Response to Comments of Michael W. I. Schmidt, Sandra Werthmüller and Jasmin Kesselring

On behalf of all co-authors I sincerely thank Prof. Schmidt and his students for their thoughtful and detailed assessment of our work. We appreciate the idea that students work on reviews of scientific papers and contribute to the discussion process. We think that it is a great opportunity for them to get an idea of the scientific publishing process and insights into the work of a researcher.

General Comments

R4: In general, we think that the manuscript has a good structure and one can follow the development of the model the way it is described in the paper. However, we think that the introduction is slightly too long compared to the rest of the manuscript.

AS: Thank you for your general positive assessment of our work. We think that after the revision of our paper with the addition of further text passages and figures, the relation between introduction and the other chapters will be better balanced.

R4: For us as beginners in the field, it is hard to understand why your model is innovative. Could you explain at the beginning of the paper what makes your model innovative compared to others in the field? And how your work is embedded in the broader work of soil water modelling? We understand that the paper is about discussing the development of a new model and is thus theoretical. However, we think a more practical description of the use of the model would be nice. For instance: For which studies is this model a must have addition? We also think that the model would have to be compared to more than one practical study to fully be called a valid model. […]

AS: Sorry, if this was not clear to you. We will revise the introduction. In short, commonly used hydrological models use the Darcy-Richards equation to simulate subsurface water flow. Many studies have shown the validity of this approach under well-mixed conditions in homogeneous soils. But also several studies have proven that the Darcy-Richards approach frequently fails when it comes to preferential flow through macropores in heterogeneous soils and due to rainfall-driven flow conditions. To overcome this weakness we propose our alternative particle-based Lagrangian approach. The differences are that we represent water masses as distinct particles and we are able to follow and describe the trajectory of each single particle through the system. We think that this until now only rarely applied approach is very promising to address the preferential flow issue and also the associated solute transport. With our study we want to evaluate and prove the validity of particle-based Lagrangian models.

And yes, you are right with your suggestion that our work is theoretical. As we are still just at the beginning of the development of our model it is difficult to describe its practical use in the future. When further adding a reactive transport routine and extending the model to 2-D it could be a practical tool to assess the risk of pesticide leaching on field sites or even on entire hillslopes.

Moreover, we consider to perform another simulation of an infiltration test and also to compare our model against the commonly used hydrological model HYDRUS 1-D in the revised version of our paper.

To this end, please see Figure 1 of this response below 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.

