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Interactive comment on "A novel explicit approach to model bromide and pesticide transport in soils containing macropores" *by* J. Klaus and E. Zehe

A. Coppola (Referee)

antonio.coppola@unibas.it

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The authors presented the results a follow-up study of the paper by Klaus and Zehe (2010). In the latter, the authors applied a spatial model explicitly accounting for preferential flow (worm burrows) in a tile drained field in terms of connected paths of low resistance. They generated 432 spatial model setups of the tile drained field. The worm burrow density was generated for each setup by assuming a Poisson distribution. Many of these setups allowed a good reproduction of the tile drain hydrograph response. Based only on the hydrographs, none of these results could be rejected. In order to reduce what they called the "equifinality" in the spatial model setups, in the current paper the authors used the best 13 spatial model setups from the previous study for describing bromide and isoproturon (IPU) transport in the tile drained

field. Their main result was that, based on the Nash-Sutcliffe efficiency criteria, the spatial model setups 1, 4, 9 and 10 reproduced the observed time series of the cumulative bromide leaching even if with a peak time error. The first setup, which provided the best discharge simulation and a relatively good match of cumulated bromide, was used with different adsorption parameter combinations for simulating the transport of the IPU pesticide, but with only inadequate results.

General comments

Based on my reading of the manuscript, the paper is well structured overall. The introduction of the paper illustrates clearly the rationale and the objectives of the work. The theoretical basis and numerical conditions for testing the index are well explained. Figures effectively summarize the results. Overall, I think the paper is significant, the objectives very clear and in general effectively supported.

Some doubts

Looking at the figures 3 to 5, it may be observed that the hydrographs are always reproduced quite satisfactorily. This means that the reconstructed preferential flow domain is generally capable to describe the actual water flow processes taking place in the porous medium.

Concerning the bromide transport, a relatively good agreement is generally observed between simulated and measured curves in terms of cumulative concentrations. If one has a look to the curves in the second columns of the figures 3-5, it may be observed that this result has to be mainly ascribed to the relatively acceptable description of the curve tails. To the contrary, as also stated by the authors, the main, and generally important for applications, the measured initial peak is never seen by simulations. At a first view, it is quite surprising this main peak be completely independent on the water flow, as may be observed in the figures 3-5 and in figure 1, the latter referring to the work Zehe and Flühler (2001) originally carried out in the same field. The most likely reason for this seemingly strange behavior is that the model describes the solute transport mainly in terms of water convection and adsorption while other important local mechanisms should be invoked and essentially related to the solute exclusion and solute exchange between the preferential flow domain and the rest of the porous medium.

My feeling is that the behavior the authors described is typically observed when the criteria for selecting the best model setups are mainly based on the outflow information (from a soil column, from a tile drain, from a watershed). This is the main reason why, for example, some methods for hydraulic characterizations of soils (one/multistep methods) cannot rely only on outflow information but need some additional information on the state variables inside the porous system. While the outflow behavior carries good information on the dynamic behavior of the system, generally it does not contain enough information for deducing what is happening inside the porous system in terms of mass storages and exchanges (see for example Abbasi et al., 2003; Comegna et al., 2001). By analyzing several transport experiments through soil columns, Comegna et al. (2001) emphasized that the agreement of outflow experimental data with a mechanistic model does not unequivocally identify the mechanism of solute transport in the soil. Different mechanistic and stochastic modeling approaches predicted breakthrough curves comparably well. It was also concluded that with the outflow experiment data used to calibrate the various models it is not possible to identify the most plausible process hypothesis, which may be deduced only through observations of transport at different locations in the porous medium. All the models in question supplied equivalent and indistinguishable interpretations when applied at only one observation position.

Looking at the breakthrough curves in figures 1 and 3-5, a long tail may be observed with a residual solute mass slowly leaving the system. The mobile-immobile concept could be one of the possible local mechanisms allowing describing such a transport behavior. On the other side, solute exclusion and solute pulse splitting could be invoked for explaining the fast peak at the beginning of the transport experiment. They are all mechanisms induced by local-scale heterogeneities which cannot be neglected

even when larger scale processes have to be described. To the contrary, the authors ascribed the fast peak to the spatially heterogeneous irrigation (page 14, lines 22-30). Unfortunately, local scale information appears to be missing (omitted?) in this study. It seems that the authors had only minor information on the internal heterogeneity of their field both in terms of storage and flow behavior. In this sense, it is quite curious to see that the study area was equipped with 25 TDR probes 30 cm length but apparently no TDR data have been used for describing the internal heterogeneity of the field.

In synthesis, what is maintained in this review is that inferring the flow field in a porous system from only water flow information may not be enough if the solute transport behavior has also to be explained from the same information. To the contrary, solute transport information is as critical as the hydrographs information for deducing the effective transport paths in the soil. Coppola et al. (2009) demonstrated that coupling approaches for analyzing both solute breakthrough curves and water flow data is the only way to preliminarily capture the existence of fast and slow flow paths in large soil columns.

With these premises, a poor description of the IPU transport was only expected. Nor allowing the retardation factor for the IPU makes physical sense.

Please, use different parameters (n) for the van Genuchten's and Freundlich's equations.

I think the authors should discuss these issues into a minor revision. It will increase the significance of the contribution of their paper.

References

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