Response to Comments of Anonymous Referee #2

On behalf of all co-authors I sincerely thank the Anonymous Referee #2 for his thoughtful and detailed assessment of our work.

Major Comments

R2: As mentioned in the Introduction and in the Conclusions this model is similar to a double-continuum one. In my opinion, it would be interesting if you could elaborate this similitude, ideally linking the parameter of your model with the ones of a classical double approach (with appropriate references)

AS: This similarity arises from the fact that both the LAST-Model and double-domain models work with two different domains. But apart from that, the two domains of our model and these of the double-domain models have not much in common because we really established a separate, physically and geometrically described macropore domain with the particle-based Lagrangian approach to simulate water flow and solute transport. The other double-domain models rely on separated overlapping continua and in some of these models water flow is again simulated by the Darcy-Richards equation assuming immobile water fractions or different hydraulic conductivities.

Both, our Lagrangian approach and double-domain models such as HYDRUS 1-D by Šimůnek and van Genuchten (2008) use, however, the same standard parameters like a spatial description of the soil domain with total length and grid element lengths, simulation time and time stepping, initial soil moisture and also soil hydraulic properties.

As proposed by you and the other reviewers, we now additionally compared LAST with HYDRUS 1-D using the same three infiltration experiments. As you can see in Figure 1, at the well-mixed study sites 23 and 31 HYDRUS 1-D performs well in accordance to the observed values and its model results are 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.

