

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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Received and published: 19 September 2013

General comments: The paper seeks to model the fate of pesticides and their transformation products in a small catchment as well as their export to a surface water body (river). I highly appreciate that the authors challenge to approach the high complexity of a catchment considering multiple transport pathways in a heterogeneous and dynamic environment. I agree with Nicholas Jarvis that the results appear plausible. However, to my opinion, the final outcome builds on so many assumptions that I would have liked to see a kind of ‘uncertainty propagation’. As a non-expert in modeling I don’t feel fine, if things cannot be tested. I will try to specify this in the specific comments down below.

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Overall, I think the attempts made head in the right direction and the manuscript represent a substantial contribution to scientific progress. The paper perfectly fits within the scope of Hydrology and Earth System Sciences. Language and presentation quality is good.

Specific comments:

P9853-L6-10: Being a biologist with only general hydrology expertise, I always thought that preferential flow is happening immediately. Here it is stated that first water infiltrates into soil and only the surplus goes into macropore flow.

P9856-L14-16: If the mixing layer is a 'thin soil layer', how can photooxidation take place there? Is this process relevant here?

P9857-L17 and following: Microbial transformation of pesticides can be very slow in the environment. Still there is Atrazine in groundwater of countries like Germany where it has been banned a decade ago. Moreover, it has been shown that there might be two different degradation rates apply for one and the same compound when being present at high concentrations and at low concentrations (Torång et al. 2003). I wonder if the factors applied accounting for lower activities (= higher DT50 values) with depth are ok. The authors relate that to gradients of bacterial cell numbers as found in different soils, however, not in the catchment. Furthermore, the fraction of total to active cells is increasing with depth. Consequently, transformation might be considerably slower than assumed.

P9860-L5: As already mentioned earlier, the outcome of the study builds on many assumptions. One example is the macropores, where the number, the size, and the orientation need to be assumed. Is no empirical data available from other studies in this catchment?

P9860-L16: How can the boundaries of a catchment be fixed to have 'no-flow' in the lateral direction. I can also follow the logic to artificially set different vertical boundaries

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in the southern (impermeable) and eastern sub-basin (permeable) of the catchment according to observations from wells. However any kind of geological records from that site would substantiate these assumptions.

P9862-L19-21: Does this mean, that in the catchment modeled there is no recharge of the aquifer? The model says 40% of precipitation is evapotranspiration, 58% is discharge (surface runoff and drainage?), but only 1% subsurface (underground) flow.

P9863-L19: I strongly doubt that 89-99% of the different pesticide compounds have been mineralized with the short time span. This is a point which, to my opinion needs to be evaluated. How big is the chance that PCs are still in the soil at higher concentrations or have left the system by other pathways (into the aquifer)? The authors conclude that the major export pathway was overland flow. Does this mean that the degradation of the PCs took place during overland transport? Neglecting sorption and taking into account the applied DT50 values 10 to 20 for the parent compounds, then did the major export events (23d after application and 60-71d after application) allow sufficient decay before the PCs should have ended up in the river?

P9867-L1-2 & L12-14: I don't agree. To support such a comprehensive and complex modelling approach hopefully leading to progress in future research, sampling and longer computation times are acceptable.

Reference:

Lars Torång, Niels Nyholm, and Hans-Jørgen Albrechtsen, Shifts in Biodegradation Kinetics of the Herbicides MCPP and 2,4-D at Low Concentrations in Aerobic Aquifer Materials. *Environ. Sci. Technol.*, 2003, 37 (14), pp 3095–3103

Interactive comment on Hydrol. Earth Syst. Sci. Discuss., 10, 9847, 2013.

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