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Modelling the transfer of pesticide transformation products from agricultural fields to the aquatic environment – state of knowledge and future challenges

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Transformation products (TP) of pesticides are found everywhere in the aquatic environment. Their dynamic formation and subsequent transport from agricultural fields to adjacent water bodies can be estimated by using environmental fate models, which is done e.g. in the registration process for plant protection products in the European Union. In this study, an overview of models, transformation simulation concepts and model applications for TP estimation including leaching and catchment scale models is given. The review is restricted to models which were tested against field data in peer-reviewed publications. The models included in this review are GLEAMS, MACRO, RZWQM(2), PEARL, PRZM, Pelmo, LEACHM, HYDRUS 1-D, ZIN-AgriTra and the Field Release Model (FRM).

Investigating model structures revealed, that six transformation schemes, i.e. possible transformation pathways, are implemented in the models. Only one of the reviewed models, PELMO, uses a completely flexible scheme. In all other models, pathways are restricted. An assessment of model complexity, including hydrological processes and transformation-affecting processes, resulted in PELMO having the highest transformation but the least hydrological complexity among leaching models. RZWQM is the leaching model with the highest hydrological complexity and ranks second in transformation processes. Among the three catchment scale models, ZIN-AgriTra ranks highest in both, hydrological and transformation complexity.

Even though the number of publications of TP model applications is rather low, the number of leaching models is adequate (eight models). At the catchment scale, however, only two models with proven applications exist in the literature. A spatio-temporal analysis of all models revealed a gap in catchment and regional-scale models with a daily or lower temporal resolution. Thus, well-developed and applied catchment-scale models should be extended by a TP module. This would enable scientists and authorities to estimate TP concentrations or to analyse the environmental fate of TPs at the larger catchment scale. At the same time, the fate processes in models should be updated to reflect the current state of knowledge, especially more flexible transformation schemes and the formation of TPs in different compartments (i.e. plant, soil, water). The integration of pathway prediction models such as the University of Minnesota Pathway Prediction System could enhance the assessment of the large number of pesticide TPs in the aquatic

environment.