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Integrated modeling of organic contaminants at the catchment scale (AquaTerra)

D. Kuntz, Y. Du, O. Kolditz, P. Grathwohl

Center for Applied Geosciences, University Tübingen, Germany,
(david.kuntz@uni-tuebingen.de / Phone: +49 (7071) 29-77452

At the University of Tübingen a powerful modeling tool is being developed, capable of uniting surface flow, unsaturated Richards flow and groundwater flow in one code. This tool is to be used to improve understanding of processes relevant for fate and transport of (organic) contaminants (PAHs, PCBs, Pesticides) at the catchment-scale.

In the last decades research on remediation of contaminated sites, extensive column-experiments and new theories on sorption- and/or reaction mechanisms have greatly increased our knowledge about these processes from grain to bench scale. The relevance of these processes at the different field scales, however, is not always clear and how to upscale them is not yet understood.

On larger scales ubiquitous contaminants (such as PAHs by atmospheric deposition, pesticides or PCBs) can be used as reactive tracers to study their fate in the soil and groundwater system at large scale. The AquaTerra integrated project allows to incorporate detailed knowledge about transport mechanism such as sorption/desorption, degradation, volatilization in models at larger (catchment-) scales.

The upscaling is extended step-by-step by monitoring small to large scale field-sites and scenario calculations which will further help to predict contaminant fate in hydrologically closed catchments.

Some specific problems to be addressed at the catchment scale are:

- How to regionalize (unsaturated) soil- and rock-properties?
- At what (time and spatial) scale(s) is the local equilibrium assumption for sorption/desorption valid?

- How to reduce computational load without increase in uncertainty (= valid simplifications?)