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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

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General Comments The paper describes a model approach that aims at predicting tracer and pesticide transport based on i) considering earthworm burrows as explicit geometric features in the grid of the 2D numerical CATFLOW model, ii) a statistically based (GLUE – Beven) procedure of selecting suitable equifinal model structures out of a number of selected initial scenarios for simulating a hillslope-scale transport experiment previously conducted in a tile-drained field. The proposed procedure is sequential in that it starts with simulation of water flow, uses the acceptable model structures to predict (without further calibration) bromide (Br) tracer transport, and again selects the acceptable model structures to simulate isoproturon (IPU) transport. The water part was described in a previous paper (Klaus, J. and Zehe, E.: Modelling rapid flow re-



sponse of a tile-drained field site using a 2D physically based model: assessment of "equifinal" model setups, Hydrol. Process., 24, 1595–1609, 2010.), whereas the Br and IPU part is presented in this follow up study. Out of 432 model setups, 67 were found acceptable for water flow simulation, and the 13 best out of these were evaluated for bromide transport prediction. Four scenarios showed cumulative water and bromide loss within experimental variation and were deemed to be equifinal realizations with valid model setups. Out of these four, stated as the scenario that 'performed best with respect to discharge and was ranked fourth with respect to bromide loss', was selected for IPU transport prediction.

I think that the approach of using an explicit structure characterization for a virtual model soil, as a means to approximate the real complexity of soil, is laudable. It should be explored more in future. The approach is here combined with a GLUE procedure based on the notion that the complexity in a field leads to equifinality in model setups, such that no single optimal setup can be identified (e.g., by inverse simulation). Instead, multiple forward simulations starting with Monte Carlo sampling are used. This combined approach (explicit structure + GLUE) seems to be new for modelling solute transport in the vadose zone.

The paper is definitely of interest for readers of HESS. The writing style leaves room for improvement regarding the English and the accuracy of many statements. Despite my generally good impression of the approach, I have several criticisms of its implementation. At least the more severe of those issues should be fixed before publication. The IPU transport simulation in its present form is not acceptable and should be repeated (see below suggestion(s) for possible improvement).

- Condensation in model setups: the number in acceptable model setups is reduced too strongly: this paper does not really follow the philosophy of the previous one in terms of accepting equifinal setups. Looking at Fig. 3-5, all 13 predictions essentially match cum. Br loss and water dynamics, however, only 1 scenario is selected for IPU simulation! That single scenario ranks even only fourth in Br simulation, so the selection seems even arbitrary. Perhaps this strong condensation is done for reasons of limited available computing resources, which would be understandable, but then this should be stated.

- 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?

- 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. 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). 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? In the simulation and experiment, was there any runoff with redistribution into macropores? 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.



- 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?

- 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%)?

- 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 correction for 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*Cˆn. 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.

- 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.

- 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.

- 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 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.

Detailed comments:

Abstract: Line 3: “. . .soils” (add: at hillslope scale.)

Line 12: “We thus simulated transport of bromide and Isoproturon (IPU) for the 13 spatial model setups (delete comma) which. . .” Comment: only 1 (not 13) model setup was used for IPU. Logic: in preceding sentence (line 11), only bromide was mentioned.

Introduction

Page 993, Line 12. Comment: The central limit theorem might still apply, only the transport regime of convection dispersion has not been reached yet.



Page 993, Line 13. Unclear statement – rephrase.

Page 996, Line 6: “NS>0.9” Comment: effective NS (adjusted for time-shift).

Methodology

Page 997, Line 4: “The focus of this study is to simulate [a] solute transport [experiment] within a tile-drained field close to the stream channel that was performed in an irrigation experiment in April 1997. . .” Rephrase this statement.

Page 997, Line 9: “three blocks” – better say ‘time intervals’?

Page 997, Line 9: “Ten minutes after onset of the first irrigation [delete: block] a bromide and [a] brilliant blue [Brilliant Blue] pulse was [were] added to the sprinkling water.”

Page 997, Line 12: Venturi flume, not ‘tube’!?

Page 997, Line 19: is it only “likely”? Is that not a proof?

Page 998, Line 1: “Soil water dynamics are [is] described”

Page 998, Line 4: use “ranges” instead of “reaches”.

Page 998, Line 9: “routing” – delete? it is not strictly speaking a routing approach.

Page 999, Line 1: “apparent worm burrows” –define apparent.

Page 999, Line 2: “assuming [that] they are. . .”

Page 999, Line 5: “Next we simulated the lengths [no: ‘length’, one macropore has a single length, how many as there may be of them] of each macropore. . .”

