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Probabilistic, sediment-geochemical parameterisation of the groundwater compartment of the Netherlands for spatially distributed, reactive transport modelling

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Pollution of groundwater aquifers with contaminants as nitrate is a common problem. Reactive transport models are useful to predict the fate of such contaminants and to characterise the efficiency of mitigating or preventive measures. Parameterisation of a groundwater transport model on reaction capacity is a necessary step during building the model. Two Dutch, national programs are combined to establish a methodology for building a probabilistic model on reaction capacity of the groundwater compartment at the national scale: the Geological Survey program and the NHI Netherlands Hydrological Instrument program.

Reaction capacity is considered as a series of geochemical characteristics that control acid/base condition, redox condition and sorption capacity. Five primary reaction capacity variables are characterised: 1. pyrite, 2. non-pyrite, reactive iron (oxides, siderite and glauconite), 3. clay fraction, 4. organic matter and 5. Ca-carbonate. Important reaction capacity variables that are determined by more than one solid compound are also deduced: 1. potential reduction capacity (PRC) by pyrite and organic matter, 2. cation-exchange capacity (CEC) by organic matter and clay content, 3. carbonate buffering upon pyrite oxidation (CPBO) by carbonate and pyrite. Statistical properties of these variables are established based on c. 16,000 sediment geochemical analyses. The first tens of meters are characterised based on 25 regions using combinations of lithological class and geological formation as strata. Because of both less data and more geochemical uniformity, the deeper subsurface is characterised in a similar way based on 3 regions.

The statistical data is used as input in an algoritm that probabilistically calculates the reaction capacity per grid cell. First, the cumulative frequency distribution (cfd) functions are calculated from the statistical data for the geochemical strata. Second, all voxel cells are classified into the geochemical strata. Third, the cfd functions are used to put random reaction capacity variables into the hydrological voxel model. Here, the distribution can be conditioned on two variables. Two important variables are clay content and depth. The first is valid because more dense data is available for clay content than for geochemical variables as pyrite and probabilistic, lithological models are also built at TNO Geological Survey. The second is important to account for locally different depths at which the redox cline between NO_3-rich and Fe(II)-rich groundwater occurs within the first tens of meters of the subsurface. An extensive data-set of groundwater quality analyses is used to derive criteria for depth variability of the redox cline. The result is a unique algoritm in order to obtain heterogeneous geochemical reaction capacity models of the entire groundwater compartment of the Netherlands.