

## Supplementary material for

### “Assessing dual continuum method for multicomponent reactive transport”

**Aitor Iraola<sup>1</sup>, Paolo Trinchero<sup>1</sup>, Satish Karra<sup>2</sup>, Jorge Molinero<sup>1</sup>**

<sup>1</sup>AMPHOS 21 Consulting S.L., Passeig de Garcia i Faria, 49-51, 1-1, 08019 Barcelona, Spain.

<sup>2</sup>Computational Earth Science Group, Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.

#### 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](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 PFLOTTRAN 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 additional calculation shown in Figures 8 and 9.