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Modelling the hydraulic and geochemical evolution of a hillslope transect

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Especially the long-term response of subsurface-surface water systems and their water quality on pressures such as diffuse pollution from agricultural activities or atmospheric deposition are not well understood at the catchment scale. The goal of this study is to quantify the factors that influence the geochemical interactions between soils and seepage water, rocks and groundwater as well the subsurface/surface water interaction in a comprehensive way. Only very recently numerical codes became available which not only couple flow and reactive transport but also unsaturated and saturated zone allowing it to follow water quality from the infiltration into the soil until discharge in a spring or river, of which the code MIN3P was used.

In order to assess groundwater quality, the origin of the recharge water and its chemical evolution pathways have to be known at the catchment scale. This involves precipitation, evapotranspiration, seepage water infiltration, interflow and perched water, and finally the groundwater as well as the effluent to rivers or springs in a watershed. Water quality is affected by rainwater pH and dissolved solids, leaching of potential pollutants from top-soils, release of CO_2 from organic matter oxidation / microbial respiration in the unsaturated zone and the water-rock interaction in the subsurface. A promising approach to identify the principal processes is the selection of vertical profiles along streamlines across the area of interest. That way, numerical simulations requiring only short computational time could be utilized to describe the water flow and solute transport from elevated parts of the catchment to the receiving stream. Eventually, this approach can be extended to capture a watershed in a three-dimensional model.

A geologic model representative for a typical valley scenario in a triassic sequence landscape composed of of sandstones and marls was set up, consisting of a i) sand and gravel aquifer, ii) underlying and hill-slope sedimentary rock formations and iii) the soil cover and weathered rock layers. The geologic model was extended into a hydrologic and hydrogeologic model by using regionally typical water budgets and hydraulic parameters. Finally hydrogeochemical reactions were implemented such as dissolution of consumption of O_2 and production of CO_2 in soils, release of nitrate and other pollutants from soils, dissolution of carbonates and other sedimentary rocks and changes of redox conditions along the flow lines of water.

Results show that subsurface water residence times range from years to many centuries. Different zones are to be expected with respect to the development of mineral equilibria such as open or closed system carbonate dissolution. Short-term responses to daily averaged changes in precipitation, however, are visible to some extent in the shallower and near-river parts of the flow system as well as in solute loads. This can most likely be explained by directional changes in flow paths. The extent of reducing zones is controlled by the presence of organic rich layers (i.e. peat deposits), the dissolution kinetics of aquifer organic matter and the subsequent mixing with oxygenated water by hydrodynamic dispersion.