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Hydrology and Earth System Sciences
Discussions

Interactive comment on "Ecohydrological particle model based on representative domains" *by* Conrad Jackisch and Erwin Zehe

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We sincerely thank referee 2 for reviewing our manuscript and highlighting some important aspects, we should convey more clearly. This reply is a response in the sense of an interactive discussion. A response addressing the revision of the manuscript in detail will be given after the discussion phase.

p. 6/7: The authors introduce here a relaxation time to LTE for a local non-equilibrium configuration of particles. What is the correspondence of this rule in a Eulerian frame, i.e., on the level of the Richards equation? Is it a type of first-order relaxation relation as used by Hassanizadeh and Gray for example?

We agree that the work of Hassanizadeh and Gray is of high relevance to the field and

our approach. Gray and Hassanizadeh (1991) give one of the rare theoretical foundations of the energy states in unsaturated flow which go far beyond our simplification for LTE relaxation. As detailed in Hassanizadeh and Gray (1990, 1993) they developed a theory for multiphase flow in porous media combining averaging of microscale descriptions and macroscopic approaches by employing balance laws and the second law of thermodynamics. Although the general lines of thought are similar in our approach, we cannot claim to rigorously derive it from first principles alone. During the development of our model, we sincerely considered their raised concerns about interfacial exchange of momentum and their microscale description of matric potential as difference of the pressure of two fluids. However within the terminology of Hassanizadeh and Gray our macroscopic description scale might be even above their REV.

Our approach to conceptualize LTE relaxation time makes use of the energetic changes associated with momentum dissipation andÂăinfiltration of water from the macropore into the surrounding matrix to overcome the well known limitation of instant LTE in current Eulerian models. The corresponding rule to our concept in an Eulerian frame would be a temporal deviation from the state determined soil water retention curve in the case of infiltration. Through the use of water particles, we can achieve a representation of a faster fraction without artificially mobilising pre-event water bound in the soil capillaries as only the new particles experience this freedom. The particle approach in combination with the binned pore approximation also enables us to analyse the dynamics of LTE relaxation. The limit to analyse this relaxation better than our rough assumption appears to be still a lack of experimental references for the process as was also noted 25 years ago by Hassanizadeh and Gray (1993). Recently Schlüter et al. (2017) published very interesting new experimental insights at the microscale.

Eq. (7): What is the mass of a water particle? The "water particles" are merely a conceptual picture, in fact, they correspond rather to "saturation particles". Equivalence between Richards equation in saturation form and the Langevin equation is achieved in the limit of infinite number of particles. The authors should clarify these points. Also *the assignation of a particle radius (how is this radius determined) to what conceptually is a point particle is unconventional.*

We agree that the use of particles is conceptual – similar to the use of particle tracking for simulating solute transport (these are not individual molecules). The equivalence between the the Richards equation and the Langevin equation is indeed when the number of particles approaches infinity (which physically does not make sense, as we have molecules).

We have shown the functional similarity between the Richards equation and the spatially explicit random walk of water particles (Zehe and Jackisch, 2016). In the model, the mass of a particle is defined by the setup of the model grid and the resolution of the porewater volume bins. This means, the finer the model grid and the better the required state resolution, the smaller the mass of water a particle represents. Obviously, this conceptual approach has limitations on both ends, when particles get too large or too small. Our test with different definitions so far did not result in massive deviations. However, we remained within "behavioural" bands and due conceptual test were left for further evaluation. Actually, we intend to reduce the number of required particles (or increase the representative particle mass) dramatically once the physical processes can be reduced to definitions of Markov-chains of higher order.

Referencing the particles as point masses with a volumetric footprint is indeed controversial. The matter arises from the combination of concepts, where the Lagrangian approach does not account for particle interaction with the solid phase but the Eulerian state control requires a translation into pore filling by means of a footprint. This receives an additional assumption in the calculation of infiltration from macropore films into the matrix, where the hypothetical radius of a spherical particle is assumed to be the threshold.

Because a particle can fill a certain fraction in the pore space which is referring to a certain capillary tension bin, I would not speak of "saturation particles" as such. The

concept is to implicitly resolve such pore-scale configurations within the soil matrix. In our first publication (Zehe and Jackisch, 2016) we especially detailed on this.

Section 3.3.3 How do the rules established for the Macropore-Matrix interaction correspond to the dual porosity models by Gerke and van Genuchten, for example?

We agree that due comparison to existing models is a valuable benchmark. Because the models require different data for their parameterisation, this task is not as trivial – especially because experimental references are scarce. We have done a series of tests to compare the model against an artificial "macropore" in a packed sand cylinder as presented by Germer and Braun (2015). These experiments are very similar to the simulations of Gerke and van Genuchten (1996).

