 |
| Sorbed phase decay rate (year ⁻¹) | 0.005 | 0.003 | 0.002 | 0.001 |
| Yield coefficient (-) | 0.0 | 0.792 | 0.738 | 0.645 |

The results are plotted against the concentrations calculated from the numerical simulator MT3D99 (1999), shown in Figure 3 -Figure 5. MT3D99 has the capability to handle first-order reaction on the sorbed phase in contrast to MT3D-USGS. Slight mismatches appear at 50 days and 100 days. The results are quite consistent overall.

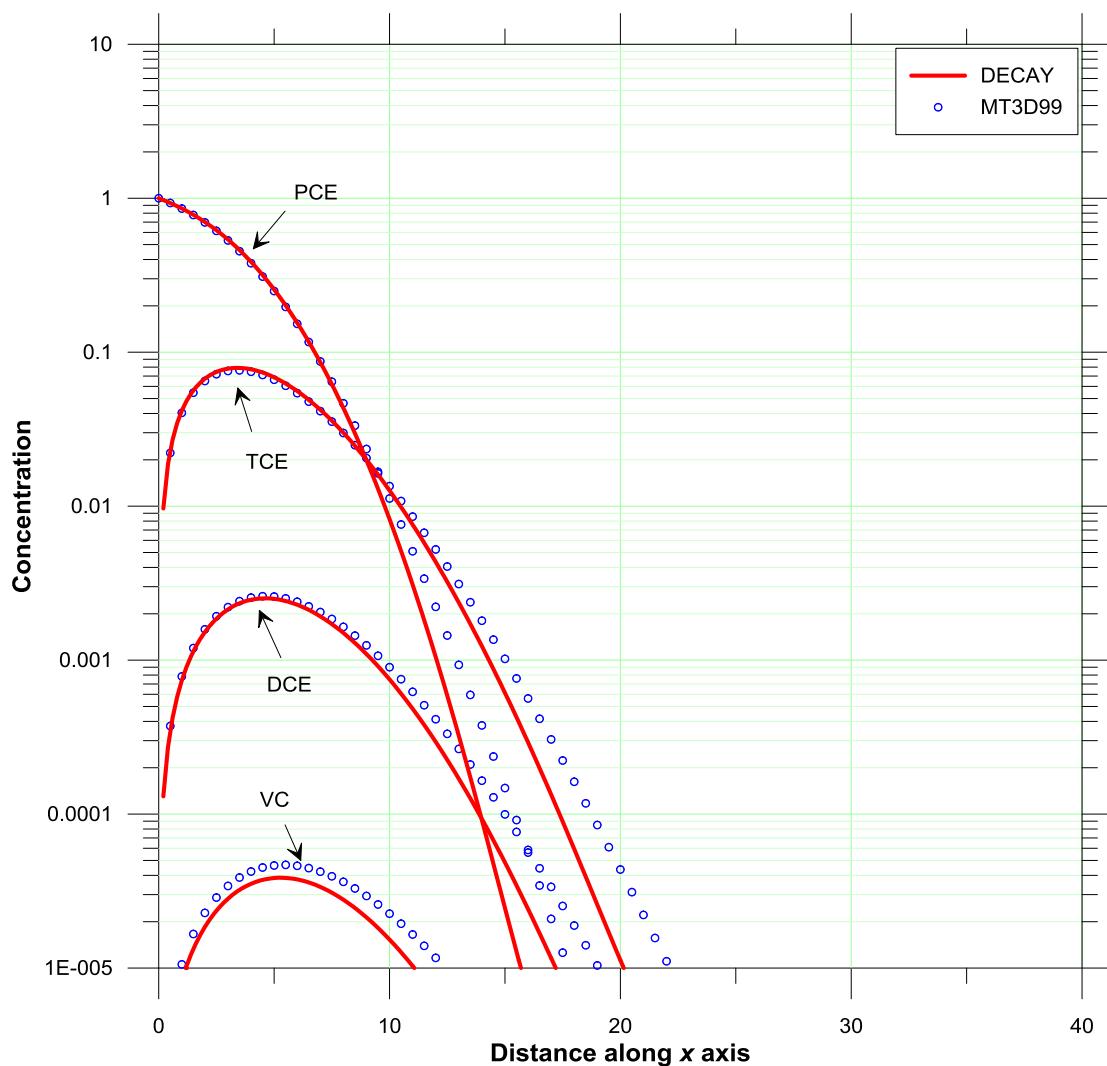


Figure 3 Concentration profiles at 50 days for PCE straight-chain decay reaction

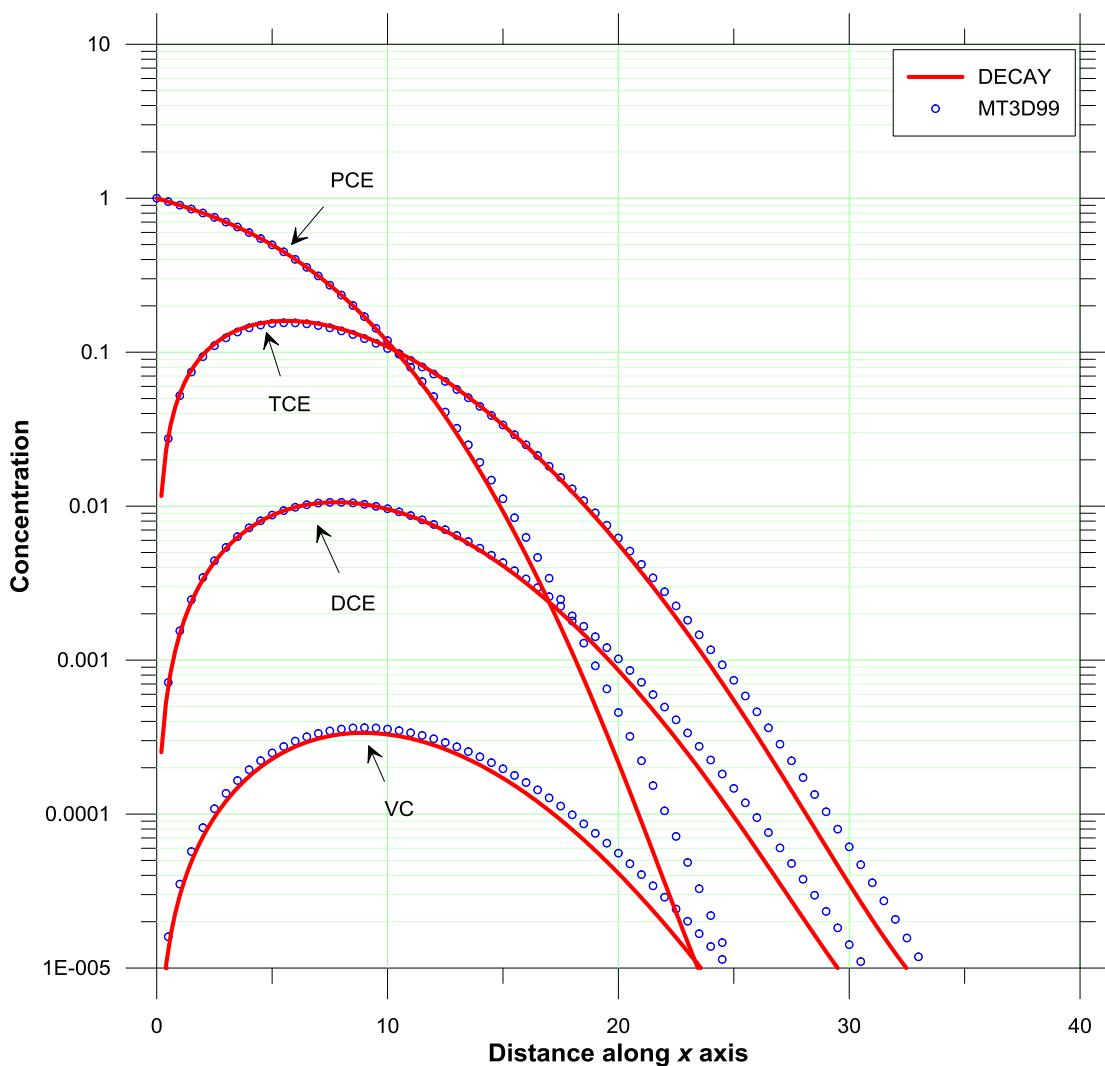


Figure 4 Concentration profiles at 100 days for PCE straight-chain decay reaction