Page 999, Line 8: Not clear; explain p_lat. Probability for vertical digging is 1-2*p_lat, so between 0.05 to 0.1 (with plat=0.05)? What does that mean?

Page 999, Line 20: “cross-sectional [area]”

Page 999, Line 24: “. . .low [water] retention [delete: properties]” properties can not be 'low'.

Page 999, Line 26: "during simulation": replace by: on the simulation results

Page 1000, Line 4: I do not think it is correct to name this a "Cauchy boundary conditions". It is just what it is, a program controlled condition that may switch between flux (Neumann) and head (Dirichlet) type.

Page 1000, "2.4 Spatial model setups [delete: used in the present study]"

Page 1001, "2.4.1 Representation of the tile drain and weighting factor for scaling length specific outflow" these are two entirely different things, so perhaps use two different subsections. "Outflow scaling factors" could be used instead of "weighting factor for scaling length specific outflow"

Page 1002: "2.4.2 Transport parameters [delete: during simulation]"

Page 1002, Line 13: "1500 g of bromide was evenly distributed within the upper layer of the model domain." Within the upper 2 cm, similar to IPU? See also General Comments.

Page 1002, Line 23: check units for kf and exponent.

Page 1003, Line 1: Are there really no site-specific kf values available from previous studies for IPU sorption for this soil at the Weiherbach catchment? At least to parameterize sorption in the matrix?

Results

Page 1003, Line 13: "time series of simulated and observed bromide concentrations (in the middle column) and cumulated bromide loss from the 13 simulations and plotted against the corresponding observation (right column)." Move this statement to the next subsection on bromide transport.

Page 1003, Line 21: The output time intervals seem to be rather coarse. This adds



artificial variation in concentrations particularly for the breakthrough curve derived by differentiation of the cumulative curve.

Page 1005, Line 3: maybe you could state that the Rˆ2 >0.95 is here for original simulation results (not time adjusted). Why is not the model efficiency used as goodness-of-fit measure?

Page 1005, Line 24: "Please note that the simulations are rather insensitive for the kf." See my General Comments. All simulations overestimate retardation. But what happens if you select Kf=0? Close to Kf=0 (retardation factor = 1), the sensitivity should increase. Otherwise, the results obtained for variation of exponent n>1 (see comments above and general comments), targeting a retardation factor of one, cannot be explained and would be a modelling artefact.

4 Discussion

Page 1007, Line 2: what are common physical parameters behind the best 13 hillslope architectures?

Page 1007, Line 11. Artificial over-reduction of scenarios? How large is the error of the 13-4=8 rejected scenarios in terms of water and tracer balance?

Page 1007, Line 24. "tile train."

Page 1007, Line 18. "differed" not really clear, what values for kf and n for matrix and macropores were chosen and based on what rationale?

Page 1007, Line 25. Comment: particle facilitated transport – would that be measured at all analytically, or would not particles be filtered prior to starting the analytics?

Page 1007, Line 29ff. Comment : I think the following discussion could probably be revised in light of revised IPU transport simulation results.

Page 1010, Line 9. remove comma after "used," Page 1010, Line 10. “singular” – single

Page 1010, Line 15 “selected” – select

Conclusion:

Page 1011, Line 6: “Generic knowledge about the origin of dominating structures is crucial to reproduce these structures in a simplified yet a sufficiently realistic manner and thus reduce equifinality in the spatial model setup to a minimum amount”. This statement might be true but was not proven here. Something like: ‘First results suggest that…’ might be acceptable. Moreover, only a single realization of geometrical earthworm burrow distribution was used (then different Ks of the biopores were assumed). Other realizations may give different results? Finally, so far no conclusions, or suggestions regarding the procedure, are given for the pesticide part.

Tables

Table 1: Soil hydraulic van Genuchten parameters… Alpha is not the reciprocal air entry point (this is not the Brooks Corey model) Why is the bulk density of the Macropore medium larger that that of the soils?? The earth worm burrows should have a lower bulk density! That affects sorption!!

Table 2. perhaps mark somehow the 4 best scenarios (if they are really significantly better, see comments above).

Figures

Figure 2: Add the drain. Caption: “effective macropore region” instead of “macropores”.

Figure 3-5 should be combined into one Figure (then say ‘continued’ on each new page). That saves the reader from reading several times those identical figure captions. Some graphs are hardly visible.

Figure 6: please be consistent with use of numbers on the color scale (all get the ‘*10ˆ-3’, or none)



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