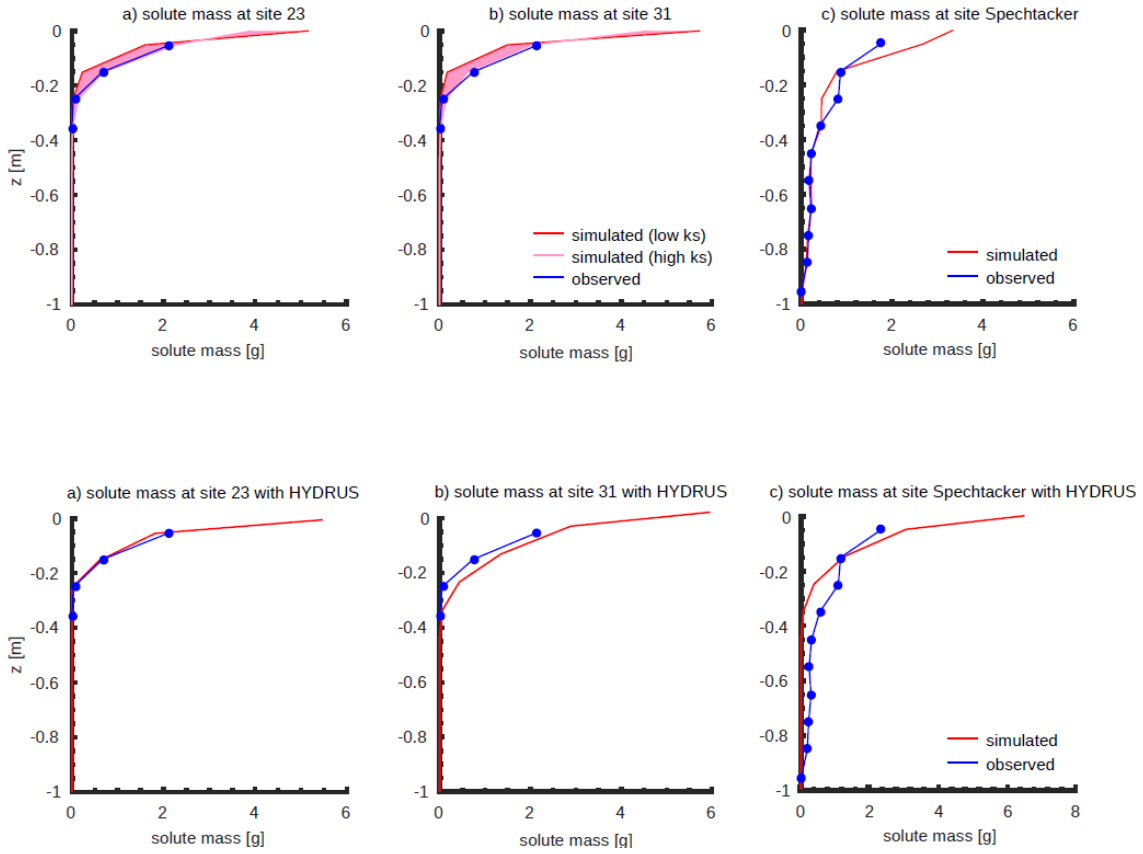

Figure 1: Solute mass profiles at our three study sites simulated with HYDRUS 1-D (lower part) and compared to the mass profiles simulated with our LAST-Model (upper part)

R2: Pag.4, line 23: here I am a bit confused about how do you compute the diffusive mixing: it is not the entire solute mass in a grid element given by the mass of all the present water particles?

AS: Absolutely true and sorry for the confusion. We will revise this part. Generally, diffusive mixing among all particles is calculated after each displacement step by summing up the entire solute mass in a grid element and dividing it by the amount of all present water particles. In this way, each particle gets a new solute mass in every time step.

R2: Pag.4, line 26: do you have some criteria to define a "sufficiently fine" grid?

AS: Generally, the grid elements of both matrix and pfd are necessary to create small spatial discretizations for the calculation of the new state variables (soil moisture, solute concentration, hydraulic conductivity) in each time step and in this way to register even slight spatial and temporal alterations of the state variables So, the grid elements have to be fine enough to ensure this proper registration of changes of the state variables and to ensure that the system remains stable without oscillations during simulation but also not too fine so that simulation times increase exorbitantly. Please also see the study of Zehe and Jackisch (2016) who determined the influences and sensitivities of different grid element sizes to the particle-based Lagrangian approach.

R2: Pag.5 line 10: could you please list all the parameters of the model and do not only refer to Figure 2 in order to better clarify how many parameters the model counts? Is the pfd characterized by the 17 parameters given in the caption of Figure 2? Is the macropore diameter "dmac" (in the text) equal to "D_M" (in Figure 2 and in Section 2.3.i)? In Table 1 we have 16 parameter for the soil description (7 for the soil type and 9 for the macropores domain) + 8 for the experiment conditions + 4 for the numerical implementation.

AS: We apologize for Figure 2 in our original paper which is indeed hard to understand. We already revised the figure and its caption, please see Figure 2 below. In general, the pfd is characterized by 9 parameters (the macropore lengths, diameter, distribution factors, grid element length). The other characteristics like the volume, lateral area etc. depend on these 9 parameters and the flow rate depends on the macropore diameter (compare Fig. 3 of this response below).

In our revised paper we will better describe how we obtained observable parameters and how we calculated or derived other parameters from those observables. And yes, dmac is equal to D_M, we will clarify this notation.

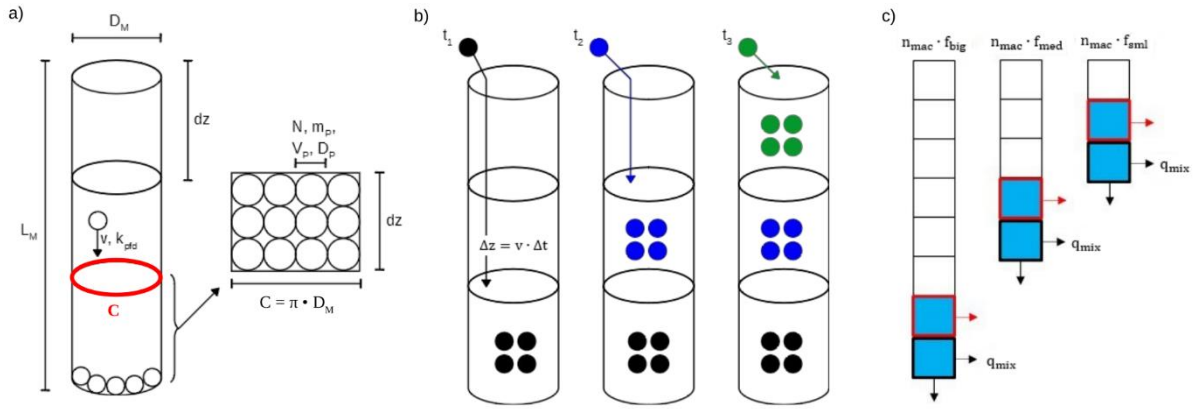

Figure 2 (i.e. Figure 2 of the revised paper): Conceptual visualization of a) macropore structure and cubic packing of particles within the rectangle of a cut open and laid-flat grid element cylinder, b) macropore filling with gradual saturation of grid elements, exemplarily shown for three time steps (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.

