Response to comments of Ehsan Ranaee

On behalf of all co-authors, I sincerely thank Ehsan Ranaee for his thoughtful and detailed assessment of our work.

***ER**: Dear Editor, Thank you for sharing this manuscript with me.*

Authors extended their previously developed Lagrangian Soil Water and Solute Transport (LAST) model; and presented a novel modeling approach of diffusive pore mixing (DIPMI). This modeling strategy is implemented for simulating reactive solute transport in partially water saturated soil domains. A key development of this modeling approach (with respect to their farmer LAST model) is that DIPMI gets rid of assuming perfect mixing of solutes among water particles. To this end, DIPMI is developed to account for the self-diffusion of water particles across a characteristic length scale of the pore space using pore-size-dependent diffusion coefficients.

Authors tested DIPMI approach to reproduce some experimental findings (from the literature) with diffusive mixing of water isotopes over the pore space of a fully saturated soil volume. They also performed simulation of mixing of a representative solute in a vertical - saturated soil column and compare results of the DIPMI approach against the ones that employed common perfect-mixing assumption.

Authors suggest that imperfect mixing of water and solutes in the pore space can result long tailing of corresponding solute breakthrough curves which agrees with experimental outcomes. Indeed, solute breakthrough curves of the simulations with the LAST approach of perfect-mixing assumption may exhibit clear differences to experimental outcomes.

This work can provide some insights to the simulation of imperfect subscale mixing in a macroscopically homogeneous soil matrix.

The original idea sounds interesting to me, and I believe this paper can be published in HESS with very mild revisions.

AS: Thank you very much for your positive assessment of our work. In line with our response to Anonymous Referee #1, we appreciate that the scope and intention of our work, as well as the provided insights into simulating diffusive mixing on the pore scale, are all clear to the reader.

***ER**: In particular, I would suggest Author to extend the work by evaluating sensitivity of the simulation responses to the variation of the molecular diffusion coefficient values.*

AS: Thanks for your interesting suggestion. In fact, we already performed a kind of sensitivity analysis by determining the breakthrough curve simulations (cf. Figure 3) with significantly different diffusion coefficients *D,* in the setups with distributed (≙ mean: $9.7 \cdot 10^{-10}$ m²/s) and constant (≙ mean: $2.29 \cdot 10^{-9}$ m²/s) *D* values (≙ range of 58 %), as well as with the instantaneous, perfect-mixing assumption (≙ infinite diffusion coefficient: 10^{∞} m²/s). Further simulations with (i) higher/faster diffusion coefficient values will result in breakthrough curves with shorter tailings gradually approaching the shape of the curve of the perfect mixing assumption, and (ii) even smaller/slower diffusion coefficient values will result in breakthrough curves with increasingly longer tailings. Hence, we think that further sensitivity simulations would not yield significantly more insights. However, we will add a statement about the sensitivity of diffusion coefficients to the discussion, to explicitly address the point raised here.

***ER**: Legends and axis of Figure 4 are hardly visible.*

AS: Thank you for this point. We will increase the font size of the axis and legends to enhance the visibility of Figure 4.

Thank you very much,

Alexander Sternagel on behalf of all authors