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Comment on hess-2021-582

Ehsan Ranaee (Referee)

Referee comment on "Stepping beyond perfectly mixed conditions in soil hydrological modelling using a Lagrangian approach" by Alexander Sternagel et al., Hydrol. Earth Syst. Sci. Discuss., <https://doi.org/10.5194/hess-2021-582-RC2>, 2022

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 former 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

HES with very mild revisions. 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. Legends and axis of Figure 4 are hardly visible.