Response to Comments of Anonymous Referee #3

On behalf of all co-authors I sincerely thank the Anonymous Referee #3 for his thoughtful and detailed assessment of our work.

Major Comments

R3: The modelling strategy have been proposed to overcome challenges related to dual domain models, however, there no quantitative comparison between the dual domain methods proposed in Seven and Germann, (1981) or Nezhad et all (2010), and the model proposed by authors in this manuscript. A further analyses is required to compare the results achieved from the extended work and the original LAST model as well as results that can be achieved via dual domain theory. These quantitative comparisons are required, particularly, for clarification of discussions in lines 25-30 if the page 12.

AS: We thank the reviewer for this comment. The main objective of our study is to propose an alternative approach to model the interplay of water flow and solute transport in structured heterogeneous soils containing macropores using a full Lagrangian approach. With their study, Zehe and Jackisch (2016) have already successfully tested this particle-based Lagrangian approach with the linear mixing assumption against a 1-D Richards solver.

Further, in the revised paper version we will additionally test the solute transport routine of our model with HYDRUS 1-D. To this end, please see Figure 1 of this response which shows the results of the simulation of our three infiltration tests with HYDRUS 1-D compared to the results of our LAST-Model.

As you can see, at the well-mixed study sites 23 and 31 HYDRUS 1-D performs well in accordance to the observed values and it is also similar to our simulation results with just slight deviations but which are in the range of uncertainty. In contrast, at the preferential flow site Spechtacker HYDRUS 1-D with its double-domain approach is not able to simulate well the highly heterogeneous, observed solute mass profile. Here, our model performs much better in comparison. We will discuss these results in our revised paper in more detail.

