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Modeling Microbial Regulation of Pesticide Turnover in Soils: Development of Up-scaled Process Descriptions

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While many pesticides show high biodegradability in soil under controlled conditions in the lab, some compounds (e.g., 2-chloro-4ethylamino-6-isopropylamino-1,3,5-triazine, atrazine; 4-chloro-2-methylphenoxyacetic acid, MCPA) persist and accumulate in the field. This poses the risk that soils become continues sources of pesticides for subsoils and groundwater. Turnover and persistence of pesticides at the pedon scale depend on the precedent encounter of pesticides and microbial degraders and therefore on small-scale (μm-mm) structure of soils. The interplay of microbial (growth, metabolism, physiology) and physicochemical processes (diffusion, convection, sorption) is a key control of pesticide biodegradation but not well understood. This project aims to improve the understanding and prediction of pesticide turnover and persistence by incorporating key processes controlling the biodegradation of the two above-mentioned pesticides into models. The objective is to find simplified but mechanistic process descriptions of pesticide turnover at the field scale. This will be addressed following a bottom-up approach. Small-scale mechanistic biogeochemical modeling will be integrated with experimental data to identify the model complexity that needs to be considered to reflect limited pesticide turnover in the field. Model development will be based on the PECCAD model (PEsticide degradation Coupled to CArbon turnover in Detritusphere). First, microbial controls such as energy-limited growth, concentration thresholds of gene expression and enzyme production will be implemented in PECCAD, ignoring spatial structure and transport processes (one-dimensional, 1D). Then, the PECCAD model will be extended to two-dimensional (2D) spatial structure and transport processes. Second, based on model analysis and model calibration of 1D and 2D models, the qualitative behavior of the PECCAD model will be evaluated to identify the key processes that control the system behavior. Third, probabilistic scenario simulations with the 2D PECCAD model will be performed to quantify the impact of degrader and pesticide encounter at the small scale on pesticide degradation at the pedon scale (0.50 – 1 m depth). Finally, mechanistic up-scaled process descriptions of pesticide turnover in soil will be derived from model analysis and probabilistic scenario simulations. We expect to find key processes and factors that determine pesticide turnover and persistence in soils under field conditions. Additionally, with the implementation and simplification of the PECCAD model, we expect to establish a basic approach of pesticide turnover in soils that represents the implications of the heterogeneous spatial distribution of pollutants and microorganisms in soils.