



EGUsphere, referee comment RC1
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Comment on egusphere-2022-1419

Albert Valocchi (Referee)

Referee comment on "Multi-phase Biogeochemical Model for Microbially Induced Desaturation and Precipitation" by Caitlyn A. Hall et al., EGU sphere,
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Overall evaluation

The manuscript presents modeling-related research funded by the Center for Bio-mediated and Bio-inspired Geotechnics at Arizona State University. One major thrust of the Center is to develop Microbially Induced Desaturation and Precipitation (MIDP) as a viable technology to modify soil mechanical properties for mitigation of earthquake-induced liquefaction. The Center integrates theory, laboratory experimentation, field demonstration and mathematical modeling. Building upon other earlier modeling work, this manuscript presents and demonstrates a biogeochemical model that includes multiple bacterial species with competition among multiple electron acceptors, inhibition, multiple gas species, general mineral equilibria and aqueous speciation, and precipitation/dissolution kinetics. These additional processes included in this 'next-generation' model are essential to account for site-specific geochemical conditions and mineralogy. A major motivation for the work is to apply MIDP in coastal regions where the local source water may be high in sulfates, which will act as a competing electron acceptor for the target acceptor, nitrate. This is the case study used in the manuscript to demonstrate model capabilities.

The manuscript is clearly written and concise. While most of the processes represented in this "next generation" model are within the capability of existing general and flexible reactive transport models (e.g., CrunchFlow, PFLOTRAN, Min3P, Reaktoro), the specific focus on MIDP processes is unique. In my opinion the model is a substantial contribution that will be of interest to researchers not only in the field of soil improvement, but also in the general area of reactive transport.

With all models of this type, there is the challenging question of parameterization and uncertainty. I recommend the authors address these issues more directly. There should at least be more discussion in the text. Even better (but perhaps not feasible)-- I recommend a limited sensitivity analysis showing how the choice of parameter values affects the results; it may only be necessary to consider a few of the more uncertain parameters, assumed initial conditions, etc. This could be reported in the Supplement. I also realize that it may not be possible to show any direct comparison with experimental data, but are there any qualitative laboratory or field observations (e.g., from the Portland Oregon field demonstration) that would give some confidence in the trends reported in Section 4?

Specific Comments

- Line 54. I like Table A.1 that summarizes the capabilities of different models. There is a paper that just was published in Water Resources Research by some of these same authors (<https://doi.org/10.1029/2022WR032907>) - should this be included?
- Consider adding a schematic 'cartoon' showing a porous medium representative elementary volume with liquid, gas, biomass phases, relevant biogeochemical processes, etc.
- 50, Sec. 2, Model Foundation. I am not familiar with the van Turnhout Toolbox. This is used to solve the coupled system on nonlinear ordinary equations, coupled with the nonlinear algebraic equations for aqueous speciation. Can you add a few sentences to explain more about the numerical techniques used?
- 81, eqn (1). I believe there are other mathematical forms to account for the impact of an inhibitory compound (e.g., Haldane Kinetics). Why is this form selected? Does this form only account for the 'inhibition' due to presence of a competing electron acceptor?
- 84. Can you comment on the assumed initial conditions for biomass of denitrifying and sulfate-reducing microbes? Are these 'typical'? I would expect that the simulation results might be highly sensitive to these values.
- 111, Table 3. The half maximum-rate constants are in units of mole/liter. Converting to mmole/L and looking at the conditions for the example simulation (Table 6) it appears that the K_d , K_a values may be much smaller than the aqueous concentrations so that the Monod terms reduce to zero-order rate expressions (max possible rate). This is just an observation and may warrant some sensitivity study since the half-max rate constants are highly variable in the literature.
- 119-120. Does the model formulation automatically switch between electron acceptors that are more thermodynamically favorable? How does the model switch to using ammonium as the electron acceptor?
- 135. The text states that K_i value is the same for inhibition of nitrate and nitrite reduction by nitric acid, however Table 4 has different values. Please explain.
- 3.3. I like the explanation in this section about computing the gas volume required to achieve target desaturation.
- 172. Sec. 3.3. As noted, the mass transfer coefficients are lumped values that are a function of the liquid-gas interfacial area. Therefore, I would expect there to be a dependence on the gas saturation. The sentence "We did not include pore-scale kinetics" is not clear. Does this sentence mean that you did not account for changing interfacial area? Given the complexity and uncertainty in modeling kinetic mass transfer, why not just use equilibrium partitioning? Is there field or laboratory evidence that kinetics are needed? I would expect the mass transfer coefficient would also be a highly sensitive parameter. The default value assumed (5 per day) is from a paper on sewer networks. I recommend checking the groundwater remediation literature (e.g., air sparging) for more representative values.
- 185. Should the symbol $[NO_3]_d$ be added to Table 1?
- 204, Eqn (8). I do not understand the statement that this rate expression is first-order with- respect-to calcium concentration, since the product $[Ca] [CO_3]$ is in the denominator. Calcite precipitation and dissolution has been studied extensively in the geology/geochemistry literature and I suggest adding a few key citations (e.g., Chou, L., R. M. Garrels, and R. Wollast (1989), Comparative study of the kinetics and mechanisms of dissolution of carbonate minerals, Chem. Geol., 78, 269–282.). As noted, calcite precipitation is a complex process and there are several calcium carbonate polymorphs of different stability.
- 217, Sec. 3.5. Does the modeling framework allow for the presence of other mineral phases at equilibrium with the aqueous solution?
- 255-260, Table 6. I am a little confused by the treatment recipes. I was expecting to see numbers in Table 6 that were 25% greater and lesser than the matched case. L. 258 implies that the matched nitrate equals 22.4 mmol/L, but the table shows 19.0

mmol/L.

- 225, Sec. 4, Case Study. Table 5. Are there any solid mineral phases present at the start of the simulation? Should the initial fluid composition be in equilibrium with solid phases? This equilibrium is then perturbed by the input of the treatment fluid? Is there any possibility of iron minerals precipitating?
- Figs 1 & 2 simulation results. Please refer to my general comments regarding sensitivity analysis.