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Comment on egusphere-2022-1016

Anonymous Referee #1

Referee comment on "CompLaB v1.0: a scalable pore-scale model for flow, biogeochemistry, microbial metabolism, and biofilm dynamics" by Heewon Jung et al., EGUsphere, https://doi.org/10.5194/egusphere-2022-1016-RC1, 2022

Review of egusphere-2022-1016

The manuscript "CompLaB v1.0: a scalable pore scale model for flow, biogeochemistry, microbial metabolism, and biofilm dynamics" by Jung et al. (egusphere-2022-1016) introduces a modular numerical model approach for reactive transport and microbial growth in fully water saturated pore structures. The model can implement/consider high resolution scans of porous media as well as microbial metabolic reaction networks from databases, two growing sources of information on subsurface environment and the processes therein. Model linking this information to reactive transport simulations are still scarce which makes the presented model a potentially very useful tool. The manuscript is well written and introduces the model and its different features. Results on the accuracy and on the model performance are shown.

I suggest publication of this manuscript after some moderate revisions. In addition to my comments below, these revisions should clarify which parts of the model have been introduced and verified before and which parts are new and need to be verified in the manuscript (if not done already). I have no worries regarding the technical accuracy of the model but more information on this would be good. This would then also allow determining where the presented model is more advanced than previous models. I also think it would help to show more results of the presented simulation examples (in the manuscript or in some supplement) to a) demonstrate the model performance and b) to allow putting the discussed results in a better context.

Specific comments:

Introduction: I am missing a bit some statements on what exists already for modeling reactive transport and microbial processes at the pore scale There are several rather recent reviews on this (e.g., König et al., 2020, doi: 10.3389/fevo.2020.00053; Golparvar et al., 2021, DOI: 10.1002/vzj2.20087; Pot et al., 2022, DOI: 10.1111/ejss.13142).

L 79: Clarify if "based on the LB method implemented in Jung and Meile" means you are using the previously established code and implement the new features or you have code new flow and transport modules based on the same LB concept. This determines which parts of the model need to be verified in this manuscript and for which parts a verification is given already in previous publications.

L 120: How is this combination achieved?

L 124: Clarify if the considered microbial dynamics are limited to specific example processes (and their kinetic expressions) or if any arbitrary (user defined) processes/rate expressions can be used.

Section 3.2.1: Related to my comment above, in case any arbitrary set of rate expressions can be considered the approach is a) not limited to microbially controlled reactions and b) would conceptually not make a difference between the concentration of biomass and chemical compounds. It is thus not clear to me why there is a distinction between these concentrations at this stage. At the end Eq. 5 is just a specific version of Eq. 6 in case of R is given as gamma*B.

L 148-162: Is there any specific reason why these variables must have the given units?

L 213-220: Were the imposed initial and boundary conditions comparable to the reference models and the experiments?

L 228-229: How is it shown that the composition of the bacteria is stable? Fig. 3 shows that after 48 all approaches exhibit approximately the same composition but not that this composition will not change later on.

L 251-253: How well could the results of the FBA simulations be fitted by a kinetic approach using a Michaelis-Menten consumption rates with the parameters given here and a constant growth yield fitted to the FBA results?

L 273: To which length scale does the Peclet number refer to?

L 312: What was the time step size?

Fig. 5 and associated text passages: It would have been interesting to see how the "traditional" KNS approach without the CA performs compared to the ANN approach. This would also show how much additional computation time the CA requires (besides the larger time for the flow (and transport?) simulation. Since most of the shown examples consider steady state conditions for the flow field but transient conditions for the transport I am wondering why only the computation time for flow and transport together is shown.

L 323-324: Following my comment above: Is this shown somewhere?

L 328 and Figure A1: Clarify that this a relative error for the biomass/metabolites in the system.

L 329-331: In this context it would be interesting to know how much computational effort was needed to run the Monte Carlo simulations for training the ANN model. I am aware that quantifying the training effort is not straight forward but some words on this would be helpful.

L 340-343: I do not get this argument. If I assume that each methods invest a given time for computation in the biomass cells and an and a given time for computation (wasted) in the non-biomass cells why should they differ in their scaling behavior? Furthermore, since detachment and attachment of the biomass is considered there would be biomass also ending on initially uninhabited surfaces. Perhaps it would be good to actually show some results of these simulations and not only the computation times. Similarly to my comment above: How is the scalability of the KNS approach without CA?

L 370: "Soil" might not be the best key word here since soils are typically only partially water saturated while the presented code considers fully saturated conditions. Better to use e.g. "porous media".