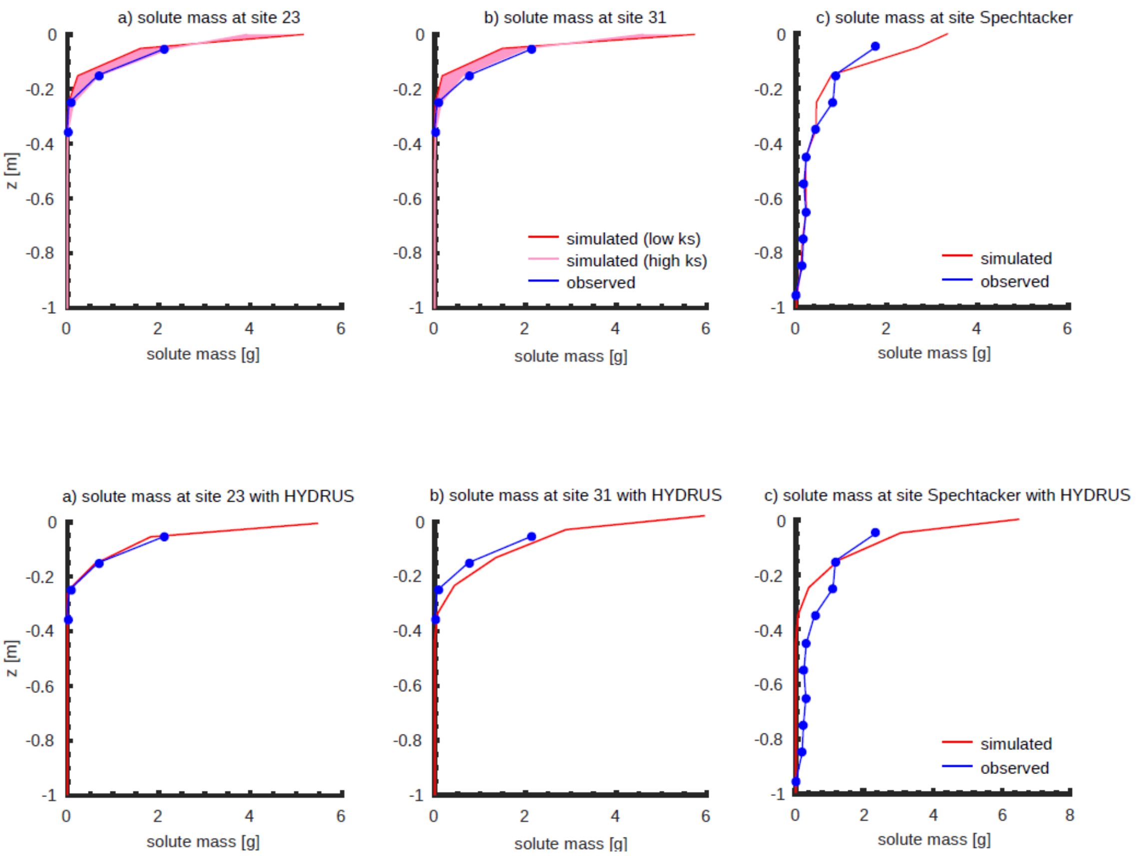

Figure 1: Solute mass profiles at our three study sites simulated with HYDRUS 1-D (lower part) and compared to the mass profiles simulated with our LAST-Model (upper part)

R3: Some new parameters have been introduced in the new model, which may not be physically measurable such as dimension of the micropores and considering the authors effort for simulation of field data, it has not been proposed/specified how values of these parameters can be identified.

AS: We thank the reviewer for this comment. Several parameters of the pfd like the number of macropores, their diameter and dephts are directly measurable in the field. We will better explain this in an additional section/paragraph in the revised manuscript and clarify how we obtained our model parameters from these observables, e.g. also with further figures (see Figure 2 below). With this Figure 2, we can explain that the dimensions of macropores (depth, diameter) are indeed physically measurable in field experiments. As you can see, horizontal soil profiles were excavated in different depths and the number of macropores, their lengths and diameters were measured. From this dataset we derived the parameters of the pfd with dmac, nmac, macropore depths and also the distribution factors. Note that also the flow rate in macropores is based on measurements of saturated flow through undisturbed soil columns, which were centered around worm burrows. These measurements revealed a clear linear dependence of the flow rate on the macropore radius, which is in line with Hagen-Poiseuille's law (Figure 3).

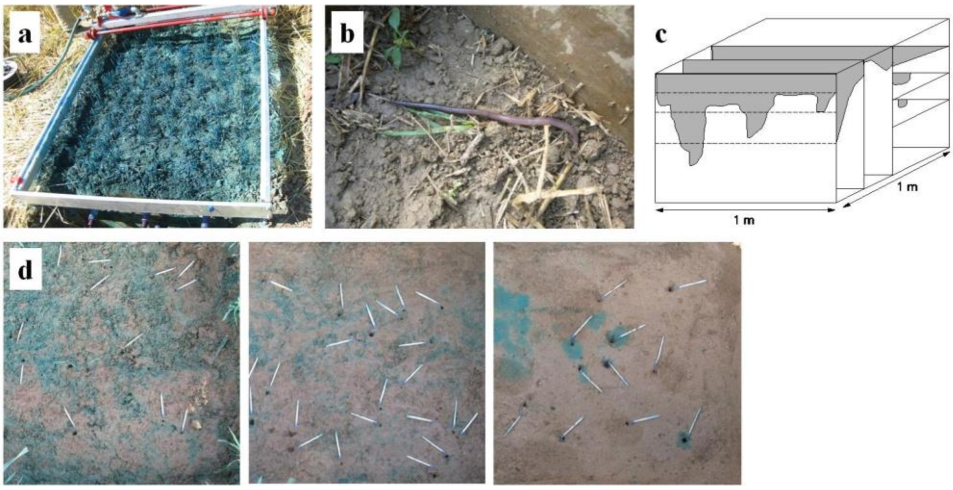

Figure 2: Patterns of dye tracer (a+d) and worm burrows as well as the measurement of distribution, lengths and diameters of those macropores in different horizontal layers (d) at the study site Spechtacker (taken from van Schaik et al. (2014)).

