Response to Comments of Anonymous Referee #1

On behalf of all co-authors I sincerely thank the Anonymous Referee #1 for his thoughtful and detailed assessment of our work.

Major Comments

R1: The proposed model is introducing a large number of additional parameters that cannot be directly related to physical properties of the soil and that require adequate calibration. I think that using 16 parameters to retrieve 10 data points (Figure 3c) might introduce a strong over-parametrization of of the model. Thus, additional examples of application of the model to real data are needed, including calibration procedures and measures of goodness of fit. In particular, a fair validation would be to compare LAST with a 1-D Richards-based model that considers a simple soil heterogeneity (e.g., hydraulic parameters changing in two or three layers of the domain).

AS: Indeed, the pfd is mainly characterized by 9 parameters (in this case the macropore lengths, diameter, distribution factors, grid element length). The other characteristics like the volume, lateral area etc. depend on those parameters and the flow rate depends on the macropore diameter (compare Fig. 1 of this manuscript, note that this relation was derived by measurements of saturated flow through undisturbed soil columns, which were centered around worm burrows). Hence, at least for worm burrows, the depth distribution and the diameters are observable (compare Fig. 2 of this manuscript) and not arbitrary calibration factors. This will be better explained in the revised manuscript by an additional chapter presenting the model database with figures and showing which observables we had and how we obtained our pfd parameters from these.

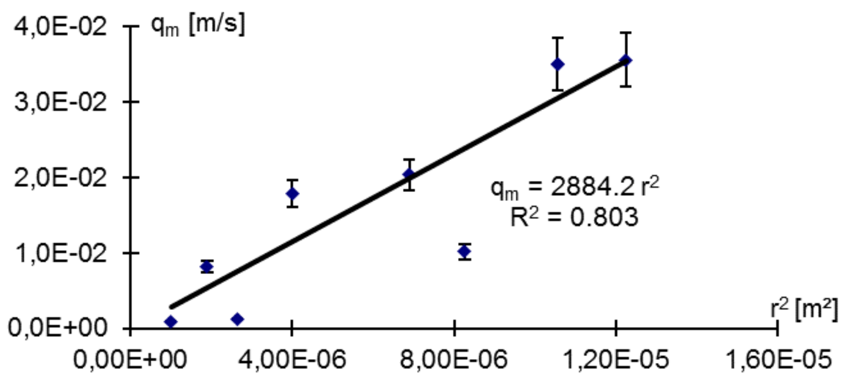

Figure 1: Linear Regression to evaluate the relation of macropore radius and flux rate within the macropore the study site Spechtacker (Zehe et al. (2001)). This relation was derived from measurements of saturated flow through undisturbed soil columns containing worm burrows.

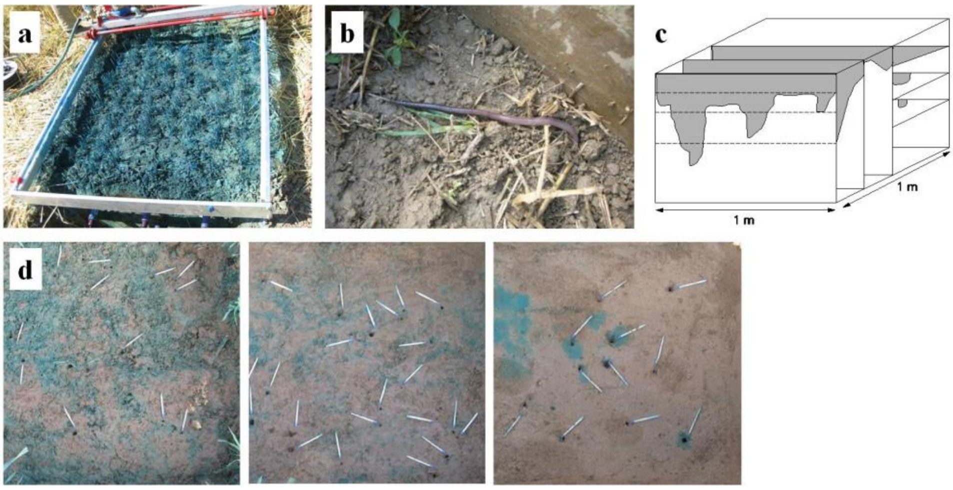

Figure 2: Patterns of dye tracer (a+d) and worm burrows as well as the measurement of distribution, lengths and diameters of those macropores in different horizontal layers (d) at the study site Spechtacker (taken from van Schaik et al. (2014)).