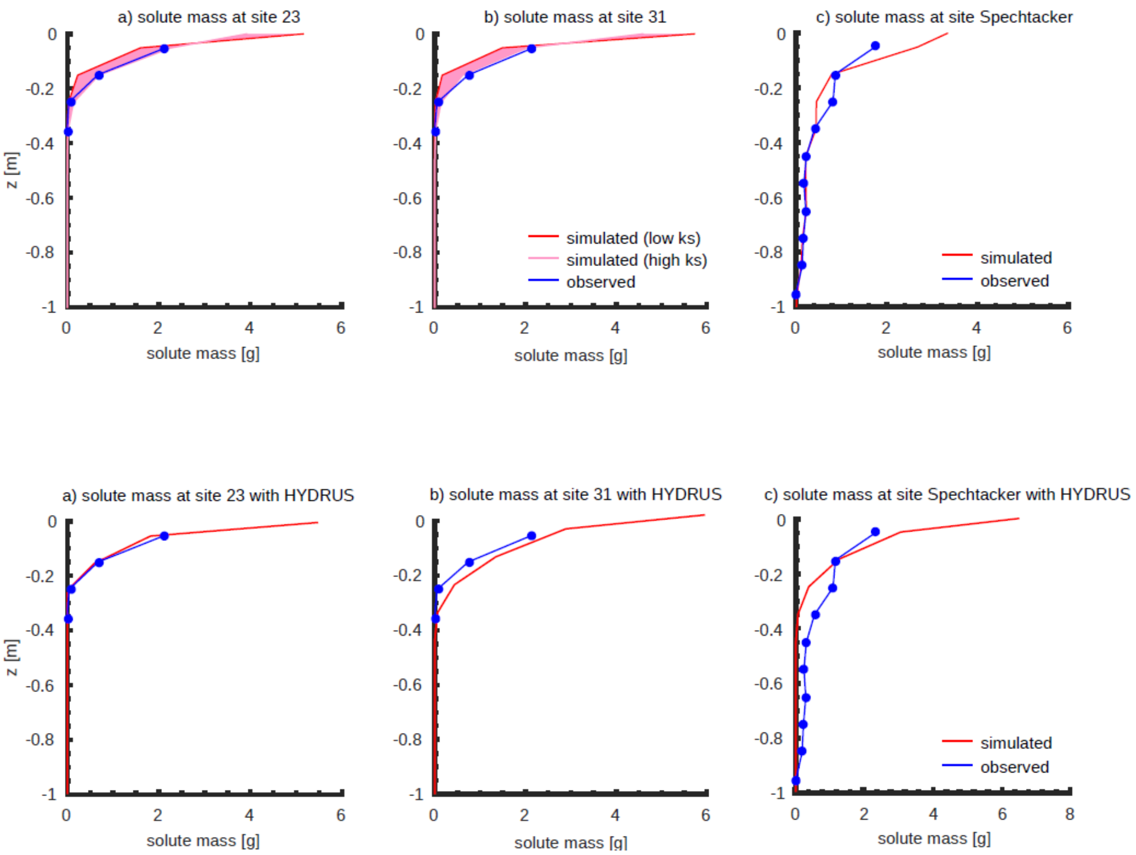

Figure 1: Solute mass profiles at out three study sites simulated with HYDRUS 1-D (lower part) and compared to the mass profiles simulated with our LAST-Model (upper part)

R4: Page 3 Line 36 ff: How is the number of bins i and the subdivision into N bins defined? What exactly is the difference between those two and how do you choose the 'perfect' number of bins?

AS: Sorry, this is indeed a bit confusing. We will revise that. N is the total amount of bins and can be predefined. Please see also the study of Zehe and Jackisch (2016), who tested how the number of bins influences the model results. In our model, we use 800 bins. And in contrast, i is the number of the current bin (between 0 - 800) within the displacement routine.

R4: Page 4 Line 30-33: Here, you list four subchapters that will follow in the next paragraph. Why not name the actual subchapters according to this list?

AS: Yes, you are right. We will adjust the list of the four subchapters.

R4: Page 9 Line 31ff: You already start the interpretation of results, why not in the dedicated section (discussion and conclusion)?

AS: Yes, sometimes we already started discussing some results in the results section. We did that, because the discussion and conclusion of these results are obvious and logical. Thus, we shortly mention them within the results section and do not come back to them in the discussion. In the discussion, we concisely refer to the main objectives of our study mentioned in the introduction.

R4: The layout of your references makes it hard to differentiate references. We also noticed that a lot of citations and references you used are from the same authors. We were wondering, if there are other scientists that are working on the same problem to which you could compare your results with.

AS: Indeed, a differentiation of the references is difficult. We consider to revise the layout. Further, there are not many studies and researchers dealing with the still relatively new particles-based approach and we think that we referenced all the crucial studies related to our topic.

Detailed comments

R4: The abbreviation for confer is cf. not c.f. It is used inconsistently in the manuscript

AS: Yes, thanks. We will correct that.

R4: Page 1 Line 34: become a major issue (change an to a)

AS: Thanks, we will correct that.

R4: Page 4 Line 24ff: This sentence is a bit difficult to understand. Maybe make two sentences e.g. ...corresponding to the molecular diffusion coefficient. Additionally, this needs to be smaller than...

AS: Ok, we will consider to revise this passage.

R4: Page 6 Line 4: k_m1 or k_m1 with a subscript 1 as in the formula above?

AS: Thanks, it should be k_m_1. We will use a consistent notation.

R4: Page 8: Has unnecessary empty space

AS: Thanks, you are right. We will revise the layout.

R4: Page 9 Line 21ff: In this sentence you suggest that the parameter hydraulic conductivity of the matrix ks, diameter of macropores dmac and the amount of macropores nmac are the most sensitive for the model behaviour and simulation results. Please elaborate why and give a reference for it.

AS: Sorry, that our description is unclear. We will explain our sensitivity analyses more properly in the revised paper. In general, due to the model structure we early assumed that it would be logical if these parameters are most sensitive because dmac and nmac mainly define the new macropore domain and ks plays a crucial role in the infiltration process, the particle displacement within matrix and even in the macropore-matrix diffusion.

R4: Page 9 Line 24ff: In this paragraph you mentioned different configurations for depth distribution and distribution factors. They have the same numbers, which is confusing and makes the text hard to understand. If possible, clarify the difference between depth distribution and distribution factors.

AS: Yes, we indeed used the same numbers for two different distributions. We will revise this issue and change the notation, e.g. macropore depth distribution with configurations 1-3 and distribution factors with configurations a-d.

R4: Page 13 Line 37 ff: You mention that your model is highly computational efficient and with a short simulations time (about five minutes). How does this short simulation time compare to other similar models? Could you give a reference time? And could you explain how this new model increased computational efficiency?

AS: The simulation of the infiltration experiment at the study site Spechtacker with the selected parametrization runs for about 5-10 minutes on a casual personal computer with moderate computing power (e.g. Intel i3, 4 GB RAM). Without an active pfd (e.g. at the other two infiltration tests) the model runs even faster (couple of minutes). When performing these simulations on a high performance computer or work station, you probably could also run several model simulations parallel within minutes.

And further, as mentioned in the introduction of our paper, the comparable echoRD model of Jackisch and Zehe (2018) has simulation times 10 -200 longer than real time.

