Geoscientific Model Development Discussions

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Comment on gmd-2022-86

Anonymous Referee #1

Referee comment on "P3D-BRNS v1.0.0: a three-dimensional, multiphase, multicomponent, pore-scale reactive transport modelling package for simulating biogeochemical processes in subsurface environments" by Amir Golparvar et al., Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2022-86-RC1, 2022

This paper describes a new open-source toolbox for simulating reactive biogeochemical processes at the pore scale. It couples OpenFoam, for interface tracking and fluid flow, with the Biogeochemical Reaction Network Simulator (BRNS), for complex reactions. An improved VoF solver is implemented based on the procedure proposed by Raeini et al. (2012). The code is validated with three test cases where analytical solutions are available. Finally, the capability of the model to represent realistic scenarios is tested on a 3D microstructure with coupled two-phase flow and bacterial growth following a complex set of reactions.

The manuscript is well written and clearly and concisely documents the model and the implementation. Coupling two-phase flow to complex reactions in a complicated pore space is a nontrivial task. However, based on the thoroughly presented benchmark tests it seems this code is able to do it in an efficient manner. Hence I believe that the P3D-BRNS toolbox will be of great benefit to the community. Provided the authors can satisfactorily answer the minor remarks below, I will recommend publication in GMD.

Minor remarks:
- E.g. in order to computationally bridge the gap between pore scale and macro scale, it is crucial to be able to scale up the system size. It is well-documented that OpenFoam is well parallelized and given that reactions are local, so should BRNS. However, the paper seems to lack a description of strong or weak scalability. Could the authors please elaborate on this?
- In at least one of the test cases 3.1--3.3, it would be useful with a discussion on how grid resolution affects the convergence to the analytical solution.
- Are osmotic forces included in the model? There is no force term in Eq. (2) due to gradients in the chemical potential, however it could be accomodated by a re-interpretation of the pressure P. Would P3D-BRNS be able to model e.g. droplet motion due to a concentration gradient and solubility difference in the two phases?
- section 3.1: How was the mesh generated? Is it skewed or staircase-like at the diagonal side? How is the sharp top corner handled? Some more information here would be useful.

Typos/formatting:
- Caption of Fig. 1 also inserted at line 115.
- line 359: incomplete sentence
- line 412: simluations --> simulations
- line 487: growth --> grow