Furthermore, other double domain models also rely on extensive parametrization. In case these models rely on the kinematic wave theory, these parameters are for instance the maximum flow rate in the macropore system, the exponent characterizing how the actual flow rate increases with saturation of the macropore domain, and an exchange length to calculate potential gradients driving macropore matrix exchange. The latter two parameters need to be calibrated as well.

Moreover, we generally agree that a comparison with a Richard solver is interesting. In case of pure water flow this has already been done by Zehe and Jackisch (2016) who revealed a good accordance of both approaches. And in this particular case, the Richards solver and the particle model had the same amount of parameters, as the diffusivity and the drift parameter of the random walk are derived from the soil water retention and the soil hydraulic conductivity curves. In the revised paper, we plan to additionally test our model against a Darcy-Richards approach, e.g. re-simulation of our three infiltration tests with HYDRUS 1-D and comparison. To this end, please see Figure 3 of this manuscript 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 study 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.

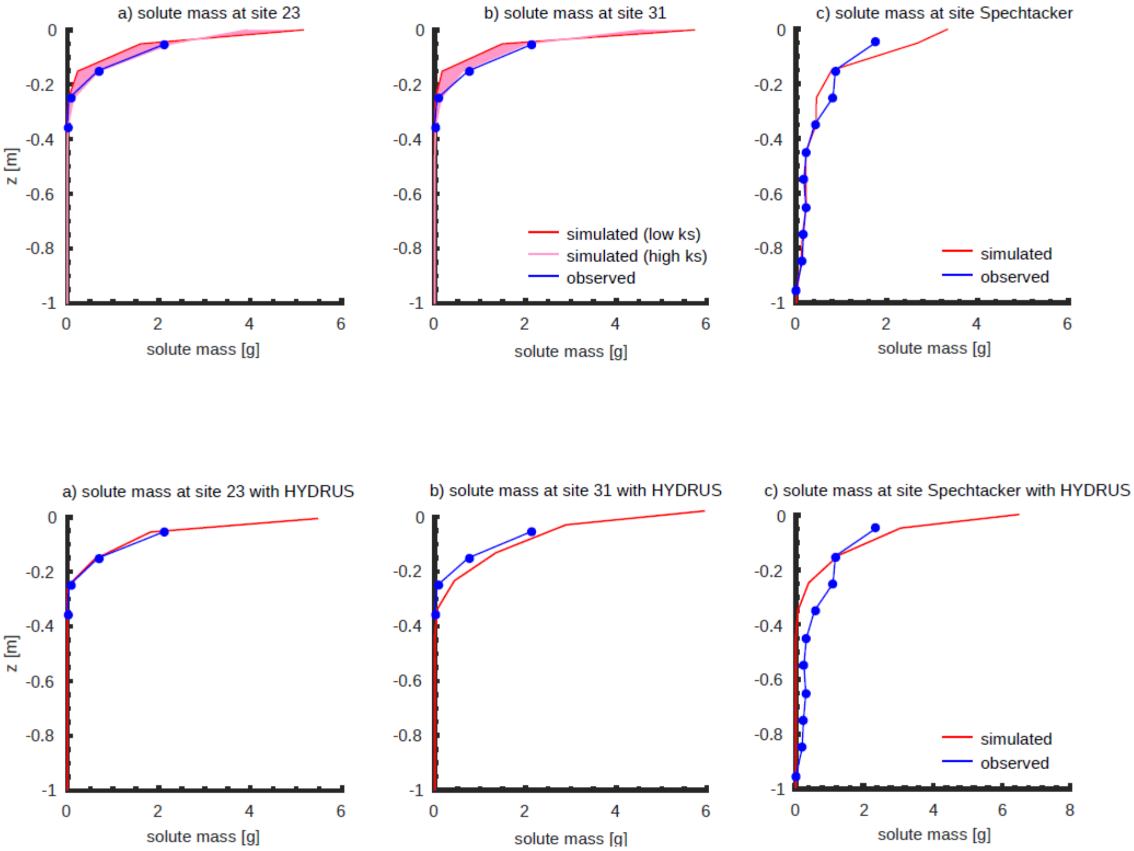

Figure 3: Solute mass profiles at our three study sites simulated with HYDRUS 1-D (lower part) and compared to the mass profiles simulated with our LAST-Model (upper part)

R1: Beside calibration, I find very difficult to apply LAST to different infiltration settings. For example, if deeper domains or longer durations of the experiment are considered, would it be always sufficient to have three classes for the length of the macropores? Why not having the classes of macropores evenly spaced along the domain? Moreover, the sensitivity of model results to the number of macropores is very low. Is it possible to consider just one macropore, and consequently adapting its diameter and the diffusion fluxes with the soil matrix?