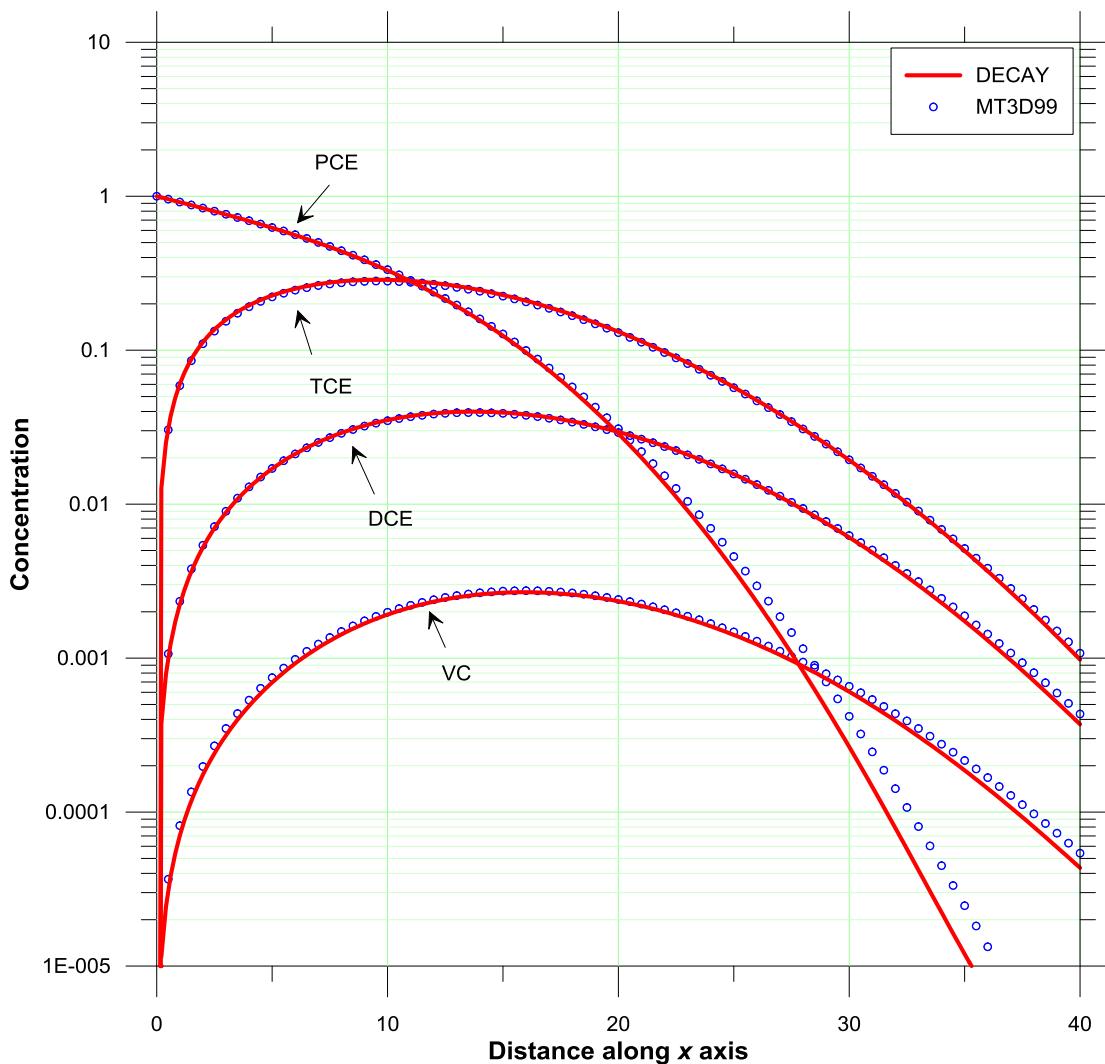
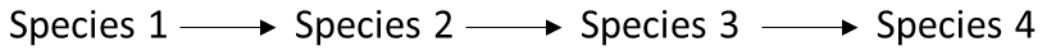


Figure 5 Concentration profiles at 200 days for PCE straight-chain decay reaction

2. A straight-chain decay reaction with Bateman source history



A test problem is designed adopting the Bateman source conditions that account for the possibility that the concentrations in the source evolve due to decay. Type III Cauchy inflow boundary condition is considered. The input parameters for the DECA^Y solutions are set up according to Sun et al. (1999) and are listed on Table 3.

Table 3 Parameters for a straight-chain decay reaction with Bateman source

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 |
|---|-----------|-----------|-----------|-----------|
| Sorption coefficient K_d (cm ³ /g) | 0.1 | 0.0 | 0.0 | 0.0 |
| Dissolved phase decay rate (hr ⁻¹) | 0.05 | 0.03 | 0.02 | 0.01 |
| Sorbed phase decay rate (hr ⁻¹) | 0.05 | 0.03 | 0.02 | 0.0001 |
| Yield coefficient (-) | 0.0 | 1.0 | 1.0 | 1.0 |

The results calculated from DECA^Y and MT3D99 are shown in Figure 6 - Figure 8. As shown in the figures, the agreement between the two results is fairly well, especially at the later time, 200 days.

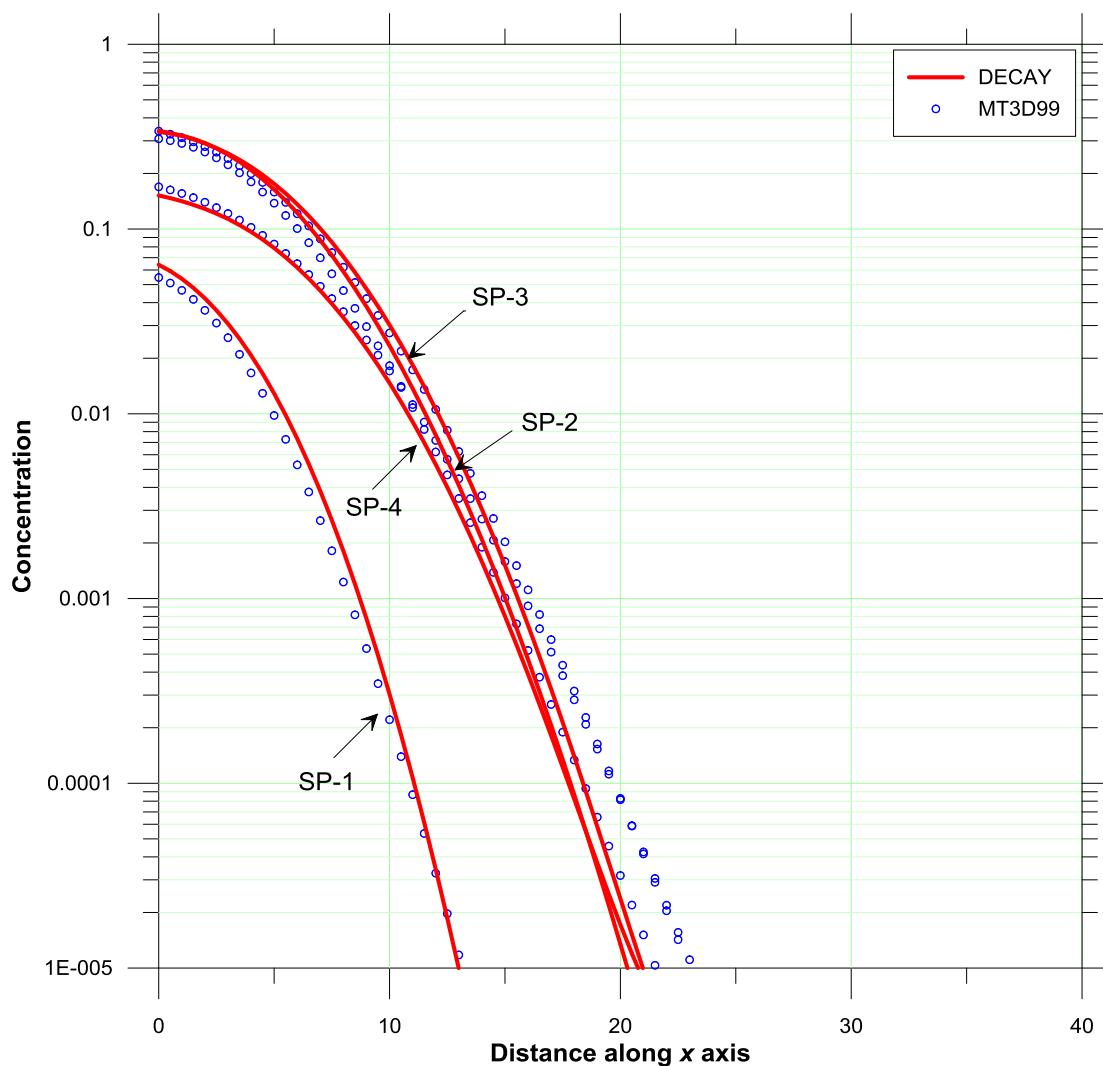


Figure 6 Concentration profiles at 50 hours for a straight-chain decay reaction with Bateman source history

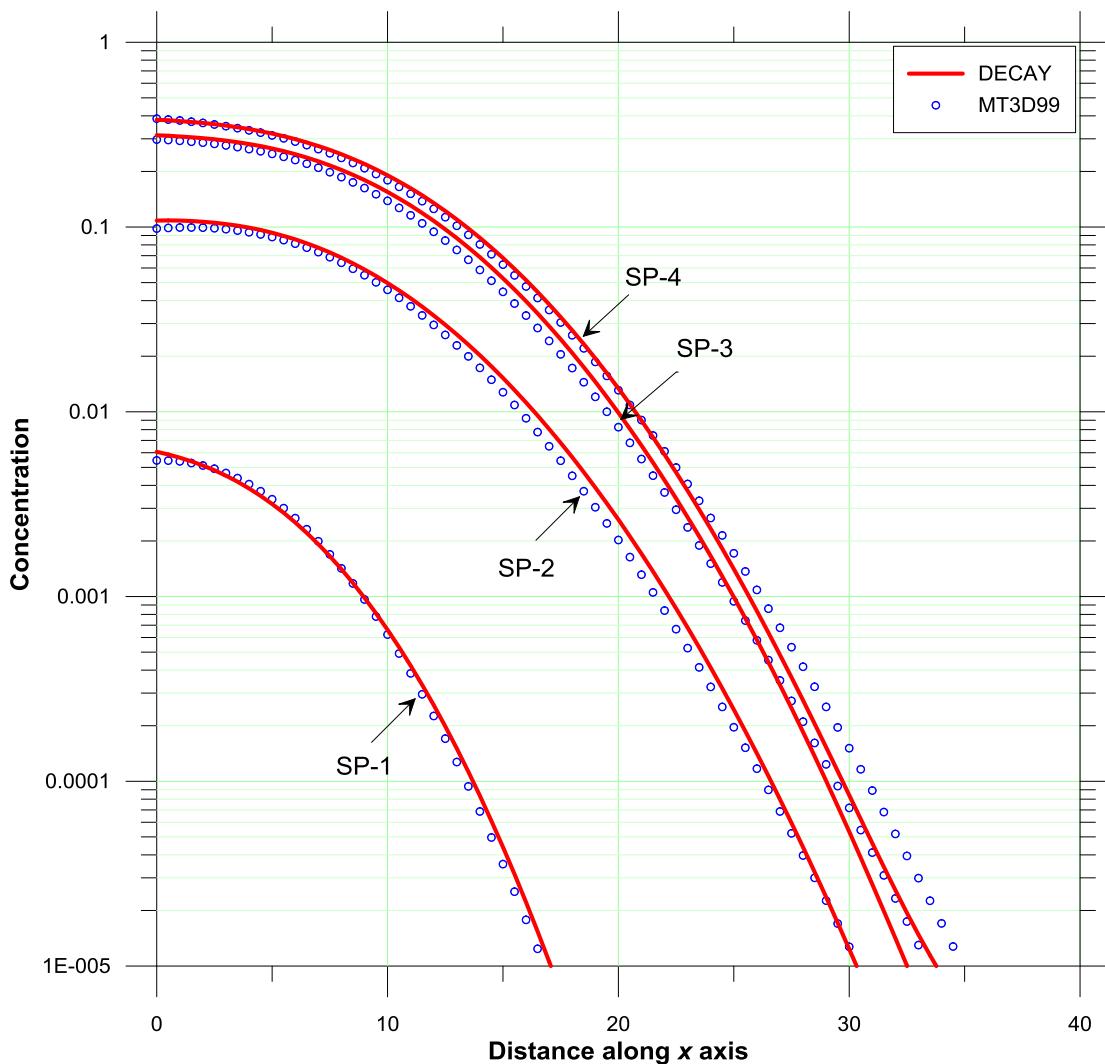


Figure 7 Concentration profiles at 100 hours for a straight-chain decay reaction with Bateman source history