They regarded exfiltration from an irrigated "macropore" into the surrounding matrix. For this a central vertical macropore (filled with coarse sand for stability) was installed in a half-cylinder filled with fine sand. The macropore was irrigated with constant flow rate until breakthrough at the bottom was reached. The exfiltration and diffusive redistribution was observed by means of time-lapse photographs and tensiometer monitoring. When parameterising echoRD according to the retention properties of the fine sand, we could reproduce the experimental observations (Fig. 1)

With respect to the rules for macropore-matrix exchange, we also can calculate a mean exfiltration time of a particle at the pore wall for different states of the surrounding soil matrix (Fig. 2).

Sections 4.2 and 5.1: The authors refer here to generic application tests as benchmarks. It is not clear however against which benchmarks the model results are compared, or in other words, which are the benchmarks? I could imagine a 2D numerical solution of the Richards equation, for example.

The benchmarks we refer to in the presented application tests are in accordance with the given aspects in section 4:

- capability to simulate 2D diffusive soil water redistribution of non-uniform states
- capability to simulate macropore-matrix exchange
- realistic sensitivity to antecedent state and soil physical parameters
- robustness of stochastic realisations of equal definitions of the representative macropore domain
- overall performance in reproducing observations of an irrigation experiment

We agree that comparisons to current model approaches have advantages with regard to the spectrum we could refer our approach to. However, we chose to emphasise experimental findings as benchmarks because the simulation of infiltration in structured soils is exactly the case, where the assumption of a well-mixed state and purely diffusive flow is critical.

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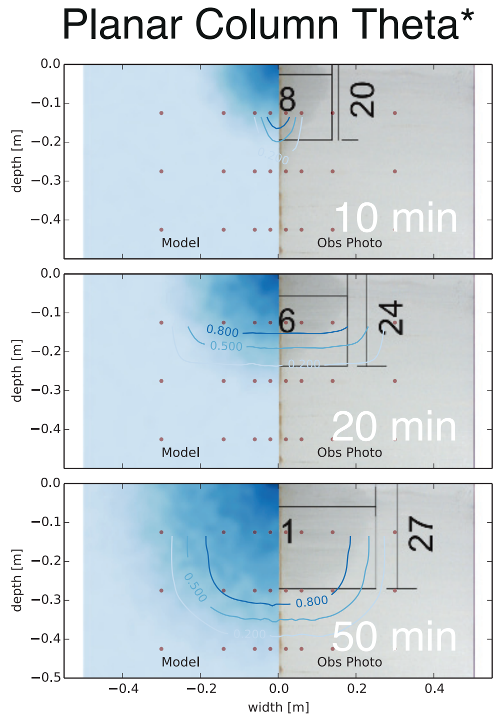

Fig. 1. Diffusive exfiltration from an irrigated artificial macropore. The irrigation rate was 3.78 L/h. Left panel: Model simulation of relative saturation (the half cylindrical column is assumed as planar

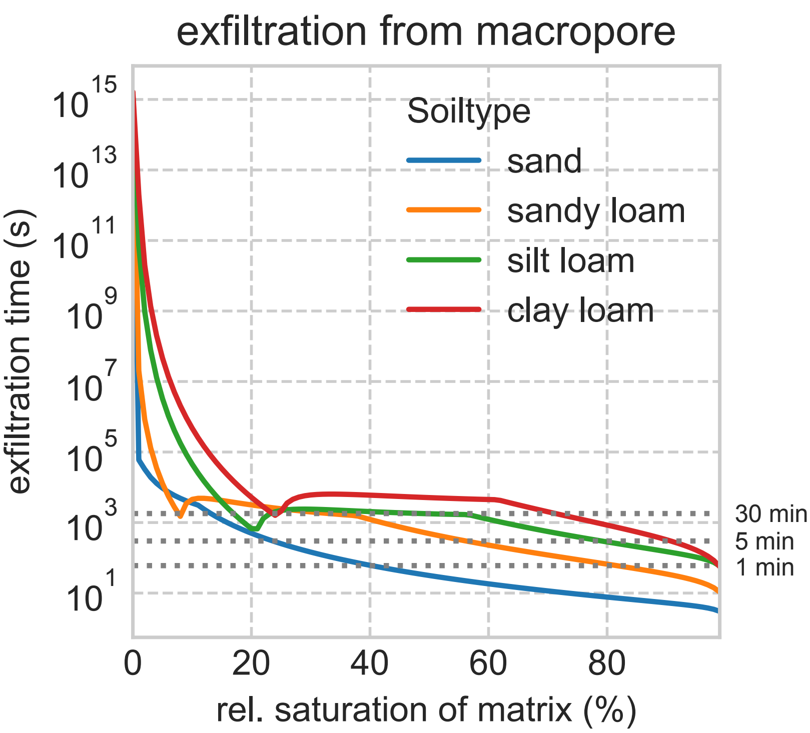

Fig. 2. Exfiltration time from macropore for different soils and matrix states.