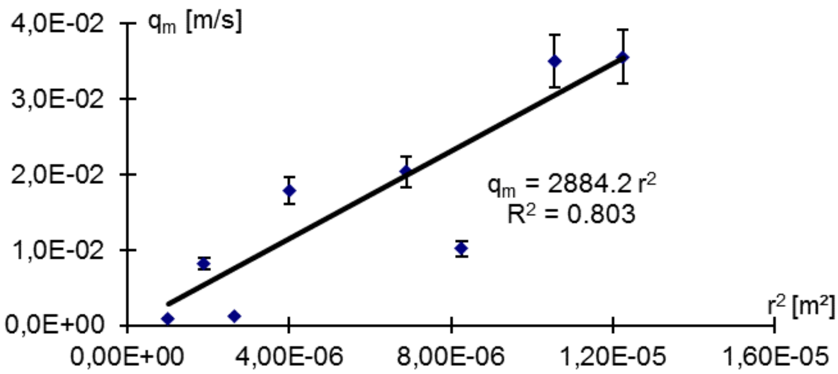

Figure 3: Linear Regression of the flux rate within the macropore on the macropore radius at the study site Spechtacker (Zehe et al. (2001)). This relation was derived from measurements of saturated flow through undisturbed soil columns containing worm burrows.

R3: Discussion regarding computational efficiency of the proposed model has not been presented sufficiently, and for example in page 13 line 39 duration of simulation has been presented without identifying which machine have been used and also duration of simulation with other possible model have not been compared. With our such complete comparisons, discussions on efficiency of the method would not add any scientific knowledge to the readers.

AS: Yes, you are right. We will add some more information about the computational setup and efficiency. We used the programming language MATLAB on a casual personal computer with moderate computational power (e.g. Intel i3, 4 GB RAM). Further, we compared our model efficiency at least against one other model, the echoRD model (see page 3, line 8) which has simulation times up to 10 – 200 longer than real time.

The simulations of the first two well-mixed cases without considering an active pfd run even faster in a couple of minutes. When performing these simulations on a high performance computer or work station, you probably could also run several model simulations in parallel within minutes. Further, the amount of total particles has a major impact on the computational efficiency: A double amount of particles results in a more than double increase of the simulation time.

R3: Some of the results presented in the paper are obvious and do not need complex modelling methods to be implemented. For example discussions presented in page 12 lines 15-20, can be achieved using other methods and perhaps developing proposed model was not required to understand these. Perhaps if authors compare their results with other results achieved using other methods which capture the effects of macropores, more valuable finding will be presented. Authors should make the results section more focused on the capacity of new strategy used for modelling micropores and their interactions with soil matrix.

AS: We agree with the reviewer that some results of the sensitivity analyses are straightforward. Nevertheless, we think their presentation is necessary to allow the reader to check if our Lagrangian approach with the macropore domain reproduces these results as the model concept is new and the exchange between both domains does not rely on an extra parameter like a leakage coefficient, e.g. used in dual models (Gerke, 2006).

We agree that the ability of our LAST-Model to reproduce the fingerprint of macropore flow observed in the tracer profile at the Spechtacker site is the main part of the results section and we will put more emphasis on this. In this respect, we are not aware of many other model studies which reproduce preferential flow fingerprints using a model structure relying on observed data. We think that the comparison with HYDRUS 1-D corroborates the feasibility of the model.

Minor comments

R3: Simulation domains have not been explained sufficiently in the text, and mainly some figures have been presented which are not enough to understand the problem being simulated.