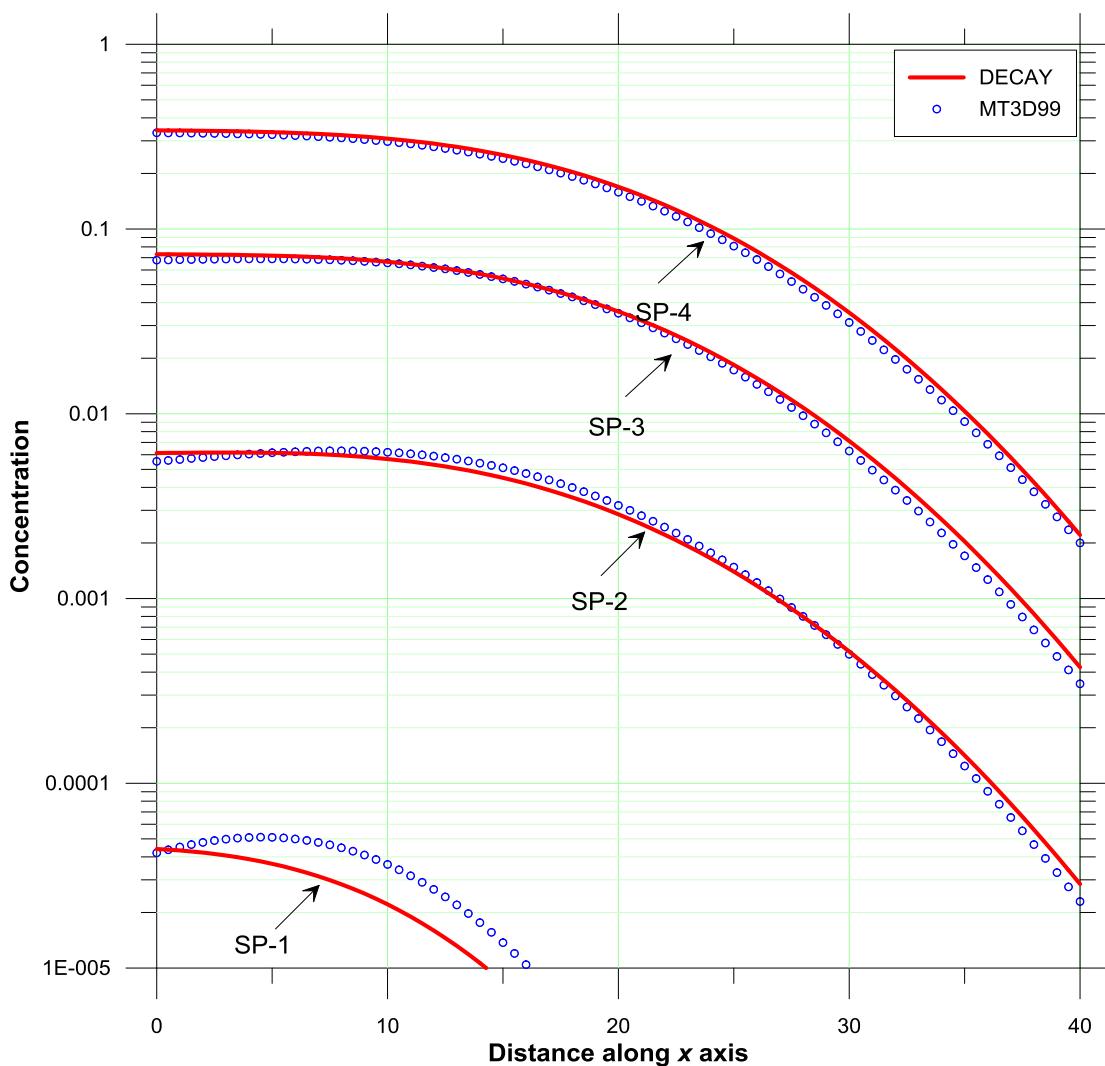


Figure 8 Concentration profiles at 200 hours for a straight-chain decay reaction with Bateman source history

3. A radioactive straight-chain decay reaction with Bateman source history



A radioactive decay chain is set up based on the second example of van Genuchten (1985) and the parameters are listed on Table 4.

Table 4 Input parameters obtained from van Genuchten (1985)

| Parameters | ^{238}Pu | ^{234}U | ^{230}Th | ^{226}Ra |
|---|----------------------|-------------------------|-------------------------|-----------------------|
| Darcy flux q (m/year) | 40 | | | |
| Porosity ϕ (-) | 0.1 | | | |
| Bulk density ρ_b (g/cm ³) | 1.6 | | | |
| Dispersion coefficient D (m ² /year) | 10.0 | 0.18 | 0.18 | 0.18 |
| Sorption coefficient K_d (cm ³ /g) | 2500 | 3500 | 12500 | 125 |
| Dissolved phase decay rate (year ⁻¹) | 7.9×10^{-3} | 2.8×10^{-6} | 8.7×10^{-6} | 4.3×10^{-4} |
| Sorbed phase decay rate (year ⁻¹) | 7.9×10^{-3} | 2.8×10^{-6} | 8.7×10^{-6} | 4.3×10^{-4} |
| Source decay rate (year ⁻¹) | 8.9×10^{-3} | 1.0028×10^{-3} | 1.0028×10^{-3} | 1.43×10^{-3} |
| Yield coefficient (-) | 0.0 | 1.0 | 1.0 | 1.0 |

The results calculated from DECAV are compared against the results retrieved from van Genuchten (1985), shown in Figure 9 and Figure 10. As shown in the figure, the concentrations of ^{234}U at 1000 years do not follow a smooth curve and a sudden change happens at around 15 along the x -axis. This arises because the numerical inversion of Laplace transform deployed in the DECAV solutions perform poorly for small numbers; however, the results calculated from DECAV are consistent with the ones from van Genuchten (1985).

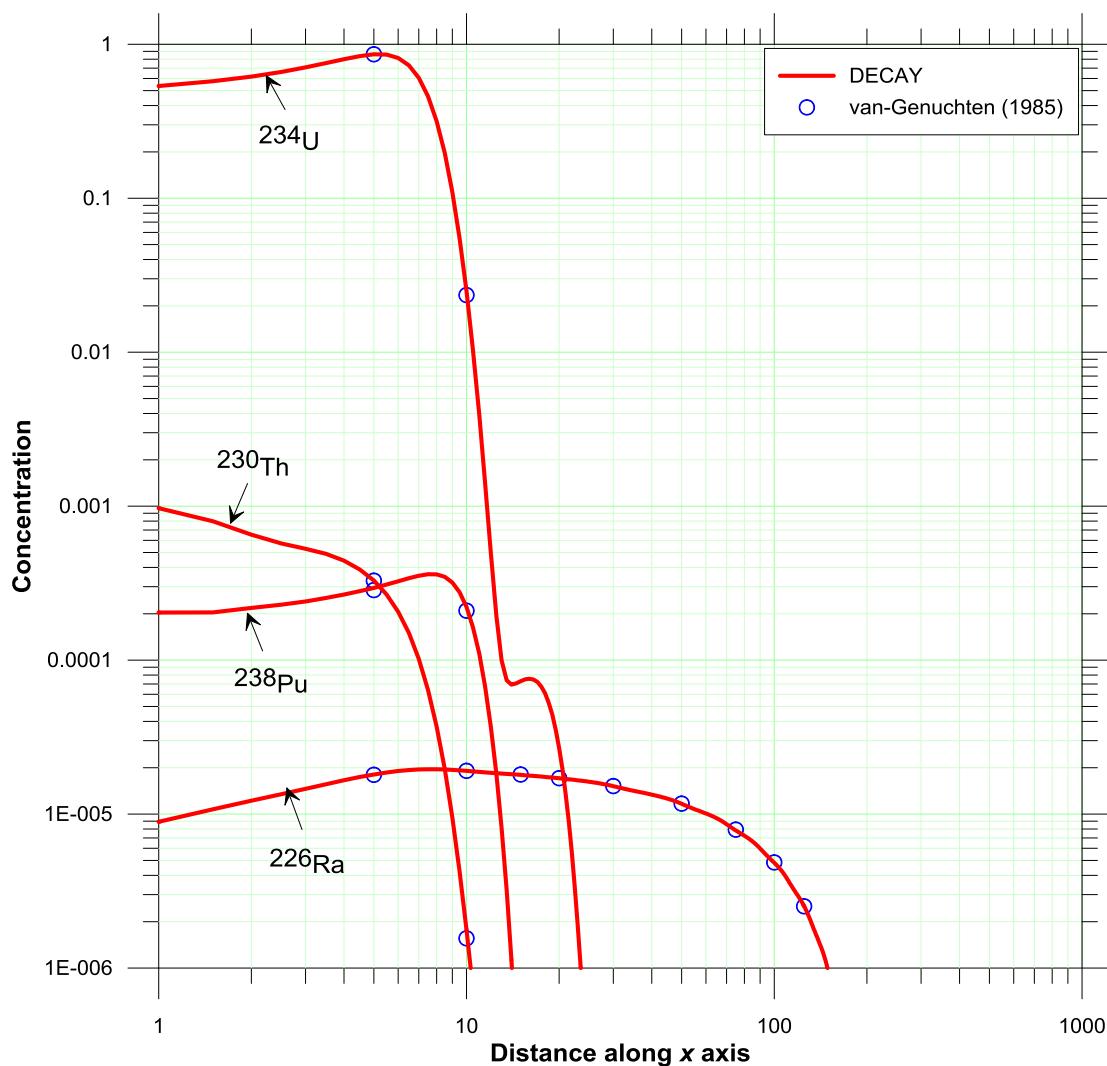


Figure 9 Concentration profiles at 1000 years for a radioactive straight-chain decay