AS: We assume that a macropore distribution with three different lengths 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 agree that the model needs to be more flexible in this respect.

Of course it is possible to represent the macropore network by just one big pore. But please note that the macropore diameter is limited in reality, in case of worm burrows usually up to a maximum of 4-5 mm. As we use a linear regression to estimate the flux rate based on the macropore geometry, we restrict the diameters of macropores to a realistic range to avoid extrapolations to unrealistic flow rates (Figure 1 of this manuscript). In an early stage of the development of the pfd we tested the idea of representing the entire macropore network as just one big macropore. In relation to volumes, masses and particle masses this would not make any difference but due to the large diameter of the one macropore the diameter-dependent flux density would be unrealistically high.

Secondly, a large macropore has a different relation of macropore cross section to the perimeter compared to many small macropores. This relation is important to calculate the fraction of particles which contribute to the exchange with the matrix and this was also the reason why we used a more realistic representation of the macropore network with a certain amount of smaller macropores. We will better explain this in the revised manuscript.

R1: The authors present three real infiltration tests, but compare the new LAST model with respect to the previous infiltration model in only the third example. Why not applying the LAST model also to the other two infiltration tests? Can you please show that proper calibration of the LAST model is suggesting to not consider the pfd component in those tests?

AS: Sorry, if our explanations were unclear and led to misunderstanding. We applied our LAST-Model on all three presented infiltration experiments. We will stress this more properly in our revised paper.

But de facto at the first two well-mixed study sites there are no or just a little active pfd because observed tracer patterns and the excavation of soil profiles did not reveal any considerable macropore network, therefore we assume well-mixed flow conditions without a considerable influence of macropores at these two sites.

We plan to perform a simulation of an additional infiltration experiment at another preferential flow site to provide more comparable model results in our revised manuscript.

Minor Comments

R1: Page 2, line 20: please insert a reference for the 'Double domain model'.

AS: Thanks, we will add a reference.

R1: Page 5, line 10: the caption of Figure 2 is not sufficient to understand the figure. The figure should be better explained in the text. In particular, which is the relation between the grid element and the macropores?

AS: We will edit Figure 2 and its caption to make it easier to understand. In general, grid elements are vertical sub-elements of a macropore, similar to the grid elements of the matrix. 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.

We will add a revised version of Figure 2 and a better explanation to the revised manuscript. Figure 4 of this manuscript gives an idea of the revised figure.

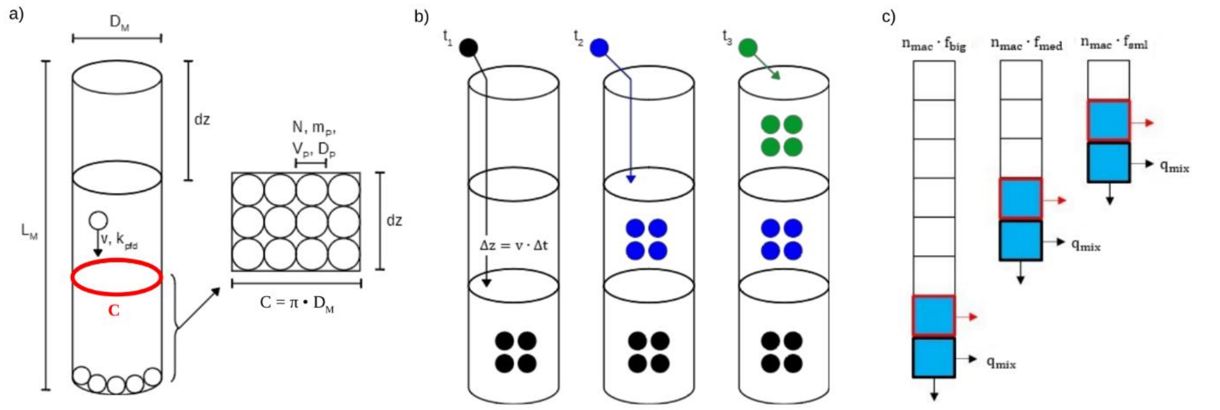

Figure 4 (i.e. Figure 2 of the revised paper): Conceptual visualization of a) macropore structure and cubic packing of particles within the rectangle of a cut open and laid-flat grid element cylinder, b) macropore filling with gradual saturation of grid elements, exemplarily shown for three time steps (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 will shorten the caption and explain the single parameters presented in the figure within the text of the methods section.

