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Modeling the fate of Diclofenac in soil-water systems

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Groundwater contamination by pharmaceuticals is a potential threat to the integrity of natural ecosystems and human health. Here, we focus on the medical drug *Diclofenac*, which poses concerns due to its recalcitrance and documented accumulation in groundwater. Experimental evidences yield controversial results on the extent of its attenuation in groundwater, a peculiar behavior being observed under reducing redox conditions. In this context, batch experiments have revealed the occurrence of a reversible biotransformation pathway of *Diclofenac* in groundwater under biotic denitrifying conditions. Such a behavior is not captured by excessively streamlined model formulations (e.g., based on first order reaction kinetics). We suggest a modeling framework which is grounded on a conceptualization (and ensuing mathematical formulation) of the molecular dynamics of *Diclofenac* biodegradation in the considered scenario. We leverage on available laboratory-scale batch experiments associated with a soil-water system and embed the resulting model formulation in a stochastic context. We address the way the available information content can be effective in characterizing specific model processes upon (progressively) reducing the complexity of the proposed geochemical model. Four levels of simplification are considered in our study. The resulting mathematical formulations represent four plausible models. These are employed in a multi-model context to interpret the considered system dynamics conditional to available data. Each candidate model is calibrated through a Maximum Likelihood approach assisted by modern sensitivity analyses techniques. This allows quantifying the impact of model structure and parametric uncertainty on relevant outputs, such as the temporal evolution of *Diclofenac* concentrations. The performance of each plausible model is then assessed (in a relative sense) through model discrimination criteria. Our results suggest that an optimal trade-off in terms of model complexity (level of parametrization) given data availability can be assessed to satisfactorily interpret the system dynamics. Our approach has the potential to be transferred also to scenarios embedding reactive transport settings, such as in laboratory flow columns. Here, various reducing conditions can take place along the system. In such contexts, application of the proposed modeling approaches can be advantageous to cope with the potential occurrence of a marked range of biogeochemical processes (and possibly high uncertainty degrees).