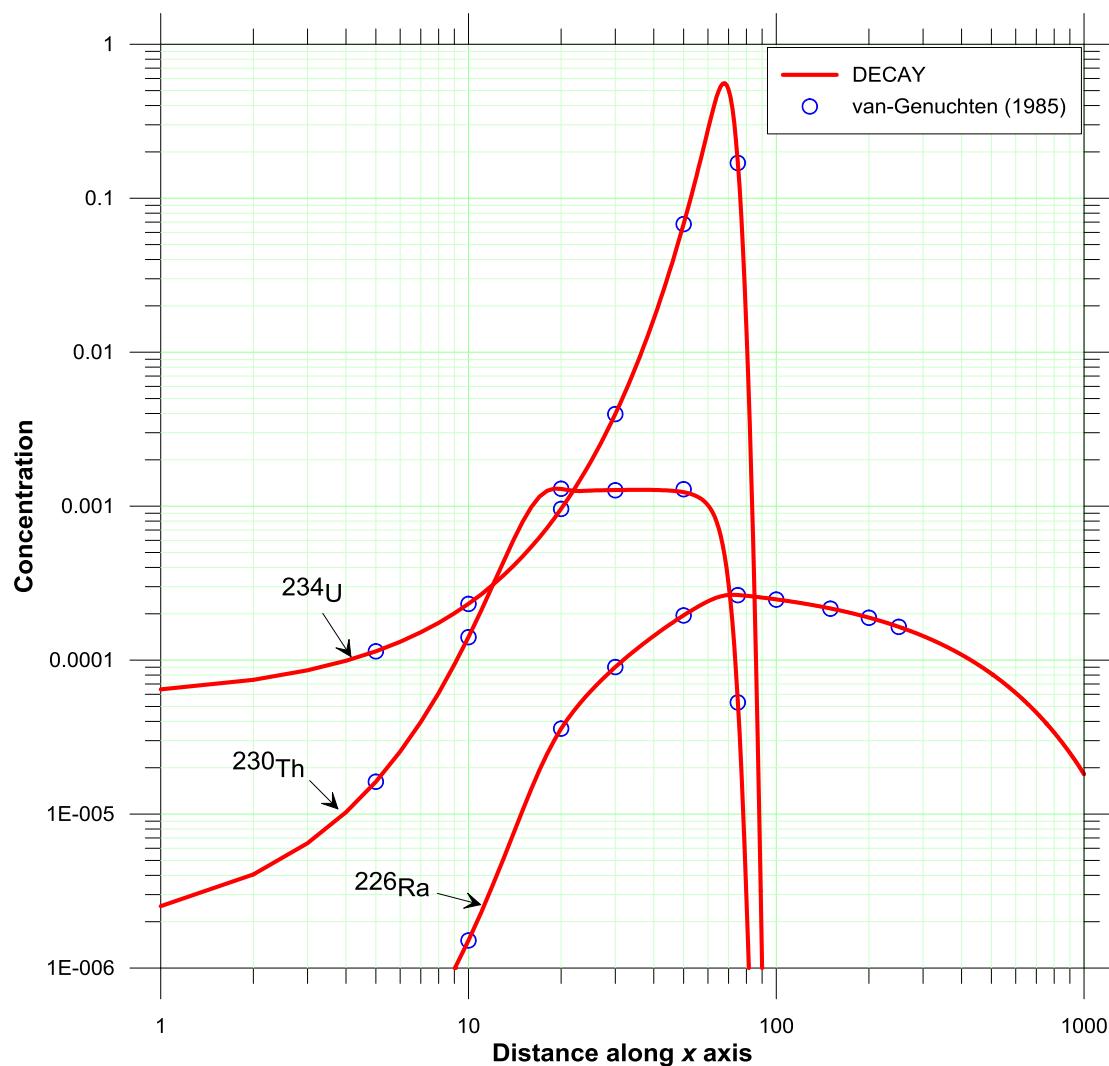


Figure 10 Concentration profiles at 10000 years for a radioactive straight-chain decay

Testing Part 2: Branching reactions

Eight test cases have been designed to test the implementation of the DECA^Y solution for branching reactions. The decay sequences considered for testing are depicted in Figure 11. The results for Test (a) are compared against Sudicky et al. (2013, Section 3.2) and Tests (b) – (h) are compared against the numerical results of MT3D-USGS (2016/01/13 update).

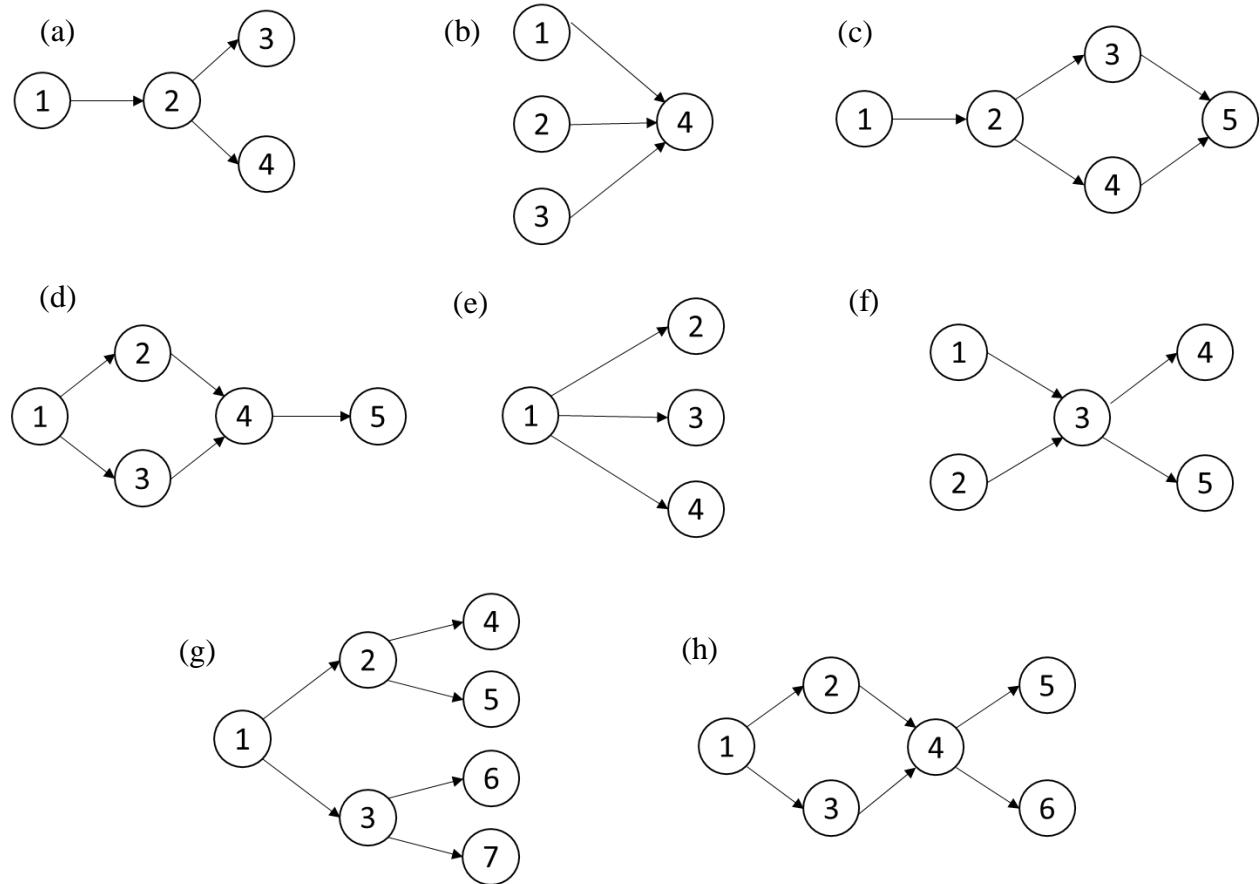
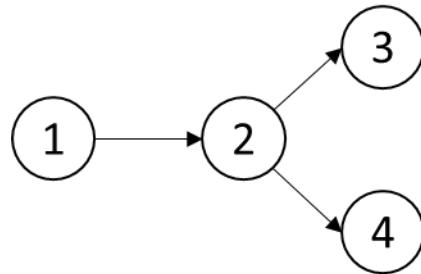


Figure 11 Decay chains for Tests (a) – (h)

1. Test (a)



The input parameters for the Test (a) are tabulated on Table 5 and the results are plotted in Figure 12.

