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Discussions

Interactive comment on "Model-based estimation of pesticides and transformation products and their export pathways in a headwater catchment" by M. Gassmann et al.

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The manuscript describes an attempt to model discharge and leaching of pesticides that were applied to arable fields within a watershed in Switzerland using a complex distributed model. The special aspect is the consideration of pesticide degradation products and to be able to simulate that these products can behave differently in space and time as compared to the applied substances. By describing preferential flow at the local scale in cylindrical macropores and lateral movement towards tiles, peaks of concentrations in river and surface water at the larger catchment scale following preferential flow events could be reproduced. To date, the fate of compounds and residues

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Interactive Discussion

Discussion Paper

of former applications (transformation products, TPs) in such a large scale watershed study is not well-known. The authors tried to consistently combine spatially-distributed watershed compartments and management-type process model components in a complex simulation system.

General comments: The topic is relevant, the text is well-written, and modelling and discussion are adequate. Nevertheless, some aspects could be clarified and others more critically reflected as pointed out below. The aspect of pathways and material characteristics in pathways is mostly not well known and solid-solution interactions or degradation in structural pores remain uncertain. The problem of equifinality could have some impact here as well. The manuscript seems to be written from a hydrologist' point of view, soil hydraulics and soil spatial variability, characterization of soil types, and soil structure as well as soil related references are relatively limited although reactive transport in structured soil is considered. With respect to testing model hypotheses about the flow pathways, tracer experiments have been carried out first with conservative tracers. The conservative tracers are used to determine the validity of assumptions on flow pathways; a step before testing pathways for the reactive solutes. If simulating reactive transport without a validated distributed water flow model, the matching of solute leaching could be ok, but could result from different reasons. I am not sure but I did not find descriptions of such an intermediate conservative tracer step for calibrating or validating the flow part here. Furthermore, for such large watersheds, studies of spatial heterogeneity at several scales (e.g., fields, the 10m by 10 m grid, the soil horizon, aggregates, or burrows) may be important (e.g., for a drained field, e.g., Gerke, Dusek, Vogel, 2013, Vadose Zone J.) at least to qualitatively characterize the relevance of the various model parameters.

Detailed comments

1. Introduction, Methods, Chapter 2.3: Indicate what is different here regarding methods and analyses in comparison to the paper of Gassmann et al 2013 Hydrol Sci J in press? Zin-AgriTra and Zin-Sed 2D needs more explanations.

2. Chapter 2.31: I did not understand why it was necessary that the soil moisture was assumed to increase within each layer according to an empirical relation (Eq. 1). If the water flow is calculated using Richards' equation as indicated before, the vertical distribution of water contents in all the layers will be calculated automatically according to the numerical discretization. It appears as a highly discretized distributed water balance model combined with some flux model and chemical reaction and sorption components.

3. The use of Hagen-Poiseuille's law for calculating the macropore hydraulic conductivity is a pragmatic possibility that means coupling a pore-scale equation for macropores with a macroscopic scale matrix flow equation. Similar approaches and their usefulness of have been discussed e.g., in Köhne et al. 2009 J Cont Hydrol., Gerke 2006 J. Plant Nutrition & Soil Science.

4. The Green-Ampt approach was used for simulating the "infiltration" (i.e., water transfer) of macropore water from macropores in to the soil matrix. How that coupling with the present layer model worked in detail here, I could not figure out. This simplification provides probably relatively stable solutions; however, transfer can be limited in just one direction; that means transfer from the matrix into the macropores for relatively saturated conditions is not considered?

5. In chapter 2.4.1, the cell grid size of 10 m was mentioned, which is of course still small compared to the size of the catchment. It is clear that with increasing cell size, the use of soil hydraulic properties and geometries will be more problematic, because of the internal heterogeneities within cells.

6. The macropore numbers and sizes are probably crucial for the outcome of this model. The parameters maybe regarded as "effective"; the question is whether these simplifying assumptions (number-diameter-conductivity-Green-Ampt mass transfer) are compensating for other unknown effects that occur in the field. Recent studies (soil) showed that earthworm burrows are not uniform, a drilosphere exists, and bur-

row walls are coated with casts; older burrows are often used by roots such that the hydraulic properties and exchange can differ in a wide range. Furthermore the wall coatings because of higher organic matter contents can have sorption properties that strongly differ from those of the matrix (such literature has not been discussed or included here). Of course, transformation product sorption along macropore walls is largely unknown.

7. Model calibration: For such a complex model system consisting of several models, each should in principle be calibrated independently and interactions separately. This can probably not be achieved using discharge and effluent concentration curves only but with additional observations in soils, drainage waters and other spatial compartments. It is interesting to have a tool for separately calculating discharge components such as e.g. tile drain via macropore; the question is how these separate components can be experimentally validated, how they may be compared with observations (which here was probably not yet possible.

8. What is the strategy here to address the problem of equifinality? The results and conclusions of this modelling study are in line with the hypotheses suggesting the important role of different pathways and physico-chemical characteristics of pesticides and transformation products. Nevertheless, it would be interesting to see how the results were affected by assumptions and calibrations of flow and transport in macropores, the exchange, or effects of the drainage network on discharge and leaching.

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