Geophysical Research Abstracts
Vol. 21, EGU2019-10662, 2019
EGU General Assembly 2019

Combining conceptual transport models with a new likelihood framework to assess high-frequency measurements of in-stream herbicide concentration

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In-stream herbicide concentrations have been shown to exceed regulatory limits in many agriculturally dominated catchments. Peak concentrations, which tend to occur during rainfall events, are especially worrisome. Modelling herbicide transport processes at the catchment scale is a promising tool for interpolation and extrapolation of available measurement data and as a basis for decision making. Our modeling study is based on a previous controlled herbicide application experiment in a small agricultural headwater catchment.

In a first step, we developed a conceptual semi-distributed transport model based on pre-existing experimentalist knowledge of the processes occurring in the catchment. The model considers fast transport processes (through shortcuts), degradation and sorption of two herbicides with different but known source areas. The model was then combined with a recently developed likelihood function, which allowed us to successfully address issues like high temporal variability, strongly autocorrelated errors in combination with varying measurement intervals, and multiple optimization criteria. Applying the Bayesian equivalent of multi-objective calibration, we performed joint inference of hydrological, chemical and error model parameters on high-frequency streamflow and concentration data. We show the resulting posterior parameter distribution and the associated output uncertainty.

Repeating this procedure with conceptual models of varying complexity representing different assumptions about the dominant transport processes, we identified suitable model configurations. By this we reveal the importance of fast transport processes (facilitated by artificial shortcuts and drainage pipes), degradation and sorption processes, and the non-linear behavior observed at small spatial scales and at high temporal resolution. These results allow for more quantitatively based estimates of the distribution of herbicide loads and concentrations to be expected in small agriculturally dominated headwater catchments.