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Interactive comment on “Modeling the impact of soil aggregate size on selenium immobilization” by M. F. Kausch and C. E. Pallud

Anonymous Referee #3

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The manuscript discusses the application of a 2D reactive transport model to assess biologically mediated selenate reduction in an artificial soil aggregate under oxic and anoxic conditions. The model appears to accurately predict selenite breakthrough under varying geochemical and redox conditions. The application of a cell death parameter is a novel way of predicting loss of reactivity due to biological inactivation. After calibration of the model to the single soil aggregate size under varying conditions, additional modeling was performed to predict the effects of varying the diameter of the soil aggregate between 1 to 2.5 cm. The accuracy of the model here is more difficult to interpret since the initial calibration was performed on a single aggregate size of 2.5 cm. Overall, the results are promising and I believe the manuscript could be published after minor revisions.

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Specific Comments p12054, In 8-9: You state that the individual soil aggregates were placed in the center of the reaction cell and then a constant flow rate was applied. Was anything else packed in the cell or was the soil aggregate allowed to move around during the experiment? Based on the larger cell dimensions and the spherical nature of the aggregate, I would imagine that the aggregate would not remain stationary while under flow conditions. Do you think this could affect your modeling results?

p12054, In 20-22: Is 15min sufficient for sparging oxygen from the input solutions? This seems a little too short.

p12055, In4-10: It would have been useful to measure both total Se and selenite in the effluent. Since selenite is an intermediate in the reduction of selenate it's difficult to assess how well the treatment is working. Also, digestion of the aggregate (as you stated) can only give the total fraction of reduced selenium (assuming no absorption of selenate by the aggregate). Although it would not be possible for the current dataset, perhaps application of an X-ray technique such as XPS or XANES would be more useful for determining the oxidation state of Se present in different sections of the aggregate.

p12056, In 3: I didn't notice this in the current explanation of the model, but did you account for permeability changes within the aggregate during selenate reduction to elemental selenium?

p12058, In 1: Regarding the predictive simulations, would it be useful to have experimental data at the endpoints (i.e., at 1cm and 2.5cm) and interpolate between the known data, rather than extrapolating all the simulations from the single 2.5cm diameter size?

p12062, In 9-10: You state that concentrations of reactants (pyruvate, selenate, and oxygen) decreased towards the core. However, movie S3 shows that selenate concentrations increase in the aggregate and reach equilibrium with the reaction cell. Can you explain this? Wouldn't selenate rapidly reduce to selenite and elemental selenium

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within the aggregate?

p12068, In 14-15: Although elemental selenium is not affected by diffusive transport by virtue of being insoluble and immobile, would precipitation of elemental selenium within the pore space of the soil aggregate affect the diffusive flux of selenite? Presumably the permeability would decrease during selenite reduction. Did you model permeability/porosity changes during the experiment?

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