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Re-design of a physically-based catchment scale agrochemical model for the simulation of parameter spaces and flexible transformation schemes

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The use of a broad variation of agrochemicals is essential for the modern industrialized agriculture. During the last decades, the awareness of the side effects of their use has grown and with it the requirement to reproduce, understand and predict the behaviour of these agrochemicals in the environment, in order to optimize their use and minimize the side effects. The modern modelling has made great progress in understanding and predicting these chemicals with digital methods.
While the behaviour of the applied chemicals is often investigated and modelled, most studies only simulate parent chemicals, considering total annihilation of the substance. However, due to a diversity of chemical, physical and biological processes, the substances are rather transformed into new chemicals, which themselves are transformed until, at the end of the chain, the substance is completely mineralized. During this process, the fate of each transformation product is determined by its own environmental characteristics and the pathway and results of transformation can differ largely by substance and environmental influences, that can occur in different compartments of the same site.
Simulating transformation products introduces additional model uncertainties. Thus, the calibration effort increases compared to simulations of the transport and degradation of the primary substance alone. The simulation of the necessary physical processes needs a lot of calculation time. Due to that, few physically-based models offer the possibility to simulate transformation products at all, mostly at the field scale. The few models available for the catchment scale are not optimized for this duty, i.e. they are only able to simulate a single parent compound and up to two transformation products. Thus, for simulations of large physico-chemical parameter spaces, the enormous calculation time of the underlying hydrological model diminishes the overall performance.
In this study, the structure of the model ZIN-AGRITRA is re-designed for the transport and transformation of an unlimited amount of agrochemicals in the soil-water-plant system at catchment scale. The focus is, besides a good hydrological standard, on a flexible variation of transformation processes and the optimization for the use of large numbers of different substances. Due to the new design, a reduction of the calculation time per tested substance is acquired, allowing faster testing of parameter spaces. Additionally, the new concept allows for the consideration of different transformation processes and products in different environmental compartments.
A first test of calculation time improvements and flexible transformation pathways was performed in a Mediterranean meso-scale catchment, using the insecticide Chlorpyrifos and two of its transformation products, which emerge from different transformation processes, as test substances.