

Supplementary material for

“Benchmarking dual continuum method for multicomponent reactive transport”

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List of input files

The PFLOTRAN input files used in the manuscript are available at https://github.com/aitorig/Benchmarking_dual_continuum_method_for_multicomponent_reactive_transport-Supplementary_material. Table 1 shows the list of files included in the repository along with an ID that is used to provide a brief description of each input file (next section).

Table 1. Input files included in the gitlab repository.

File name	ID
matrix_2d_C.in	f1
regions.h5	f2
velocity_fracture.h5	f3
hanford.dat	f4
1D_multicontinuum_N20_slab.in	f5
1D_multicontinuum_N50_slab.in	f6
1D_multicontinuum_N75_slab.in	f7
1D_multicontinuum_N500_slab.in	f8
1D_multicontinuum_N20_NC_1_10_minus_2.in	f9
1D_multicontinuum_N20_NC_1_10_minus_3.in	f10
1D_multicontinuum_N20_NC_6_10_minus_4.in	f11
1D_multicontinuum_N60_NC_6_10_minus_4.in	f12

Brief description of the input files

f1 is the PFLOTRAN input deck that corresponds to the 2D independent solution used in Figure 3 to Figure 9 of the manuscript (Benchmark#1 and Benchmark#2). This simulation uses f2 and f3 as input files (definition of regions and velocity file) along with the thermodynamic database (f4). Files f1 to f4 are located inside the “2D_input” folder in the repository.

f5 to f8 are the input decks used to produce the results of Figure 3 (Benchmark#1) and Figures 4 and 5 (Benchmark#2).

f9 to f11 are the input decks used to produce the results of Figures 6 and 7 while f12 is the input deck for the additional calculation shown in Figures 8 and 9.