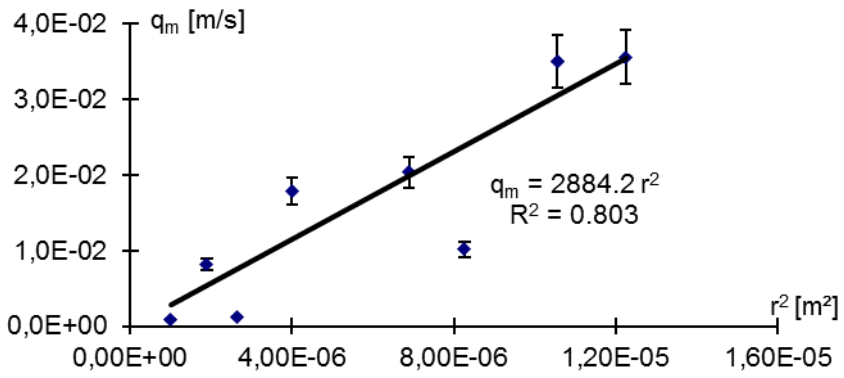

Figure 3: Linear Regression of the flux rate within the macropore on the macropore radius at the study site Spechtacker (Zehe et al. (2001)). This relation was derived from measurements of saturated flow through undisturbed soil columns containing worm burrows.

R2: Pag. 6, line 6: how is the matrix potential gradient between the first two grid elements computed?

AS: It is calculated as the difference of psi between the first two grid elements in each time step at the beginning of the infiltration routine. Please note, that the first grid element belongs to the soil surface (z = 0) and the second actually to the first grid element right beneath the soil surface (z = 5 cm). We will revise the explanation of this calculation.

R2: Pag. 7, line 11: why does your model "generally" divide the total amount of macropores into 3 parts? Could you please explain the meaning and the effect distribution factor?

AS: We assume that a macropore distribution with three different depths is a sufficient approximation of the observed macropore depth distribution at the study site Spechtacker. Nevertheless, as a variable macropore depth distribution might be observed at other sites we think that the model needs to be more flexible in this respect.

The distribution factors distribute the total amount of macropores among the three defined depths and determine in this way in which depths and to which extent water and solute masses are diffusively exchanged between the macropore and the matrix. This distribution is based on real-observed data of the macropore network at the Spechtacker site. As already mentioned, we will implement an additional section/paragraph to properly explain the model database and the derivation of all the parameters.

R2: Pag. 7, line 20: why do you use the harmonic mean to compute a sort of "effective" hydraulic conductivity? Usually, the effective hydraulic conductivity for heterogeneous media in parallel configuration is computed as the arithmetic mean of the 2 conductivities…is your model sensitive to this choice?

AS: Yes, you are of course right for parallel configurations. But here we use the harmonic mean because we assume a row configuration at the calculation of the lateral diffusive mixing fluxes between macropore and matrix as there is a vertical interface between the two domains. We will add this explanation to the revised paper.

R2: Eq(7): is the number "2884.2" result of a calibration? Could you please provide some details about it? Have you calibrate some parameter of your model to fit the experimental data? Could you please provide some details about how to use the model to interprete experimental data?

AS: The relation of the macropore flux rate or the k_{pfd} to the radius of a macropore was measured by Zehe and Flühler (2001) at the Spechtacker site. This relation was derived by measurements of saturated flow through undisturbed soil columns which were centered around worm burrows with the assumption that flow through these macropores dominated. When normalizing the measured flow with the cross sectional area of the macropores, they obtained a linear dependence of the average flow rate with the macropore radius which is in

line with Hagen-Poiseuille. Please see Figure 3 of this response which shows the linear regression to determine this dependence. We will explain this relation in our revised paper in more detail.

