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Simulating the fate and release of metazachlor and its transformation products metazachlor oxalic acid and sulfonic acid in a small-scale agricultural catchment

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The unwanted release of pesticides after use in agriculture is a known concern for water quality. Thus, a monitoring campaign was carried out in 2016 and 2017 by the project MUTReWa to determine the release of herbicides from the 180 ha area of the Loechernbach catchment. In which the herbicide metazachlor and its transformation products (TPs) metazachlor oxalic acid and sulfonic acid were measured regularly in the base flow and during rainfall-runoff events even in high concentrations in the Loechernbach catchment. The study area is characterized by vineyards on large terraces and an intensive agricultural use in the valley. A dense road and drainage network accelerates the drainage of the catchment area.

Based on these measurements, the aim of this study was to adapt an existing catchment model, which simulates the transport and transformation processes for pesticides in the Loechernbach catchment, for the modeling of the herbicide metazachlor and its TPs oxalic acid and sulfonic acid and to make these available for further simulation studies.

For this purpose, the spatially distributed and process-based catchment area model ZIN-AgriTra was used. The hydrological sub-model was successfully calibrated for a 6-month high-resolution time series of discharge data for 2016 (Nash-Sutcliffe efficiency = 0.8). The metazachlor and TPs modeling was done for single rainfall-events using literature parameters for sorption and degradation behavior. The application of metazachlor was adjusted within the scope of recommended spray rates to the measured output.

The simulation results of outflow and metazachlor concentration fit well with the measurements at the catchment outlet. The first event after application causes a strong leaching of metazachlor with maximum concentrations up to 10 μg/L. Thereafter, measurements and simulation results show significantly lower concentrations in the range of maximum 200 ng/L. In the model, metazachlor is almost completely degraded in the soil by the end of the application period. The results for the simulated transformation products show a maximum concentration of 100 ng/L for the sulfonic acid and 400 ng/L for the oxalic acid. The simulated TPs concentration of event and base outflows are in the range of the observation. The main discharge path for the TPs is the subsurface flow from the fields, with most of the TPs release being caused by the degradation of the previous year's application.

Concluding, the catchment model ZIN-AgriTra can be seen as a suitable tool for the simulation of the dominant processes of the metazachlor release. In addition to the results of the measurement campaign, the model application provided new insights into the behavior and fate of metazachlor and its TPs metazachlor oxalic and sulfonic acids.