Table 5 Input parameters for Test (a)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 |
|---|-----------------------|-----------------------|-----------------------|-----------------------|
| Darcy flux q (m/year) | 0.03 | | | |
| Porosity ϕ (-) | 0.1 | | | |
| Bulk density ρ_b (g/cm ³) | 1.0 | | | |
| Dispersion coefficient D (m ² /year) | 3 | 3 | 3 | 3 |
| Sorption coefficient K_d (cm ³ /g) | 0.05 | 0.2 | 0.0 | 0.0 |
| Dissolved phase decay rate (year ⁻¹) | 6.93×10^{-3} | 3.47×10^{-3} | 1.16×10^{-3} | 1.00×10^{-3} |
| Sorbed phase decay rate (year ⁻¹) | 6.93×10^{-3} | 3.47×10^{-3} | 1.16×10^{-3} | 1.00×10^{-3} |
| Yield coefficient (-) | 0.0 | 1.0 | 1.0 | 1.0 |
| Branching ratio (-) | 1.0 | 1.0 | 0.5 | 0.5 |
| Initial concentration (-) | 1.0 | 1.0 | 1.0 | 1.0 |

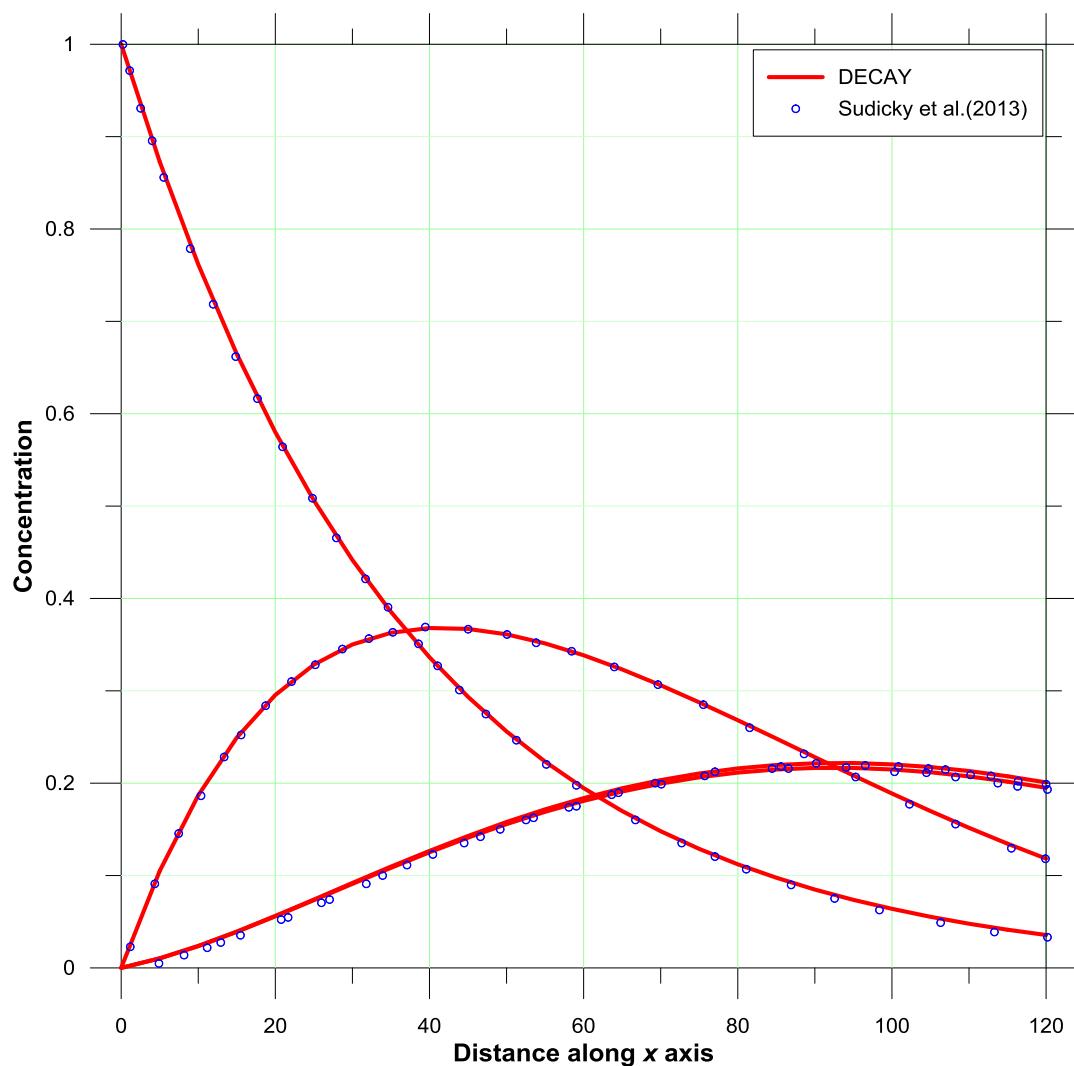
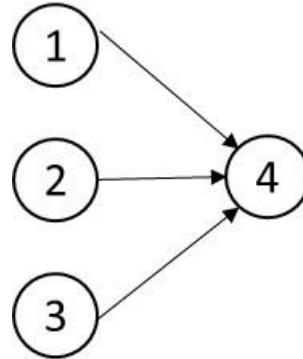


Figure 12. Concentration profiles at 600 years for Test (a)

2. Test (b)



A numerical model was set up to assess the results of the analytical solution for Tests (b) – (h). Because MT3D-USGS cannot handle reactions on the sorbed phase, sorbed phase decay rates for each species are assigned zero in the DECA input file. The values of Darcy flux, porosity, bulk density and dispersion coefficient are identical and are presented on Table 6.

Table 6 Common input parameters for Tests (b) – (h)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 |
|--|-----------|-----------|-----------|-----------|
| Darcy flux q (m/day) | 0.01 | | | |
| Porosity ϕ (-) | 0.1 | | | |
| Bulk density ρ_b (g/cm ³) | 1.0 | | | |
| Dispersion coefficient D (m ² /day) | 0.18 | 0.18 | 0.18 | 0.18 |

The other parameters of Test (b) required by DECA are listed on Table 7.

Table 7 Other input parameters for Test (b)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 |
|---|-----------------------|-----------------------|-----------------------|-----------------------|
| Sorption coefficient K_d (cm ³ /g) | 0.0 | 0.0 | 0.0 | 0.0 |
| Dissolved phase decay rate (day ⁻¹) | 6.93×10^{-3} | 3.47×10^{-3} | 1.16×10^{-3} | 1.00×10^{-3} |
| Yield coefficient (-) | 0.0 | 0.0 | 0.0 | {1.0,1.0,1.0} |
| Branching ratio (-) | 1.0 | 1.0 | 1.0 | {1.0,1.0,1.0} |
| Initial concentration (-) | 1.0 | 1.0 | 1.0 | 0.0 |

The results generated from DECY and MT3D-USGS are plotted in Figure 13. The slight mismatches at the ends of the profiles arise because the analytical solution assumes a semi-infinite domain whereas the numerical model terminates with a zero dispersive-flux boundary condition.

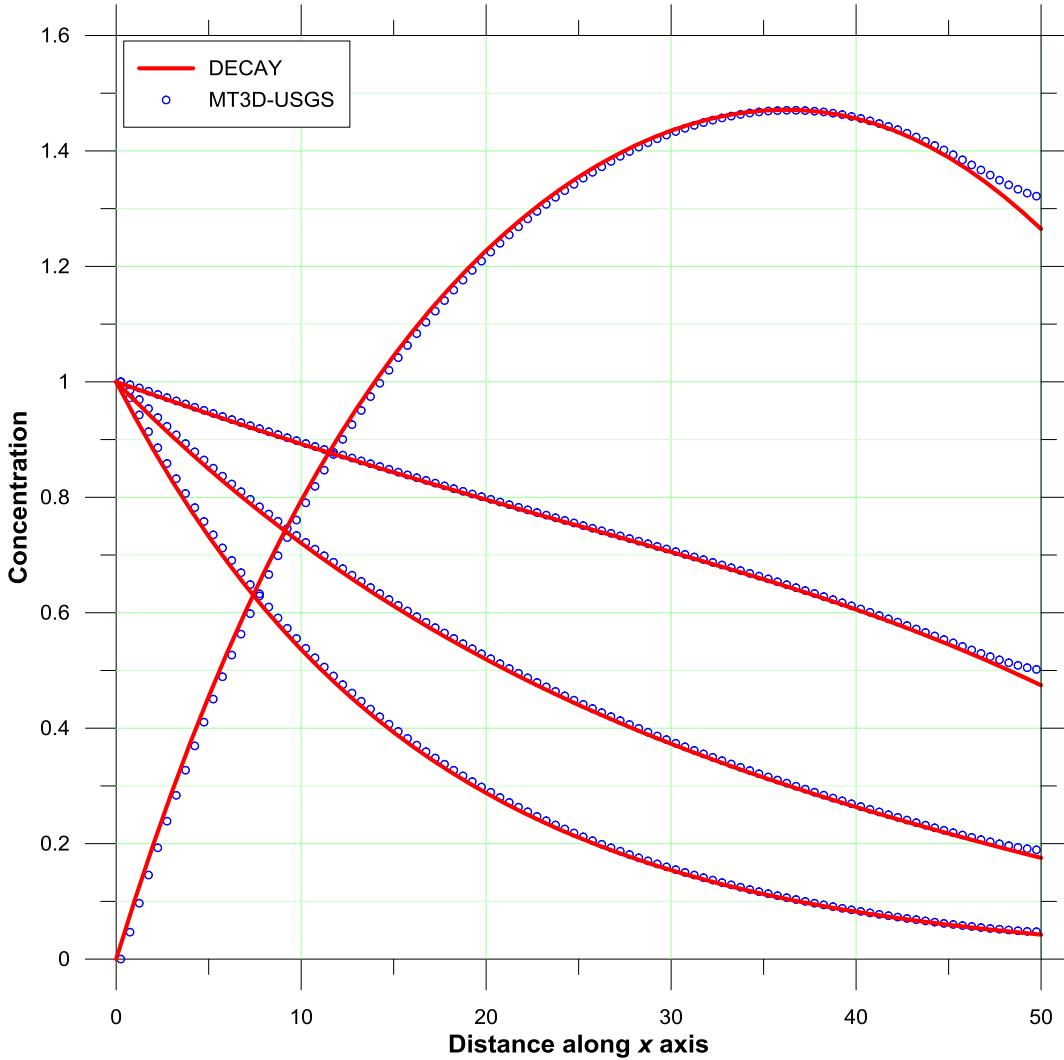
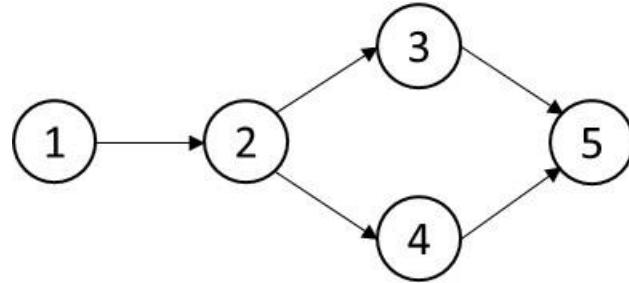


Figure 13 Concentration profiles at 600 days for Test (b)

3. Test (c)



The input parameter and the results are presented on Table 8 and in Figure 14, respectively.