R2: Pag.9, line 21: in my opinion, the way you describe your sensitivity analysis is a bit vague.. how do you conclude that ks, dmac (=Dm?), nmac are the most sensitive parameters? How do you conclude that ks is "probably the most sensitive parameter" (Pag.9, line 31) ?

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 were 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 the macropore-matrix diffusion.

R2: Pag. 10: Result section: I am sorry, but for me it is not clear how do you select the parameters of your model to simulate the tracer mass in the respective depths, could you please state more clearly which observables you had, which parameters you compute from measurements etc.

AS: We agree that this needs to be better explained. We will implement an additional chapter to properly explain the model database and the derivation of all the parameters. Due to the extensive mapping of the macropore network at our study site Spechtacker, we had a detailed database containing information on macropore numbers, depths and diameter distributions. From these data it was able to derive our nmac, dmac, depth distribution and the distribution factors. Please see the following Figure 4 to get an idea of these observations.

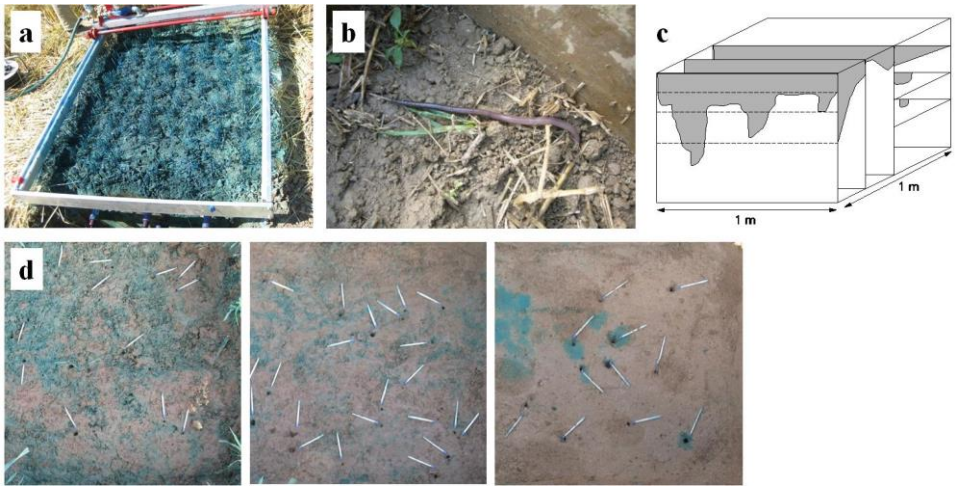

Figure 4: Patterns of dye tracer (a+d) and worm burrows as well as the measurement of distribution, lengths and diameters of those macropores in different horizontal layers (d) at the study site Spechtacker (taken from van Schaik et al. (2014)).

R2: Pag. 10, line 23: do you have an explanation about the greatest difference in profiles between 0.15 and 0.35m depth?

AS: Good question. We think that simulation in this region is difficult a) because of the lateral network of endogeic worm burrows which are completely unknown and not represented in the model and b) due to the influence of the nearby plow horizon in 30 - 35 cm depth. We will stress that soil properties are uncertain in this region.

R2: Pag. 10, line 32: here, as in Figure 9, it looks that the results are sensitively depending on the Configuration (1,2,3) … there is a way to parametrize the different configurations in order to study and quantify the sensitivity of the model to the different configurations?

AS: Yes, there is again the problem with the imprecision of our description of the database and model parametrization. As already mentioned, we will implement an additional section/paragraph to address this issue and to explain how the different configurations were parametrized.

R2: Pag.12, line 28: here, you conclude that macropore-matrix exchange should be modelled deriving an "effective conductance", even if it is the first time you introduce this term. I suppose you refer to the coefficient in Eq.6, but I would specify it.

AS: Yes, you are right. We indeed refer to the diffusive mixing flux calculated by equation 6. We think we will introduce this term at the presentation of equation 6 in the methods section.

