

***Interactive comment on* “Simulation of reactive solute transport in the critical zone: A Lagrangian model for transient flow and preferential transport” by Alexander Sternagel et al.**

Anonymous Referee #2

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Comments on the paper HESS-2020-527 entitled “Simulation of reactive solute transport in the critical zone. A Lagrangian model for transient flow and preferential transport”, by A. Sternagel et al.

This contribution proposes an interesting Lagrangian technique employing random walkers to solve both unsaturated flow and solute transport in a one-dimensional soil column. My understanding is that the so-called LAST model has been already published in HESS, but the present work would improve the model by giving it a preferential transport module in the form of advection in a macropore compartment. It also faces model results to actual experiments of water and reactive solute percolations from the

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surface in various soil columns.

The key fact that would justify the eventual publication of the paper is in the Lagrangian approach to flow (and incidentally transport), which is not very much widespread in the ongoing literature. The Richards equation is manipulated to form a non-linear Fokker-Planck-Kolmogorov equation (FPKE), then solved by classical advection-dispersion conveyed random walkers. These represent water parcels, to which a solute mass is added with the aim of solving transport. As there is no other set of particles specifically allotted to solve transport, the transport process is mainly advective but accounts for solute dispersion-diffusion by a “full mixing” process which states that all particles mapped onto a discrete cell of the soil column will share after a given time step the same solute mass, as the mean of the mass beard by all the particles within the cell. . . The process is slightly rough, but, provided that the time spent in the cell is enough, and provided that the macropore compartment is not assigned the same diffusive process, the whole is receivable.

The major concerns I have with the present writing are mainly associated with lacks in the depiction of the model. I remind that this model is the key justification for providing an innovative study. The authors often refer to the previous work by Sternabel et al. 2019, but the present writing becomes sometimes fuzzy and not self-containing, with the meaning that any reader should understand at first glance how physically the model works without relying upon multiple other readings.

The model manipulates particles as water parcels that, I guess, bear an elementary mass (or a volume) of water. Because of the non-linearity of the Richards equation, the particles have to be periodically mapped onto a regular grid discretizing the modeled domain, the aim being to evaluate the local water content, which in turn conditions the motion of the particles. It is unclear how the particles are mapped. If it is only their number, then this number needs for calibration for being transformed into a water content. If the particles are mapped as mass or volume, then compared to the local open pore space, then a water content is affordable.

It is clear that for small one-dimensional systems, the boundary conditions deeply influence both flow and transport within the system. Nothing is told about these boundary conditions, e.g., prescribed infiltration at the top, free drainage at the bottom, how they are handled with particles etc. . . This does not help to be confident in the reliability of the LAST model.

The implementation of the macropore compartment is very evasive. My understanding is that in wide open pores, the capillary pressure is almost zero, which makes that the open void is either water-saturated or empty. This feature changes the physics of flow and could also change that of transport, for example, with a “mixing” process that does not apply in the macropores. It is not clear at all how the macropore compartment is calculated. It is stated that the macropore compartment is only filled up with “event particles” (rapid infiltration?) I do not see why. It is also stated that there exist some exchanges between particles in the matrix and in the macropore compartments. How does that work? Is there any probability for an elementary particle to fall, for a given cell, within either the matrix or the macropore? What is the transition probability for a particle to pass from one compartment to the other, etc. The physics handled and how it translates into algorithms should be detailed, all the more this macropore compartment seems to be an improvement of the LAST model compared with previous attempts.

The present writing is always referring to Sternagel 2019, to the point that, for example, parameters reported in tables 1 and 3 are not documented. It is clear, for a non-novice reader, that these parameters inherit from the Van-Genuchten model linking effective conductivity and capillary pressure with water content. This is not a reason to not mention the Van-Genuchten model, the significance of parameters, and with what they are associated. Otherwise, the reading may become cumbersome.

By the way, I also find the Appendices useless, since results have already been published and do not really fit the aim of the present writing.

Finally, the application of the LAST model to actual transport data is interesting, but

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needs moderate rewriting to be picky on what the model does and what it does not. Otherwise, it is easy to fit model outputs onto data, but without saying too much on the way the model outputs are acquired. For the rest, nothing really pivotal to mention; the authors do their best for mimicking experiments, which is always a hard task.

Other suggestions.

P.2, lines 8-12. I do not understand why dual porosity approaches would not work, but macropores within a matrix would work. In both cases, this is a representation merging two compartments with interactions between both.

P.3, line 18. Mention the characteristic times of what is stated as being a long-term simulation

P.4, line 24. State that z is counted positive upward.

P.4, Eq. (4). Rigorously speaking, it should be $-v$ (and not $+v$) which corresponds to $K/\theta - dD/dz$. Otherwise, Eq (3) is not a FPKE.

P.4, Eq. (5). In the second term (within brackets) of the RHS of (5), the sign in front of dD/dz should be a minus sign.

P.4, Eq. (5) notation Δt_i not explained at this stage.

P.5, line 5. z should be a number drawn from a Gaussian distribution of zero mean and unit variance. It is right that a uniform distribution of z can render Gaussian spatial distribution of particles, but only after, say, 20-30 jumps. I would stick to a Gaussian distribution of z , even if in the effective algorithm a uniform distribution can be employed.

P. 6 lines 23 and 27. Matric? Is it meant matrix?

P.8, Eq. (6). Slightly rearranging eq. (6) results in a concentration on the LHS compensated in the RHS by a concentration to the power beta. The Freundlich coefficient cannot be dimensionless. By the way, I do not see why a retardation factor associated with Euler approaches to sorption could not be applied to Lagrangian models. Inciden-

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tally, Eq (6) is very similar to a kinetically-controlled Freundlich sorption process. Has the time step dt in LAST any influence on the sorption. If instantaneous equilibrium is suggested (as mentioned by discussing on a retardation factor), then (6) has no meaning because the mobile concentration in a given cell should equilibrate with that onto the solid phase. . . I fear that I do not understand.

P.8, Line 7. Which form is given to the concentration onto the solide phase? Is that the so-called reactive mass in (6)?

P. 9, Eq. (8, 9) Do not use k as a notation in (8) and (9), simply because the constant has not the same significance as in (7). Or refer to k in (7) as a value in h^{-1} and specify that (8) is a first-order approximation of the exponential in (7) for small arguments of the exponential.

P.12. Line 21, Specify how much water volume (mass) corresponds to the initial number of 2 million particles.

P. 14, 15, tables 1 and 3. . . Van Genuchten parameters? Specify it both in the text and in the table captions.

P. 18, lines 1-5. As suggested above, it seems that the Freundlich adsorption is mainly insensitive to the Freundlich coefficient in an equation close to a x -order kinetics. . . Too large time step for moving the particles from one cell to the other? Too rapid kinetics, thus rendering instantaneous equilibrium?. If so, why not to discuss simply on local equilibrium?

Next Pages. . . With data, hardly available, a thing that I understand, it is hard to take all the wording in Sections 5 and 6, as not partly conjectured. . . Fitting an accurate model onto sparse data will never inform on the model reliability, its capability of mimicking actual systems, and is sensitivity to parameters. This point does not jeopardize publication; it simply underlines that LAST needs for confrontations with synthetic test cases. . . Perhaps a concluding remark to add, of an appendix to rapidly build

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