Table 8 Other input parameters for Test (c)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 | Species 5 |
|---|----------------------|----------------------|----------------------|----------------------|----------------------|
| Sorption coefficient K_d (cm ³ /g) | 0.05 | 0.05 | 0.1 | 0.1 | 0.1 |
| Dissolved phase decay rate (day ⁻¹) | 5.0×10^{-3} | 3.0×10^{-3} | 1.5×10^{-3} | 2.0×10^{-3} | 1.0×10^{-3} |
| Yield coefficient (-) | 0.0 | 0.792 | 0.738 | 0.738 | {0.645,0.645} |
| Branching ratio (-) | 1.0 | 1.0 | 0.2 | 0.8 | {1.0,1.0} |
| Initial concentration (-) | 1.0 | 0.0 | 0.0 | 0.0 | 0.0 |

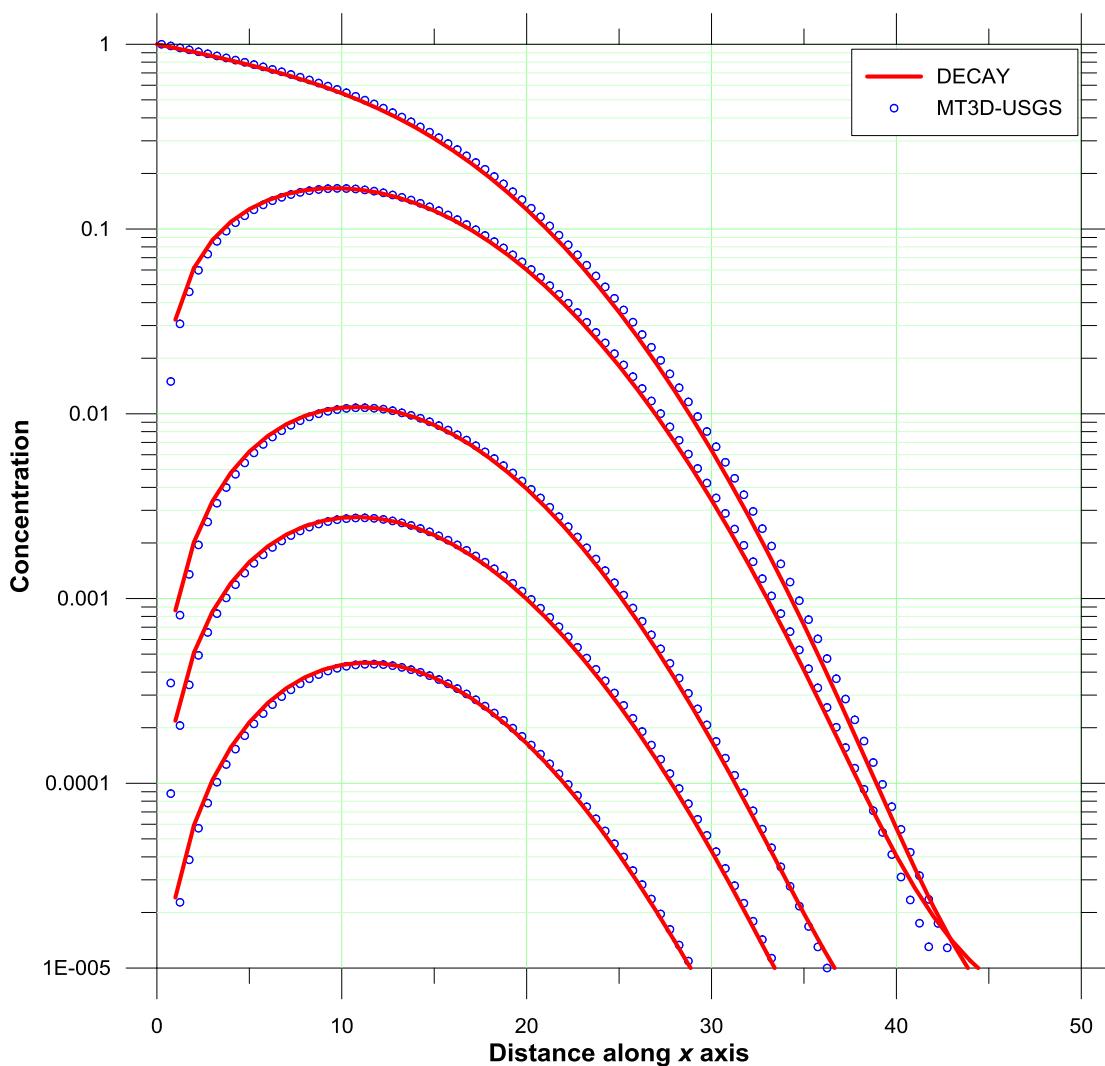
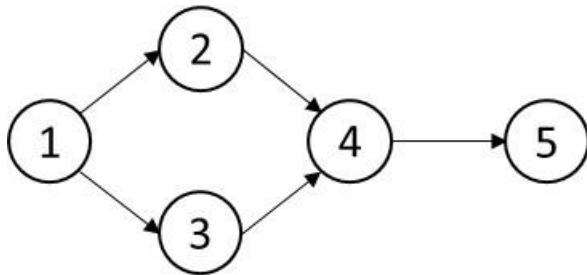


Figure 14 Concentration profiles at 200 days for Test (c)

4. Test (d)



The input parameter and the results are presented on Table 9 and in Figure 15, respectively. For simplicity, sorption is not considered for Tests (d) – (h).

Table 9 Other input parameters for Test (d)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 | Species 5 |
|--|----------------------|----------------------|----------------------|----------------------|----------------------|
| Dissolved phase decay rate (day^{-1}) | 3.0×10^{-3} | 2.0×10^{-3} | 2.0×10^{-3} | 1.0×10^{-3} | 5.0×10^{-4} |
| Yield coefficient (-) | 0.0 | 0.738 | 0.738 | {0.645,0.645} | 0.449 |
| Branching ratio (-) | 1.0 | 0.2 | 0.8 | {1.0,1.0} | 1.0 |
| Initial concentration (-) | 1.0 | 0.0 | 0.0 | 0.0 | 0.0 |

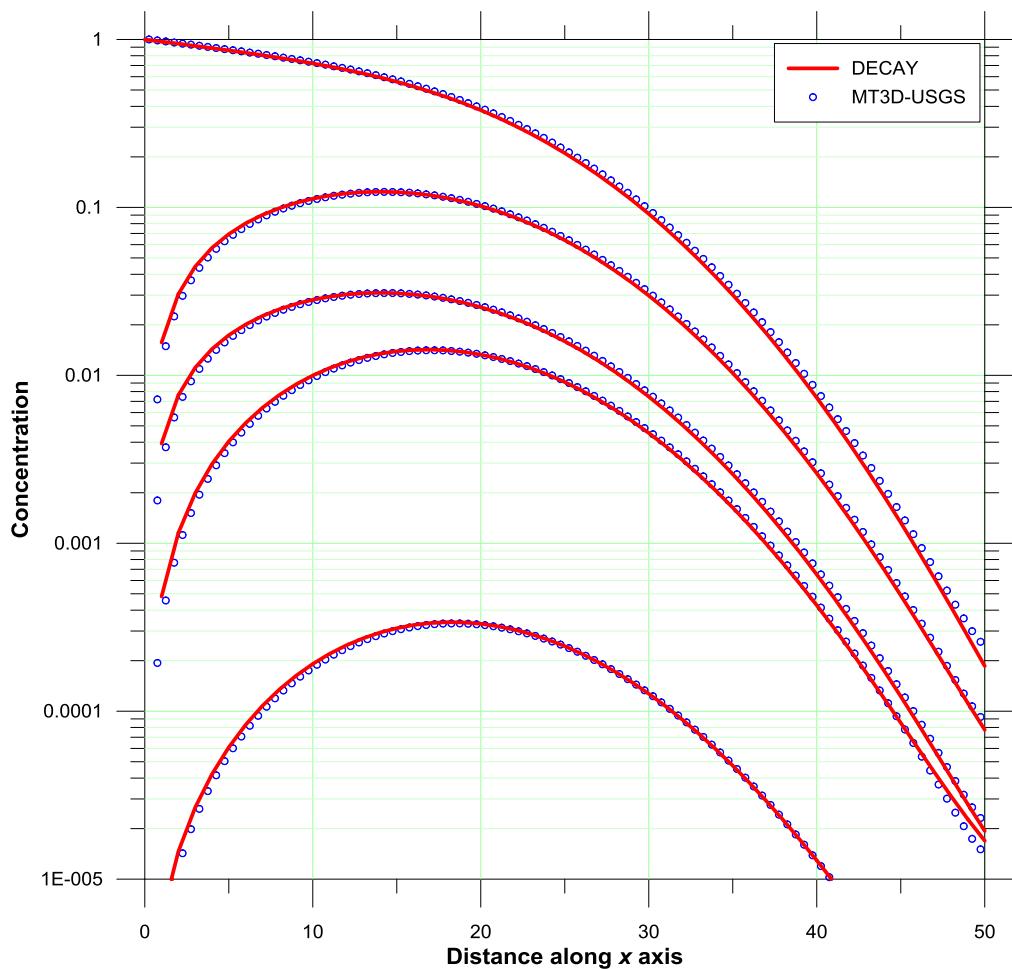
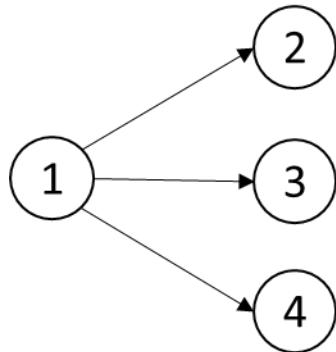


Figure 15 Concentration profiles at 200 days for Test (d)

5. Test (e)



The input parameter and the results are presented on Table 10 and in Figure 16, respectively.