The reason for the computational efficiency of our model is the fact that we tried to keep the model structure as simple as possible using a combination of appropriate assumptions and basic physical rules.

R4: Figure 1: Why are pore size and soil water content equal to each other? (x-axis) Maybe mention in the figure caption how the bin width is calculated.

AS: Good question. Related to the velocity or hydraulic conductivity of the matrix (y-axis) the water content and pore size can be seen as equal because big pores contain more water and also the binding forces in these big pores are reduced. Both facts lead to a higher flow velocity. The calculation of the bin width is explained in the text but we will consider to also mention it in the figure caption.

R4: Figure 2: In line 3 of the caption: describe DM, LM, dz separately like the other parameters and not as a group. We do not understand what figure b) means. What do the different colours stand for? Describe it better in the text where you reference it as well as in the figure caption

AS: Thank you. Your criticism on Figure 2 of our paper is adequate and in line with the other referee comments. We will add a revised version of Figure 2 and a better explanation to the revised manuscript. Figure 2 of this manuscript gives an idea of the revised figure. We will move the definitions of the parameters of Figure 2 to the text.

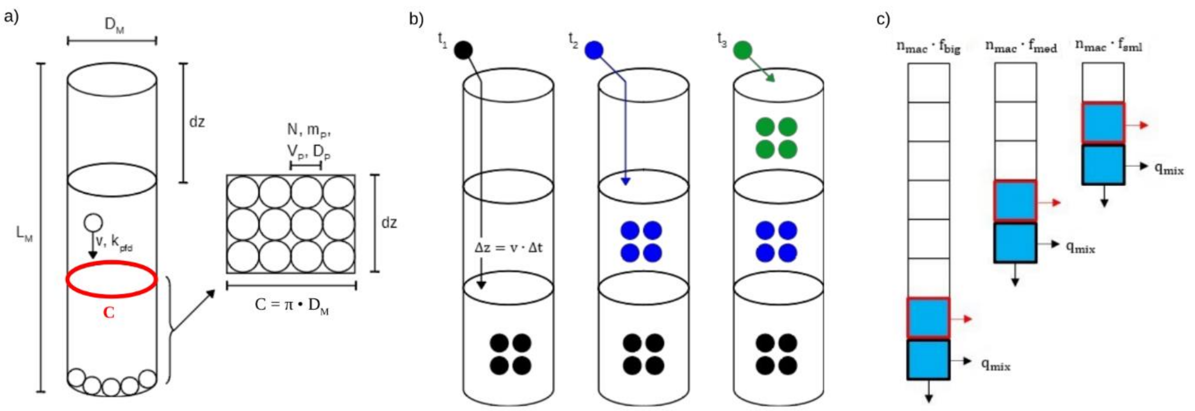

Figure 2: Conceptual visualization of a) macropore structure and cubic packing of particles within the rectangle of a cut open and laid-flat grid element cylinder, b) macropore filling with gradual saturation of grid elements, exemplary shown for three time steps (t_1-t_3) whereby in each time step new 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.

R4: Figure 3/4: Is the coloured in area the uncertainty range? Are these different parameters in figures 3 and 4 or why do they have different colours? For us the graphics are also a bit small which makes it difficult to read them. It would be better if the graphics were a bit bigger.

AS: Sorry, if this is unclear. Figure 3 of our discussion paper shows the simulated mass profile at the three study sites compared to the obtained data of the real infiltration tests. The rose area shows the model uncertainty/ -changes to different model setups. And Figure 4 of our discussion paper is part of the sensitivity analyses and the blue area shows the range of different model results dependent on different ks values. Thus, as both figures relate to different issues (Figure 3: re-simulation of real infiltration test, Figure 4: sensitivity analyses with different ks values), we used different colours to emphasize the difference.

R4: Figure 9: In all four plots use the same colour for the same configuration number. This makes it easier to see the influence of the different factors on the configurations.

AS: Sorry, if there is a misunderstanding. We deliberately used different colours in Figure 9a+b) and 9c+d) as they relate to two different configuration setups (Figure 9a+b): distribution of macropore depths with three different configurations 1-3; Figure 9c+d): Four different configurations 1-4 of distribution factors). We will revise Figure 9 of our paper and the explanation of the different configurations in the text. Please see also our response to your previous comments.

Thank you very much,

Alexander Sternagel on behalf of all authors

References

Jackisch, C., Zehe, E.: Ecohydrological particle model based on representative domains, Hydrol. Earth Syst. Sci. 22 (7), 3639–3662, doi:10.5194/hess-22-3639-2018, 2018.

Zehe, E. and Jackisch, C.: A Lagrangian model for soil water dynamics during rainfall-driven conditions, Hydrol. Earth Syst. Sci., 20, 3511–3526, https://doi.org/10.5194/hess-20-3511-2016, 2016.