R1: Page 5, line 15: also the concept of cubic storage is really vague from the text and the figure and it is not in agreement with the cylindrical shape of the macropores.

AS: Maybe cubic packing is a better wording, as the macropore is cylindrical but the water particles are spheres. The particle diameter is determined by the stored water mass, the density of water and the number of particles in the pfd. The amount of spheres which can be packed into a macropore cylinder is calculated from the cubic packing. This means that the particles are arranged in the way that the centers of the particles form the corners of a cube. The concept of cubic packing facilitates the calculation of the proportion of particles having contact to the lateral surface of a grid element. The rectangle in Figure 4a (i.e. Figure 2a in the revised manuscript) of this manuscript describes such a lateral surface of a grid element, with the height dz and the circumference C as length, which can be obtained when a macropore grid element is cut open and laid-flat. The number of particles which fit into this rectangle have then contact to the lateral surface.

R1: Page 5, line 33: in Case 3 the accumulated water should create a ponding volume for both the soil matrix and the macropores. Why this is not taken into account in equations (3) and (4)?

AS: As the infiltration rate into the matrix is based on Darcy's law we are generally able to account for an additional hydrostatic pressure due to a ponded surface. This will indeed increase the infiltration rate into the matrix domain and we will implement this into the model. But given our investigated cases with a precipitation rate of roughly 10 mm/h we suggest only small ponding heights with marginal effect. This might be of relevance when the model is used to calculate double-ring infiltrometer experiments with related great ponding heights. In other cases, we expect that the water will runoff as overland flow. Up to now this is not within the scope of the model and we will better explain this in the revised manuscript.

R1: Page 5, line 36: mmatrix and mpfd described in equations (3) and (4) should be the infiltration capacities, not the mass of water that infiltrates as stated in line 36.

AS: Yes and no! As the model works with particles with a discrete mass, the infiltrating fluxes of water ($m^3/(m^2 *s)$) needs to be transferred into a mass to calculate the number of infiltrating particles per time. This is the reason why we present the infiltrating masses in both equations. We will better explain this in the text.

R1: Page 6, eq. 3: at my understanding, this equation is approximating the infiltration capacity for the first grid element. Why does it involve the potential gradient in the second grid element?

AS: Sorry, for the misunderstanding. 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). Maybe this is not clear enough within the text. We will clarify this.

R1: Page 6, eq. 4: the power 2 should be outside the parenthesis.

AS: Absolutely true. Many thanks, we will correct that.

R1: Page 6, lines 20-23: does this mean that the time step changes at each temporal iteration? In fact the deepest unsaturated grid element changes in time. Do the macropores fill at the same speed? From what I understand at lines 10 and 11, the water reaches different depths during the same time step, depending on the depth of the pdf. I think this should be clarified.

AS: Generally, our model can work with variable time stepping as it is not subject to numerical 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 manuscript) and this further implies that particles reach the bottom of shallow macropores even faster.

R1: Page 6, line 25: what is the boundary condition at the bottom of the macropores? From this description, the model can handle only no-flow condition, which is a big limitation.

AS: In this case, we indeed used a no-flow lower boundary. Generally, we agree that it is of course important to allow flow at the lower macropore boundary. This can be achieved by using the same formula as for the lateral exchange but we have to account for the hydrostatic pressure in the saturated parts of the macropores. We will revise the model accordingly.

R1: Page 6, line 14: what does the term 'coupled' means here? Does this mean that the water in these grid elements entered the system at the same time (and thus have the same tracer concentration)?

AS: Yes, you are right, and it also means that at the pfd-matrix mixing the diffusive flow from the coupled grid elements happens simultaneously (please, see also our response to your comment below).

R1: Page 7, line 10: why three depths? This seems a very arbitrary choice without areal physical meaning.