Table 10 Other input parameters for Test (e)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 |
|---|-----------------------|-----------------------|-----------------------|-----------------------|
| Dissolved phase decay rate (day ⁻¹) | 6.93×10^{-3} | 3.47×10^{-3} | 1.16×10^{-3} | 1.00×10^{-3} |
| Yield coefficient (-) | 0.0 | 1.0 | 1.0 | 1.0 |
| Branching ratio (-) | 1.0 | 0.5 | 0.3 | 0.2 |
| Initial concentration (-) | 1.0 | 0.0 | 0.0 | 0.0 |

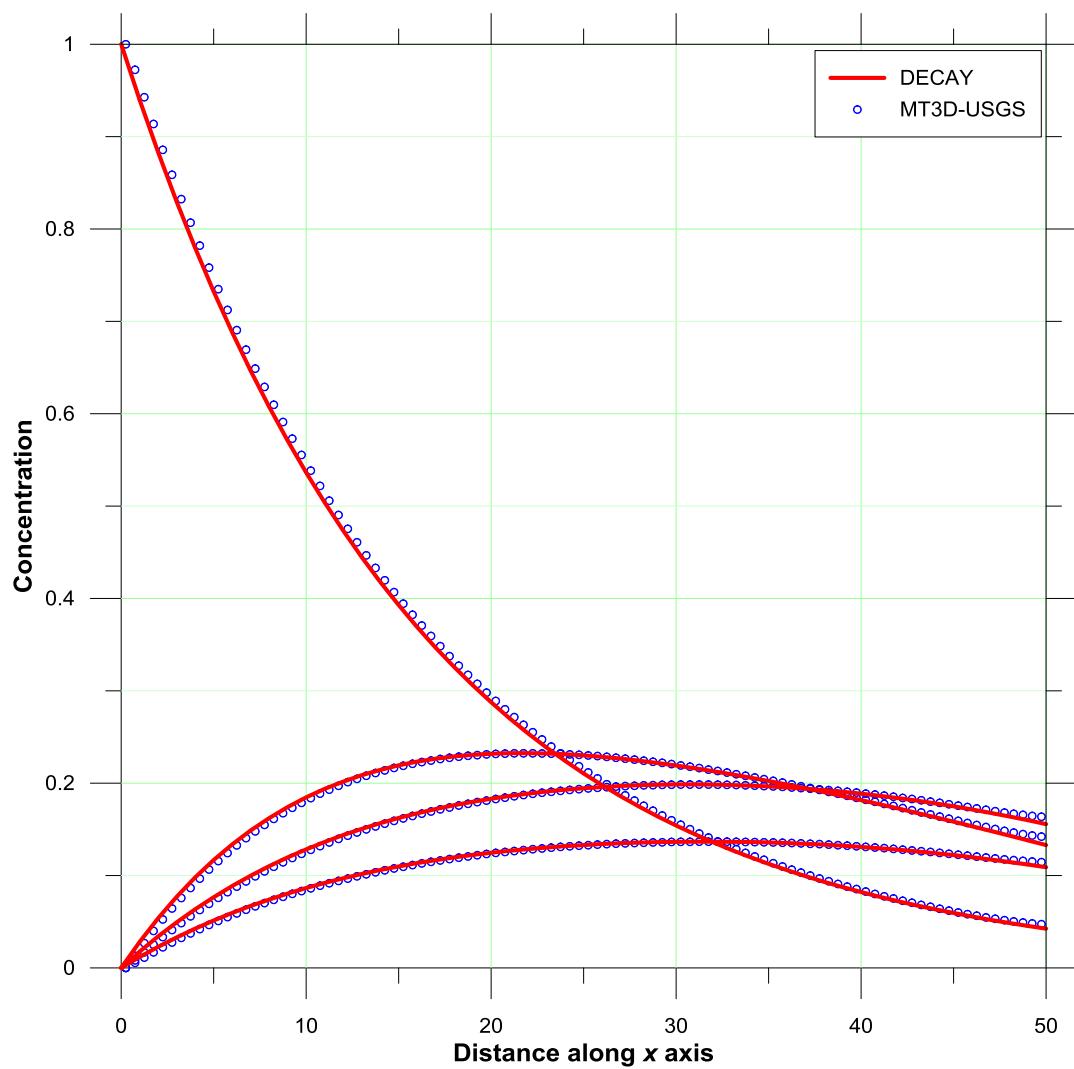
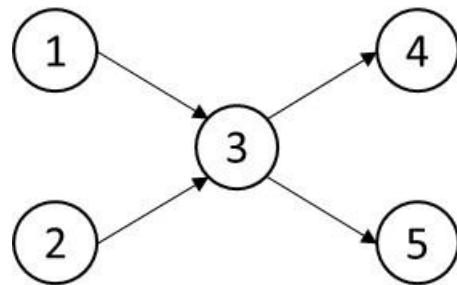


Figure 16 Concentration profiles at 600 days for Test (e)

6. Test (f)



The input parameter and the results are presented on Table 11 and in Figure 17, respectively.

Table 11 Other input parameters for Test (f)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 | Species 5 |
|---|----------------------|----------------------|----------------------|----------------------|----------------------|
| Dissolved phase decay rate (day ⁻¹) | 5.0×10^{-3} | 3.0×10^{-3} | 1.5×10^{-3} | 2.0×10^{-3} | 1.0×10^{-3} |
| Yield coefficient (-) | 0.0 | 0.0 | {1.0, 1.0} | 1.0 | 1.0 |
| Branching ratio (-) | 1.0 | 1.0 | {1.0, 1.0} | 0.6 | 0.4 |
| Initial concentration (-) | 1.0 | 1.0 | 0.0 | 0.0 | 0.0 |

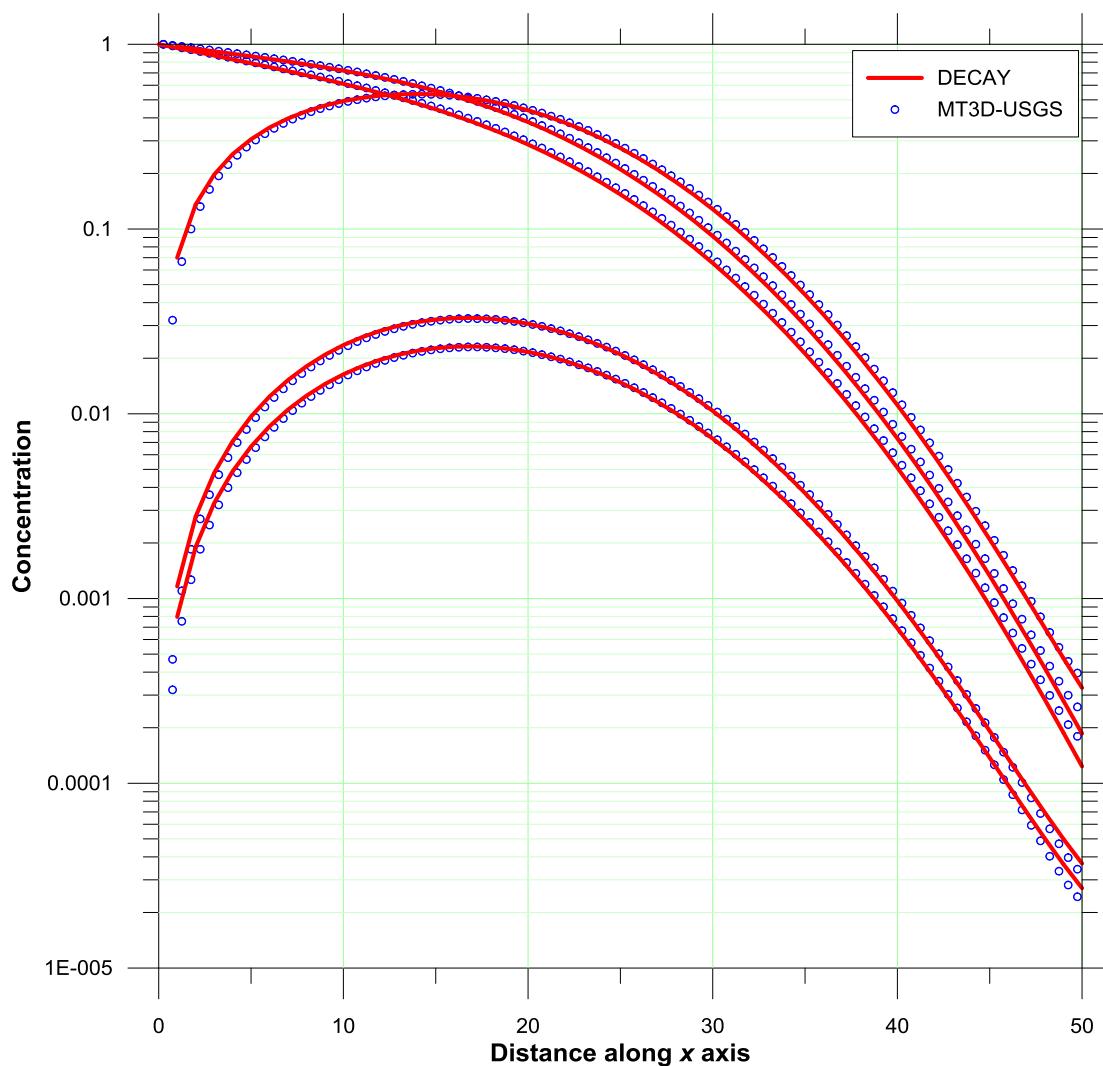
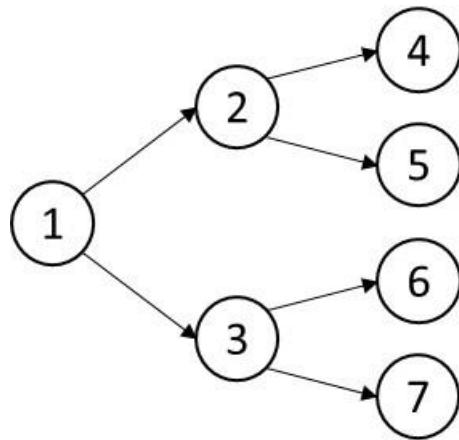


Figure 17 Concentration profiles at 200 days for Test (f)

7. Test (g)



The input parameter and the results are presented on Table 12 and in Figure 18, respectively.

