**Hydrology and
Earth System
Sciences
Discussions**

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

J. Klaus and E. Zehe

j.klaus@bv.tum.de

We acknowledge the comprehensive review and the several suggestions of Maximilian Köhne on our Manuscript. In the following we will address his questions and suggestions.

Considering the reviewers suggestion that the manuscript does not follow the philosophy of the previous paper:

This is an interesting point risen by the reviewer. The purpose of our study was however to shed light on three initial questions. - How far can we get with the proposed approach to represent structures in an explicit manner? Successful predictions of water flows at the tile drain outlet, even bromide mass flows or event pesticide mass flows. - Does

the inherent uncertainty in our data cause equifinality in particular do we find several flow path networks (i.e. different areal densities of worm burrows that link the surface and subsurface) that compile the same integral response behavior? -Does additional information from additional data help us to reduce the set of acceptable model setups?

We can only address the last questions if we proceed in the proposed three step procedure, that uses the best model setups from a previous information level for istance just using discharge (without additional tuning of model structures) to the next information level were us additional bromide to falsify the model structures.

It would surely be interesting to reduce the level of accepting models in the first stage and thus to evaluate more model setups against the bromide data (much more work though). Evaluating all the model setups against the bromide data, also those that failed to reproduce the tile drain discharge response, is to our point of view not justified. Simply, because we want to have model structures that perform well with respect to both signatures. We think that our proposed three step procedure is a parsimonious to assess such structure. (Eating is the proof of the pudding). We agree there could be other ways, but this is not the scope of the study.

It will be an interesting question to compare also less good results of water transport and the corresponding solute transport.

Reviewer#3 concerns about just using one model setup for the transport modelling of IPU:

Choosing only one model setup for IPU was indeed for reasons of computing time. Nevertheless, the chosen run suits in the work philosophy, using the run that describes the water transport best and is also successfully in modelling the bromide transport. Nevertheless, in the final version of the paper we will mention that the computation resources limit modelling IPU transport for several runs in a way as it was done for one run.

'Reviewer#3: The underlying combination of physical factors of suitable setups for Br simulation is not discussed (initial water content, flow rate in macropores, flow rate in drains, etc.). This discussion was done in the water part and should be conducted here as well to help understand the system. Some information could not be measured in the field, such as water content in the subsoil, but it was measured with TDR in the top soil, right?'

To add a small discussion/conclusion about the parameter runs that allow the sufficient simulation of the water and solute transport is a good suggestion. We will revise the paper accordingly.

'Reviewer#3: The description of boundary conditions is partly incomplete and appears partly inconsistent with the experiment, thus limiting the understanding of the system. Overall the system to me falls short of a black box.'

We will provide additional details in the revised manuscript.

'Reviewer#3: Following details were unclear to me: in the experiment, IPU was applied 1 day before irrigation, while Br was applied with the sprinkler. However, in the model Br and IPU were incorporated in the upper layer. Particularly in case of preferential flow, BCs may have a large effect (Gerke et al, 2007).'

True, although the reviewer mixes initial and boundary conditions. We represented initial conditions of IPU in our model setup accordingly to the field experiment. We agree that applying Bromide in the proposed way is a simplification that could lead to a too early breakthrough of Br. The boundary conditions is however high intense rainfall in a three step procedure, which is again well represented in the mode setup.

'Reviewer#3: I assume the simulation left one day for diffusion and sorption before the irrigation simulation, and irrigation was simulated using the same time intervals and rates as in the experiment?'

We accounted for this redistribution as IPU in reality is applied to the surface and slowly

diffuses into the upper soil, and we simulate that IPU totally entered the soil.

'Reviewer#3: In the simulation and experiment, was there any runoff with redistribution into macropores?'

The model accounts for overland flow and thus also for these effects, we did however not analyse surface redistributions and leave this for future research.

'Reviewer#3: It seems to me that the drainage simulation does not exactly represent tile drainage, since it presumably considers drainage of unsaturated soil: the lower boundary considers free drainage, so there won't necessarily be groundwater buildup, and drainage will kick in once the hydraulic conductivity of the drain layer will increase above a certain value, is it like that? And is it possible that drainage starts in other scenarios only when the reservoir below the drain will wet up, leading to a mixing of Br and IPU from zones below and above the drain? How will this mixing affect the results? What are the spatial concentration patterns of Br and IPU and how do they evolve in time? By these questions I want to point out that this is a highly complex system, and given the present information, it is difficult to understand the simulation results.'

The reviewer is right, that a build up of groundwater is not necessary for a start of the tile drain. Flow in the drain starts if the tile drain grid cells exceed a certain threshold and the water supply to the drain layer is at least the same as the water leaving the drain. Field studies in the Weiherbach showed that tile drain discharge can significantly increase if the macropore network becomes saturated that has not to be accompanied by rising groundwater level (Klaus, unpublished data; see Klaus et al., EGU 2011). Mr. Köhne describes a case, where drainage might start when the reservoir below the drain went up. This process did not occur in the different model setups. Figure 6 of the manuscript presents the spatial distribution of bromide at different time steps. Bromide transport, and high bromide concentrations can be attributed to the preferential flow grid cells and the surrounding cells, while an absent of preferential flow paths leads to nearly no solute concentrations in the grid cells. We think Figure 6 should supply

enough information to gain impression of the internal dynamic and the solute transport of the tile drained field site.

'Reviewer#3: Is the sequential procedure (water – Br – IPU) valid at all? Several papers using other model approaches have shown that a drainage hydrograph just does not include the information for simulating preferential solute transport. Can you prove that your approach using explicit structure characterization permits to use the sequential procedure?'

See our comments above.