AS: Please see the response to your second major comment as we think we already answered your question there.

R1: Page 7, line 15: how can the diffusive water flow be simultaneous? The water in the small macropores reaches the deepest unsaturated level much faster than the water in the big macropores, thus it should start the diffusive flow before.

AS: We agree with you, that there might be cases where a temporarily resolved treatment is necessary. In the presented cases and the selected time stepping, particles travel along the maximum vertical depth of the pfd within one time step (dt = max. length/vmak). So, the different arrival times are not resolved in this case due to the high advective velocity in the macropores and the relatively small distances. The difference of arrival times and the saturation velocities of the different macropores can be assumed as marginal.

When assuming the particles travel along the minimum vertical depth of the pfd within one time step (dt = min. length/vmak) it would also have just a marginal effect on the different arrival times as the diffusive flow from the big macropores would then probably start just one time step later due to the general high velocities within the macopores.

R1: Page 7, line 20: Why are the Authors using a harmonic mean in (6) and an arithmetic mean in (3)?

AS: Good question. We use the harmonic mean here 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 justify the use of the different means in the revised paper.

R1: Page 7, line 24: it is still not clear what are C and DM and their meaning is the opposite of what is defined in the caption of Figure 2.

AS: Yes, you are generally right with your criticism on Figure 2 and its caption. Please see our revision of Figure 2 above (Fig. 4). As you can see, we added the equation for the circumference of a macropore grid element which shows that the circumference is a function of the macropore diameter. We will also describe the underlying concept of the pfd in more detail in the methods section.

R1: Page 8, Lines 4, 7: what is the depth of the soil samples? Please specify also the initial soil saturation used in the model.

AS: We will explain this in our revised paper in more detail. There was a 1 m^2 plot which was subdivided into 10 depths (every 10 cm vertically) and in each of the depths, there were ten samples taken (every 10 cm horizontally) (in total 100 soil samples).

Furthermore, you can see the sampled depths at the observed mass profile in Figure 3c of our paper. And the initial soil moistures at the three sites are listed in Table 1.

R1: Page 9:, eq 7: how was this coefficient computed?

AS: Please see Figure 1 and our response to your first major comment. The relation of the flux rate of a macropore or the k_{pfd} with the radius of a macropore was measured by Zehe et al. (2001) at the Spechtacker site. Flow experiments with soil cores containing differently sized macropores were conducted to determine the hydraulic conductivity of macropores with different radii assuming macropore flow is dominating in these soil cores. We will clarify this context within our revised paper.

R1: Page 9, section2.4.3: the proposed macropore structure has many degrees of freedom. Is it possible to calibrate / validate such a model with infiltration measurements?

AS: Thanks for this comment. 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 1 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.

R1: Page 9, line 20: Which kind of sensitivity analyses is performed? Sensitivity of which output of the model? From table 2 I understand that the parameters used in the sensitivity analysis are evenly spaced in the parameter space. Usually in MC approaches the parameters are randomly selected from the parameter space.

AS: Good point, we indeed used evenly spaced parameters within the presented range in Table 2. We will therefor rename our sensitivity analyses and leave out the label "MonteCarlo". Generally, to check the sensitivity of our model to various input parameters we used the simulated solute mass profiles and checked if they show explainable behaviours in relation to the input parameters.

R1: Page 9, lines 31 – 33: this part should go in the discussion.

AS: We think that a short introduction and explanation why we especially chose these three parameters (ks, dmac, nmac) is important for the understanding of the presented sensitivity analyses and thus, we will leave this short passage in the methods section.

R1: Page 10, line 1: This sentence is not clear here. I suggest to describe the observations (and the possible difference with the mode outputs) in the methods section. Please provide more information about how these observations are obtained. The real process is three-dimensional. How are these concentrations obtained? Are they an average of the concentrations in different layers?

AS: Yes, we think you are right here. We will replace this sentence to the methods section and will provide further details on the underlying field experiments (please, see also our responses above). But yes, bromide concentrations were averaged over each sample depth to compare them with our 1-D results.

R1: Page 10, line12: change 'suggest' with 'suggests'

AS: Thanks, we will correct that.

R1: Page 11 , line 3: please specify which are the three values of ks considered

AS: low ks: $1 \cdot 10^{-6}$ m/s; medium ks: $2,5 \cdot 10^{-6}$ m/s; high ks: $1 \cdot 10^{-5}$ m/s. Actually, the range of these values is also listed in Table 2 but we will also insert these values into the text.