Table 12 Other input parameters for Test (g)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 | Species 5 | Species 6 | Species 7 |
|---|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| Dissolved phase decay rate (day ⁻¹) | 5.0×10^{-3} | 3.0×10^{-3} | 1.5×10^{-3} | 2.0×10^{-3} | 1.0×10^{-3} | 5.0×10^{-4} | 5.0×10^{-4} |
| Yield coefficient (-) | 0.0 | 0.0 | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 |
| Branching ratio (-) | 1.0 | 0.4 | 0.4 | 0.6 | 0.4 | 0.6 | 0.4 |
| Initial concentration (-) | 1.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

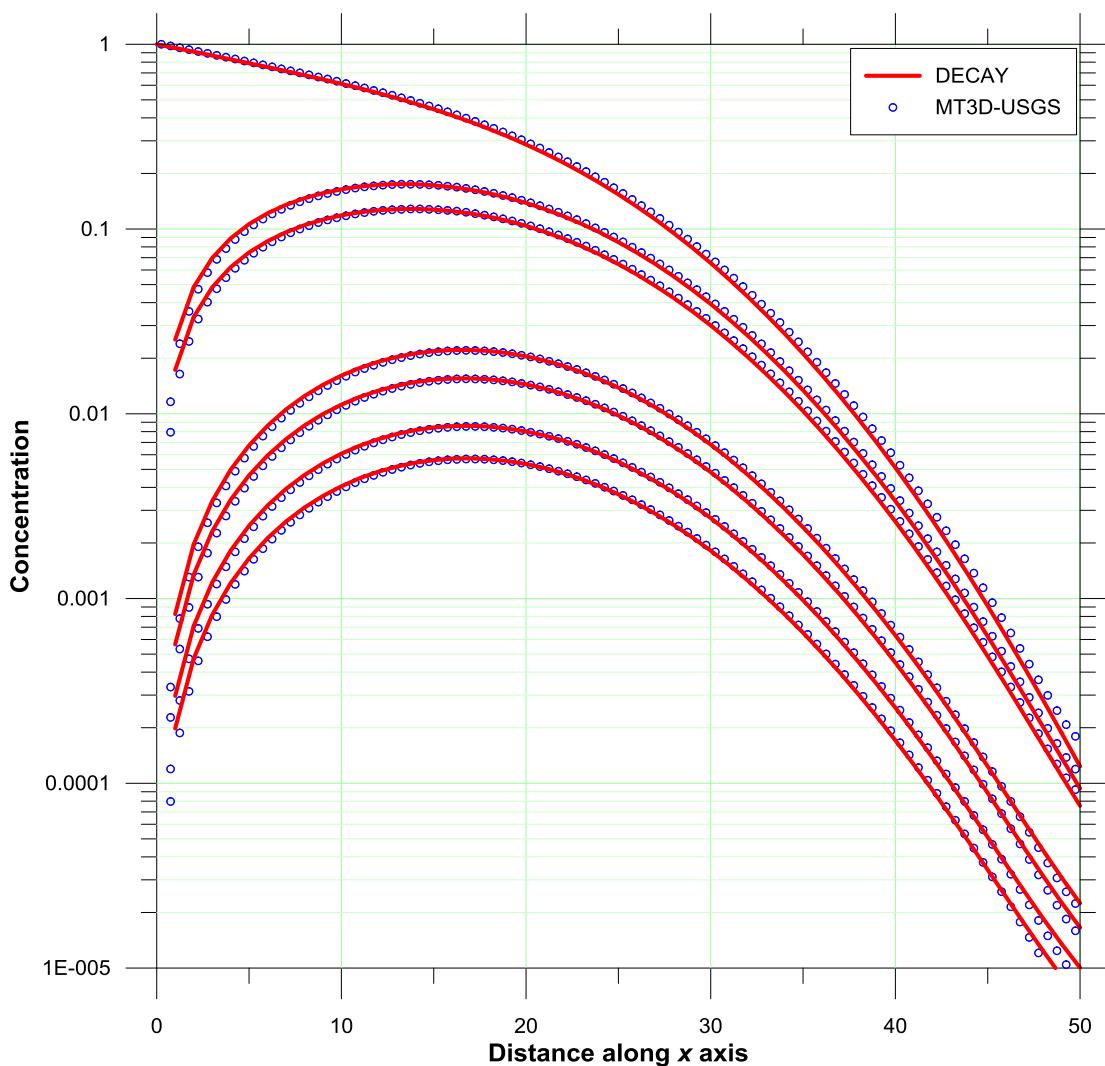
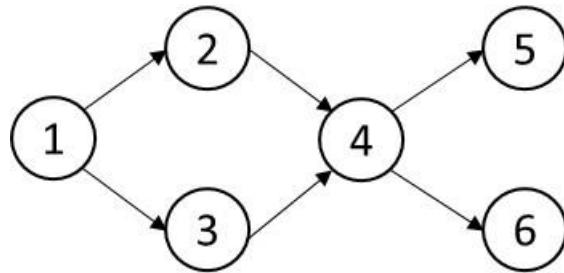


Figure 18 Concentration profiles at 200 days for Test (g)

8. Test (h)



The input parameter and the results are presented on Table 13 and in Figure 19, respectively.

Table 13 Other input parameters for Test (h)

| Parameters | Species 1 | Species 2 | Species 3 | Species 4 | Species 5 | Species 6 |
|--|----------------------|----------------------|----------------------|----------------------|----------------------|----------------------|
| Dissolved phase decay rate (day^{-1}) | 5.0×10^{-3} | 3.0×10^{-3} | 1.5×10^{-3} | 2.0×10^{-3} | 1.0×10^{-3} | 5.0×10^{-4} |
| Yield coefficient (-) | 0.0 | 1.0 | 1.0 | {1.0, 1.0} | 1.0 | 1.0 |
| Branching ratio (-) | 1.0 | 0.6 | 0.4 | {1.0, 1.0} | 0.6 | 0.4 |
| Initial concentration (-) | 1.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |

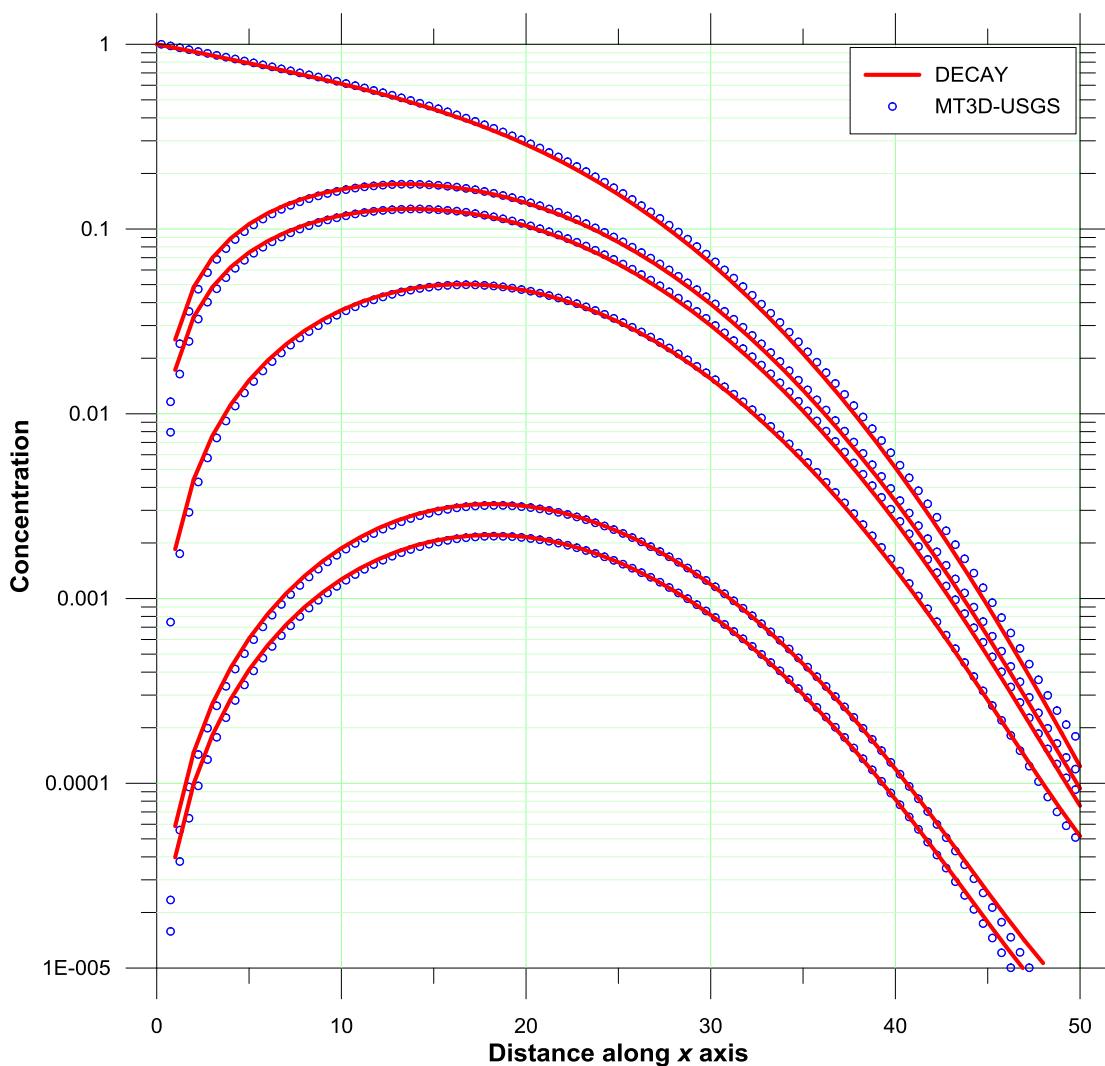


Figure 19 Concentration profiles at 200 days for Test (h)

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