Interactive comment on “Ecohydrological particle model based on representative domains” by Conrad Jackisch and Erwin Zehe

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We sincerely thank referee 1 for the constructive comments. With this reply, we respond to these as part of the interactive discussion process. A response addressing the revision of the manuscript in detail will be given after the discussion phase.

It is assumed that solutes are moving like water to define the macropores. This is not obvious, since solute can diffuse in existing saturated dead end pores as it is often the case in unsaturated transport. Please comment on this.

The referee is correct that the model cannot account for diffusive solute transport at the current state. Because we consider non-uniform flow during and shortly after events as most critical, the model has a clear focus on this initial phase with high potential for advection. The time scales for diffusive solute transport are generally much longer. At the same time, diffusive mixing of solute mass among the particles is planned for future versions, which is important when going to long time simulations. With regard to dye staining and tracer experiments an accordance of the solute redistribution with the water movement is generally assumed. Being based on such experimental findings, the macropore domain in our model is defined based on this assumption, too. A deviation of solute and water movement during unsaturated transport is a common phenomenon. However by reducing the information to a binary existence of stained patches at a given depth level, the actual diffusive infiltration reach is not considered during the preprocessing.

Is the methodology restricted to 1d vertical macropores? It seems to me that it could be extended to single macropores that have more complicated geometries.

It is imaginable to extend the methodology to more complex geometries. However, this will require more information and explicit handling of the friction within such macropores. So far, different and more complex geometries are subsumed in a rather bold assumption based on the deviance of literature and theoretical values of the maximal transport velocity. Instead of handling complex geometries explicitly, we suggest to extend the data basis about such frictional losses in different structures and different states.

The drift term (velocity) is not trivial to me. It is uniform inside a macropore when saturation is reached, it is not before saturation. How is the derivative of the diffusivity handled numerically with macro-pore – matrix interactions?

The drift term is used to describe the directed, gravitationally driven component of the soil water movement in the matrix. It is not trivial in its implication on the processes, but rather straightforward with regard to its numerical application. Advection in macropores is describes as film flow constrained by the impulse balance with macropore matrix interaction. If the matrix is above field capacity, the frictional losses minimise and...
particles start to be in concurrence for free slots for infiltration or sufficient freedom for exfiltration from and into the matrix respectively. Inside a macropore the film water is not considered for diffusive flow. This is justified by the subordinate time scales of diffusive processes during macropore advection. But the referee is correct that situations with saturated dead end macropores and slow infiltration might not be fully captured.

p. 7, line 16: Where is the 0.7 percentile coming from?

This percentile is hypothesised based on the assumption that all free bins need to be considered but do not contribute evenly. The number 0.7 was arbitrarily chosen to compensate for a skewed distribution here.

*Solutes are injected at high concentrations (5g/l KBr).* Density effects may affect the fluid velocity.

This is an interesting point. Currently, the model is foreseen to update the soil water viscosity based on temperature and pressure (which is held static at the moment). We agree that solute concentrations could also be considered. However, first test with dynamic viscosity resulted in rather subordinate effects as long temperature ranges near freezing were avoided. Actually, this is an additional capacity of the model that such hypotheses can be tested.

*I did not understand how the particle breakthrough is computed over the domain. Is it an arithmetic average? Flux averaged? This holds for water and contaminant BTCs.*

The Lagrangian approach allows us to flag and track any particle. For the breakthrough curves in the manuscript we calculated the depth-distribution of new particles of the respective event. As such it is representing the result of the described diffusive and advective soil water redistribution. With regard to contaminants we so far neglect particle interaction and diffusive dilution, which is assumed reasonable given the short time scales. Thus the water and solute breakthrough is calculated by converting the depth distribution of the number of new particles to water mass/volume or mass of based on an initial concentration, respectively.

*The authors are slightly too enthusiastic by interpreting the simulation of the irrigation experiment. First, they provide a comparison for short time (infiltration over 20cm). At this time, it is difficult to identify biases. Second, there is a preferable flow which transported the tracer to a depth of 30-40 cm (see fig. 10) and which is not reproduced by the model. Despite these differences, I agree with the authors that their alternative model is able to simulate that experiment.*

We agree that the presented approaches are only a first step. Especially applications under different setups and further experimental references are needed and foreseen. Moreover, there are numerical concerns to be solved to enable longterm simulations. The model setup presented in Figure 10 could only be evaluated until 45 min after irrigation onset so far due to the high computational demand in the film flow routine. Thus the second hump in 30-40 cm did not yet establish in that time.

*Concerning the comparison with TDR measurements, how is the support volume defined and how is it taken into account in the modelling?*

The support volume of the IMKO IPH tube probe is very large. Especially the vertical extend of the signal guides of the probe (18 cm) is important here. The probe was manually applied and the mid point of the probe is taken as reference. It was lowered in increments of 10 cm. The measurement procedure was considered to calculate the references by averaging the total soil moisture of the depth increment referring to the respective probe depth.