R1: Page 11, Section 3.3.2: please discuss why in figures 7a and 8d the concentration increases between depths -0.15 and -0.4 for all the macropores diameters considered.

AS: Thank you very much for pointing this out. A prerequisite for exchange between the pfd and the matrix is saturation in the grid elements of the pfd and this occurs at first in the shallowest macropores. The exchange is then driven by two concurring factors a) the potential gradient which increases with depth, reflecting the decline of the soil water content with depth and b) the harmonic mean of ks and k(?) which strongly decrease with depth. This leads to a tradeoff and likely to a maximum. We will further explore this and show the concurring controls in an appropriate figure of the revised manuscript.

R1: Page 12, line 30: This sentence in not correct: to prove this sentence, the sensitivity analysis should be performed by perturbing the parameters of the real-case experiment. However the parameters of the real-case experiment are not among the ranges considered in the sensitivity analysis.

AS: Thank you. At the revision of the parameters we have found a mistake in the values of the macropore diameter. We correct it and now the parameters of the study site Spechtacker are indeed within the range used in the sensitivity analyses (Table 1).

Table 1: Value range of saturation conductivity (ks), diameter of macropores (dmac) and number of macorpores (nmac)

Parameter	Value range
k_s [m/s]	10^{-6} - 10^{-5} (step: $1\cdot10^{-6}$)
dmac [m]	0.0035 – 0.008 (step: 0.0005)
nmac [-]	11 – 20 (step: 1)

Table 1 shows the revised parameter ranges of the sensitivity analyses. The parameters at the study site Spechtacker are within the same ranges: ks = $2.50 \cdot 10^{-6}$ m/s; dmac = 0,005 m, nmac = 16.

R1: Page 12, lines 31-33: this modelling detail should be specified in the model setup. Which is the computational cost of the model when using 2 million particles?

AS: Sorry, but the 2 million particles here were a mistake. It should have been 1 million. The simulation of the Spechtacker experiment with 1 million particles runs about five minutes.

R1: Page 13, line 18: From figure 5, the sensitivity of the results with respect the considered variation of ks is quite small. What are the differences when changing kpfd?

AS: Sorry, but we do not really see that the sensitivity of the model towards different ks values is small. There are significant differences in the solute concentration profiles at the end of simulation (24h) as shown in Figure 5 of our paper. You are right when referring to earlier simulation times. In the first few hours, there is indeed just a slight difference between the different ks values but we also discuss this issue.

Changing k_{pfd} would probably have just a marginal effect because the hydraulic conductivity and velocity of macropores are always so high and the distances small that particles get instantaneously transported to the bottom of the macropores or to the last unsaturated grid element, respectively.

R1: Figure 2, caption: the saturated hydraulic conductivity of a macropore here is indicated with ks, while in the main text (page 5, line 8) it is indicated with kpfd. I think the same notation should be used for these two variables. From the figure I am not sure to understand the difference between the diameter of macropore (DM) and the circumference of a grid element (C). Why the length of a grid element is expressed as dz(z) ?

AS: Yes, you are right. Figure 2 of the original paper has some weaknesses. Please see our revised Figure 4 above and its caption and also our previous responses. We hope that the difference between macropore diameter and the circumference are now obvious. Further, we will use a consistent notation for the parameters.

R1: Figure 2b: this figure is really not clear and not well explained in the caption. Do the three cylinders correspond to three different time-steps? The times should be better indicated in the figure and the caption should describe what is happening in the three steps.

AS: The revised figure also contains a new and better understandable presentation of the macropore filling (Figure 4b). Yes, the three cylinders correspond to three exemplary time steps and we also indicate and explain these time steps in the figure caption.

R1: Table 2: please consider using a parameter range that covers the parameters used in the Spechtacker test. Not only it is important to see the sensitivity of the model in this test, but I think the results obtained for the Spechtacker are quite interesting, having a very deep infiltration.

AS: Thanks, and as already mentioned above we revised the parameter ranges.

R1: References: please check the references: Zehe and Bloshl in not in the correct place. Sometimes there is an 'and' before the last author, sometimes not.

AS: Thank you, that is right. We will correct that.

Thank you very much,

Alexander Sternagel on behalf of all authors

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