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Integrative modeling of water flow dynamics and nitrogen biogeochemistry in the soil-unsaturated zone-groundwater System

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Nutrient inputs in soil, groundwater, and rivers are still one of the most important problems in agricultural areas in Germany. The assessment of the groundwater pollution risk by diffuse immissions from, among others, agricultural practice as well as the recommendation of effective counteractive measures and optimized agricultural practices requires a qualitative and quantitative understanding of the fate and effect of nutrients in the soil-vadose zone-groundwater system. Within a joint research and development project, we are under development and application of a physical, process-based distributed numerical simulation framework to model water-flow dynamics and nitrogen biogeochemistry on the catchment scale. Among others, the model considers both unsaturated and saturated flow and transport, different nitrogen species, biogeochemical N-transformation reactions as well as different land use. In accordance with the EC-Water Framework Directive (WFD), the federal state of Thuringia has issued surface water and groundwater quality monitoring programs in different regions of Thuringia. From those, the Erlbach sub-catchment in Eastern Thuringia was selected as prototypical region for model development, implementation, parameterization, calibration, and validation. The Erlbach catchment is effected by intensive pasture and crop-farming with medium to high N-loads by fertilizer and manure inputs. Information and prescience on the pedologic and hydrogeologic situation, land use and land use history is available. Lithology is dominated by Triassic formations of the Mittlere und Untere Buntsandstein, covered by pleistocene and holecene sediments and deposits. The soils found are typical for these parent materials and include in particular cambisols, luvisol, fluvisols, and colluvisols. Flow and transport of water and nitrogen is affected by a complex interplay of hydraulic, physicochemical, and biogeochemical processes in the soil, the vadoze zone and the groundwater. Unfortunately, there is not one single software solution for the simulation of all the relevant process in these different subsurface compartments. Moreover, we face the situation that immense financial and personal effort has been invested in the set up and application of partial solutions, e.g., the implementation of a groundwater flow model or water-balance models. Thus, one of our goals was to integrate already existing, but heterogeneous numerical solutions provided by existing software tools. The tasks of the first phase of this project were to develop a comprehensive conceptual model based on given constraints of existing and software solutions, the definition of interface functionalities and the requirements for the GUI. During the second and running project phase, the tasks are to implement, test, adapt and validate the model. The numerical backbone of our simulation framework is a data and simulation engine based on a distributed spatial approach employing biogeochemical and hydropedological response units. This engine acts as an interface and GUI. Yet, its major function is to link, synchronize and drive the interplay of three different numerical tools. These are (i) the land-surface-restricted hydrological and water balance model J2000S (FINK et al., 2007) for the simulation of the catchment hydrology, climate and land use data, (ii) the HYDRUS code (ŠIMŮNEK & van GENUCHTEN, 2008) for water flow, N-dynamics and heat transport in the unsaturated zone parameterized based on concepts developed for agricultural and forest sites (HUWE AND TOTSCHE 1995; MATZNER et al. 2001), and (iii) FEFLOW (DHI-WASY GmbH) for simulation of water, heat and solute transport in the aquifer. We will present the unique features of the data/simulation engine and the basic concept of the implementation. Preliminary results on prognostic scenarios employing pedological, hydrogeological and land use data from the Erlbach catchment are discussed.

Literature

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