'Reviewer#3: A reference simulation without macropores would be good to see how large the macropore flow effect is in the first place. On the other hand this may not be required, since the setups with weak influence of macropore flow were already excluded in the water part. I suggest to discuss a bit the relative influence of macropores and matrix. Is there a strong mass exchange? How much of the leached mass of water, Br and IPU comes from macropore flow (for IPU presumably it is 100%)?'

Figure 5 of the previous paper (Klaus and Zehe, 2010) presented modelling results when no macropore are included in the model domain. Nearly no increase in tile drain discharge could be observed in these cases. The percentage of mass leached by macropore flow can not be determined, since the mass can always interact with the soil matrix grid cells.

'Reviewer#3: The approach to IPU simulation probably contains (at least) one principal error! That is, the sorption isotherm is used for the 30-cm macropore domain without correctionfor the fact that reactions should occur only within the earthworm burrows. Of course the available surface area is much smaller in those burrows. A surface area weighted correction factor should yield much smaller effective KF-values for the macropore zones, as seems required here. Other issues are: I do not understand using n=5 in $C_a = kf*C Ë Ę n$. n=5 gives an extreme increase in sorption for C>1. So did you mean n=1/5? But I would rather reduce Kf instead of using an exponent>1.'

We will include useful runs with lower kf values near zero, to support the IPU modelling with parameters of a better physical meaning and address the concerns of Mr.Köhne. Nevertheless, for C<1 the approach of n>1 is appropriate to reproduce retardation coefficients of 1 (see also comment to review#1). We attached a figure that shows the development of the retardation coefficient for n>1 (and C«1) to underpin this.

'Reviewer#3: While once again the approach is good pioneering work, my feeling is that here the second step is taken before the first one. The structure characterization relies on some effective description of the macropore region (and of the drain region as well), but this is done a priori (without upscaling) for water and bromide and not at all for pesticide reactions. A systematic study with a synthetic data set should be conducted in future to (upscale and) evaluate equivalent parameters for these regions.'

We slightly disagree. Structures like macropores emerge genericly at a certain scale and cannot be derived from upscaling procedures. Simply because the worm digs the structures in a way that serves the survival of his species. The underlying cause why such structure look the way they do is thus behaviour of ecosystems engineers which cannot be inferred from physical principles. The main advantage of our study is use genetic knowledge about this structures and their topology and that is may be parameterized according of observable data we can collect in the field. The approach allows furthermore to quantify change impacts (dye back of worms) but also surface preparation (ploughing).

'Reviewer#3: Important transport parameters are seemingly ignored: Dispersivity and degradation rate. Zehe has shown in a previous study that degradation of IPU in earthworm burrows proceeds very fast, at 'top soil rates'. Dispersivity is a key parameter in transport simulation, although after separation of the domain into two different flow zones, its importance may be less. Please comment on your model assumptions regarding these parameters.'

Degradation is completely ignored, since the simulation time is based on 10 hrs, and

the existing observations only covered 6 hrs. With half lifes of 7-10 days or more, the absolute degradation can be ignored. For the dispersivity we have chosen one fixed value. This was done to avoid additional uncertainty/equifinality be possible variation of the dispersivity. We ad a small section about the sensisitivity of the dispersion coefficient, when we change the dispersivity in the range of observed values.

'Reviewer#3: The 2D approach is an 'effective' one, as is revealed by the calibrated narrow zones of influence ('catchment') for drainage, of only 1-3 m. A simulation perpendicular to the tile drain could help assess how large the real zone of influence is. Was there only one tile drain, or else, what was the spacing between tile lines? The standard assumption is to take half the drain spacing as zone of influence.'

The exact construction/location of the tile drains at the field site is unknown. There might be additional tile drains located about 20 m away. A simulation perpendicular to the tile drain (with one or more drains) only revealed 'catchment widths' under steady state conditions. With several drains that were exactly between the drains, with one drain, of course all distances to the drain contributed to drainage. We may have to take into account for further studies that not the full area between two tile drain tubes are active in the drainage but the water can percolate to deeper regions

'Reviewer#3: The introduction could be shortened and should lead to the objectives of the study. I would suggest to leave out most of the two-region case studies mentioned, but rather discuss the few studies with explicit structure characterization, (see also Allaire et al., Role of macropore continuity and tortuosity on solute transport in soils: 1. Effects of initial and boundary conditions, Journal of Contaminant Hydrology 58 (2002) 299– 321, //AND// 2. Interactions with model assumptions for macropore description, Journal of Contaminant Hydrology 58 (2002) 283– 298), briefly discuss GLUE and the rationale for using it here (what is its advantage over multi-objective global inverse methods, where in principal one could also define several equifinal model setups), and report how this study builds upon the water study, and then state objectives.'
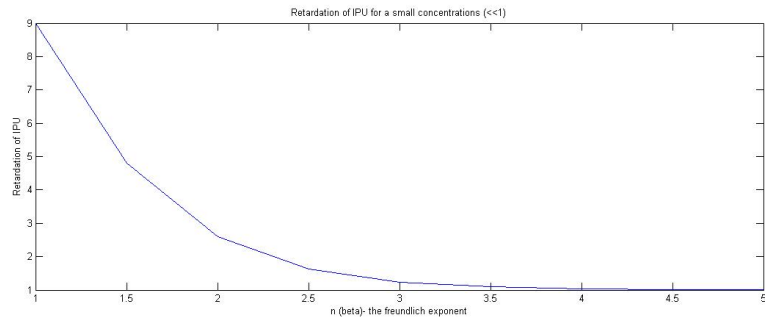
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Thanks for supplying additional literature. After the three reviews we see some weakness of the introduction. The main intention was to show the existing approaches and there limitations, and to point out that the use of an explicit representation may be one possible solution. We will render that more precisely.

Fig. 1. Retardation for n>1

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