AS: Yes, you are right. Your criticism is in line with the other reviews. We will add further information on the simulation domains in the text and also revise the Figure 2 of our paper and its caption, e.g. with this revised Figure 4 and caption:

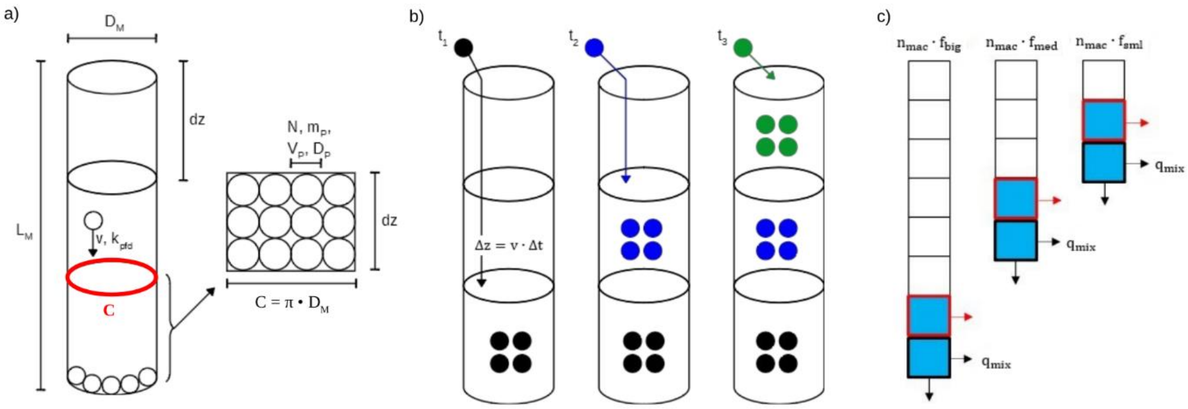

Figure 4 (i.e. Figure 2 of the revised paper): Conceptual visualization of a) macropore structure and cubic packing of particles within the rectangle of a cut open and laid-flat grid element cylinder, b) macropore filling with gradual saturation of grid elements, exemplarily shown for three time steps (t_1-t_3) whereby in each time step new particles (differently coloured related to the current time step) infiltrate the macropore and travel into the deepest unsaturated grid element c) macropore depth distribution and diffusive mixing from macropores into matrix.

We think the revised figure is now easier to understand. The explanation of all pfd parameters was moved from the caption to the text.

R3: A complete description of boundary conditions and initial conditions for simulation domains are required.

AS: We will add more information on the boundary conditions. At the upper boundary we have a variable flux boundary describing infiltration of precipitation water into the soil with a Darcy flux and at the lower boundary we assume no-flux conditions.

The initial soil moisture of the matrix is listed in Table 1 of our paper. Further, there is no solute initially stored within the soil and the macropres as well as the surface storage are also completely empty at simulation begin. We will add more information on the boundary conditions in the revised paper.

R3: discussion on time step in page 6 lines 20-25 is vague and needs to be clarified. It will be helpful that author visualise the discussion and king it more understandable.

AS: Yes, we have to revise the section about the time stepping and macropore filling. Generally, our model can work with variable time stepping as it is not subject to numerically stability criteria. In fact, we select the time step such that the particle displacement per time step equals the maximum depth of the pfd and subsequently we shift excess particles to the deepest unsaturated grid element. In this way we gradually fill the macropores from the bottom to the top (see Fig. 4b of this response above).

R3:)If I understood correctly LAST model is the same as the model developed by Zehe and Jackisch (2016). I suggested that author call it as their model or the model developed by

Zehe and Jackisch (2016), i.e., rewrite lines 9-11, I suggest "Our LAST-Model (Lagrangian Soil Water and Solute Transport) developed by Zehe and Jackisch (2016) relies on the movement of water particles carrying a solute mass through the soil matrix and macropores. We advance this model by two main extensions: a)..."

AS: Sorry, if there is a misunderstanding. We try to make it clearer in the revised paper. Zehe and Jackisch (2016) just developed the basic idea of using a particle-based Lagrangian approach to simulate water flow in well-mixed soil domains. Now, with this study we extended this basic model by solute transport and a macropore domain and also developed the name of this new model: “LAST-Model”. As this name already suggests, it is mainly about solute transport and therewith essentially different to the original model of Zehe and Jackisch (2016) only treating water flow.

Thank you very much,

Alexander Sternagel on behalf of all authors

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