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Regional coupling of unsaturated and saturated flow and transport modeling – implementation at an alpine foothill aquifer in Austria

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For many European countries nitrate leaching from the soil zone into the aquifer due to surplus application of mineral fertilizer and animal manure by farmers constitutes the most important threat to groundwater quality. Since this is a diffuse pollution situation measures to change agricultural production have to be investigated at the aquifer scale. In principal, the problem could be solved by the 3 dimensional equation describing variable saturated groundwater flow and solute transport. However, this is computationally prohibitive due to the temporal and spatial scope of the task, particularly in the framework of running numerous simulations to compromise between conflicting interests (i.e. good groundwater status and high agricultural yield).

For the aquifer 'Westliches Leibnitzer Feld' we break down this task into 1d vertical movement of water and nitrate mass in the unsaturated zone and 2d horizontal flow of water and solutes in the saturated compartment. The aquifer is located within the Mur Valley about 20 km south of Graz and consists of early Holocene gravel with varying amounts of sand and some silt. The unsaturated flow and nitrate leaching package SIMWASER/STOTRASIM (Stenitzer, 1988; Feichtinger, 1998) is calibrated to the lysimeter data sets and further on applied to so called hydrotopes which are unique combinations of soil type and agricultural management. To account for the unknown regional distribution of crops grown and amount, timing and kind of fertilizers used a stochastic tool (Klammler et al, 2011) is developed that generates sequences of crop rotations derived from municipal statistical data.

To match the observed nitrate concentrations in groundwater with a saturated nitrate transport model it is of utmost importance to apply a realistic input distribution of nitrate mass in terms of spatial and temporal characteristics. A table is generated by running SIMWASER/STOTRASIM that consists of unsaturated water and nitrate fluxes for each 10 cm interval of every hydrotope vertical profile until the lowest observed groundwater table is reached. The fluctuation range of the phreatic surface is also discretized in 10 cm intervals and used as outflow boundary condition. By this procedure, the influence of the groundwater table on the water and nitrate mass leaving the unsaturated can be considered taken into account varying soil horizons.

To cover saturated flow in the WLF aquifer a 2-dimensional transient horizontal flow and solute transport model is set up. A sequential coupling between the two models is implemented, i.e. a unidirectional transfer of recharge and nitrate mass outflow from the hydrotopes to the saturated compartment. For this purpose, a one-time assignment between the spatial discretization of the hydrotopes and the finite element mesh has to be set up. The resulting groundwater table computed for a given time step with the input from SIMWASER/STOTRASIM is then used to extract the corresponding water and nitrate mass values from the look-up table to be used for the consecutive time step. This process is being repeated until the end of the simulation period.

Within this approach there is no direct feedback between the unsaturated and the saturated aquifer compartment, i.e. there is no simultaneous (within the same time step) update of the pressure head - unsaturated head relationship at the soil and the phreatic surface (like is shown e.g. in Walsum and Groedendijk, 2008). For the dominating coarse sand conditions of the WLF aquifer we believe that this simplification is not of further relevance. For higher soil moisture contents (i.e. almost full saturation near the groundwater table) the curve returns to specific retention within a short vertical distance. Thus, there might only be mutual impact between soil and phreatic surface conditions for shallow groundwater tables. However, it should be mentioned here that all other processes in the two compartments (including capillary rise due to clay rich soils and groundwater withdrawn by root plants or evaporation losses) are accordingly considered given the capabilities of the used models.

If we impose the computed groundwater table elevation as the outflow condition of the hydrotope for the next time step we postulate that the associated water volume of the saturated storage change will lead to the same change of the phreatic surface in the hydrotope column. This is only valid if the storage characteristics of the affected unsaturated soil layers can be adequately described by the co-located porosity of the saturated model. Moreover, the current soil moisture content of the respective soil layers is not being considered by the implemented new outflow boundary condition. Thus, from the perspective of continuity of mass it might be more correct, to transfer

the same water volume that led to the saturated change (rise and fall) of the groundwater table to the unsaturated hydrotope column and compute the adjusted outflow boundary position for use in the next time step. Due to the hydrogeological conditions in our application, for almost all hydrotopes we have the same soil type (i.e. coarse sand) in the range of groundwater table fluctuations and thus, we expect no further impact of transferring the groundwater table from the saturated computation to the unsaturated domain.
Summarizing, for the hydrogeologic conditions of our test site and the scope of the problem to be solved the sequential coupling between 1d unsaturated vertical and 2d saturated horizontal simulation of water movement and solute transport is regarded as an appropriate conceptual and numerical approach. Due to the extensive look-up table containing unsaturated water and nitrate fluxes for each hydrotope at a vertical resolution of 10 cm no further feedback processes between the unsaturated and saturated subsurface compartment need to be considered.

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