R2: Pag. 13, line 3: I agree that "further field experiments on a variety of differently structured soil is necessary", however, from my point of view, it is not clear how do you parametrize these differently structured soils as well as do you parametrize the spatial heterogeneity of the macropores network (Pag. 13, line 35)

AS: In general, our model is able to consider also several, differently structured soil layers with different soil parameters and not just one homogeneous soil type. As stated above, several of our parameters are observable in the field and in the presented case we were able to derive them from detailed data. If these data are not available, but we still work at sites where anecic worm burrows are the dominant macropore type, we still rely on the regression shown in Figure 3 because its functional form is in line with the law of Hagen-Poiseuille. We would of course remain with the macropore diameter distribution and the depth distribution as unknown, which need to be calibrated on tracer data. This will however be a subject to equifinality (because this is a generic problem), as shown in e.g. Wienhöfer and Zehe (2014). We will better explain this in the discussion of the revised manuscript.

R2: Pag. 13, line 13: in my opinion it is not so straightforward how do you transfer the concept of cubic particle storage and hydraulic radius to any kind of macropore geometry.

AS: Good point, we agree that these concepts have certain limitations especially for complex geometries. This is a generic problem with respect to frictional loss and exchange. Such complex geometries could be expected when dealing with soil cracks but when referring to biologically generated macropores like worm burrows, degraded plant roots or even for example ant channels, we think that the resulting macropore geometries would be simple enough to apply the concept of cubic packing and hydraulic radius.

Minor Comments

R2: Eq. (1): please check this equation. I suppose a "+ z_i(t)" after the equal is missing and the format is different from the other equation in the manuscript.

AS: Yes, you are absolutely right. Thank you. We will correct that.

R2: Pag. 4 line 5: could you provide some details about the soil water retention curve used to compute the diffusivity from the hydraulic conductivity?

AS: It is a typical soil water retention curve with the relation $\frac{\partial \Psi}{\partial \theta}$. Multiplied with the hydraulic conductivity you can obtain the diffusivity. Thus, in each time step in the particle displacement routine we compute this relation with the current values for psi and theta to obtain the diffusivity for each particle.

R2: Pag. 4, line 6: I guess that Z is a random uniformly distributed number "between 0 and 1";

AS: Actually, it is between -1 and 1. But thanks for calling our attention. We will clarify this in the text. With this range the particles are allowed to move vertically up- and downward.

R2: Pag.4, line 21: could you please provide some details about the numerical implementation of the model (e.g. programming language etc)?

AS: Yes, you are right. This is something that is still missing in our paper. We will add some information on this issue. The programming language is MATLAB and the model runs were performed on a casual personal computer with moderate computational power (e.g. Intel i3, 4 GB RAM).

R2: Pag. 6, line 4: typo: please write consistently k_m1 with Eq.(3) as well as n_mac introduced in Pag.5, line 6.

AS: Sorry, yes. We will revise the text for a consistent notation.

R2: Pag 6, line 8: is the simulation time step “dt” or “Delta t”?

AS: Again, we will look for a consistent notation. Simulation time step will be “Delta t”.

R2: Pag 7, line 22: please correct a typo: “matric” potential

AS: Thank you, we will correct that.

R2: Pag. 12, line 33: Here you say that you need at least two million particles, but I suppose the minimum number of particles you need is proportional to the observation area, isn’t it?

AS: We are sorry, because there is a mistake. We have to correct the particle number to 1 million.

Further, we think that the total amount of particles does not necessarily depend on the domain extent. We think that it instead depends on the total amount of water stored within the domain. Particles must have a sufficient volume and mass, and to scale these measurements you can adjust the total particle number, e.g. at high water masses within a domain you have to select a higher particle number to avoid that a single particle carries an immense water mass and consequently has also a too large volume. This case can also arise in small domains.

But yes, when simulating a hillslope you generally need more particles because the large spatial extent of the hillslope usually implies also a high number of stored water masses.

R2: Pag. 13 line 38: you conclude that your model provides high computational efficiency with short simulation times, could you please provide further details?

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. 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 in 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.

We will expand our discussion to provide this information in the revised paper.

Thank you very much,

Alexander Sternagel on behalf of all authors

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