**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.