Geophysical Research Abstracts
Vol. 14, EGU2012-**PREVIEW**, 2012
EGU General Assembly 2012

Statistical characterisation and stochastic parameterisation of sedimentary geological formations on their reaction capacity for sustainable groundwater quality management

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The fate of contaminants in groundwater aquifers is determined by the buffering capacity of those aquifers together with the composition of inflowing groundwater. A nationwide characterisation of the environmental geochemistry of the shallow subsurface (down to 30 m below surface) has been started in the Netherlands. This covers: 1. the reaction capacity of sediments as buffer for contamination, and 2. typical elemental composition of geological formations and the association between trace elements and major minerals. For this purpose, the Netherlands is subdivided into 27 so-called geotop regions each having a unique geological build-up of the shallow subsurface. Here, four types are recognised based on vertical hydrogeological build-up. The regions are statistically characterised on their geochemical composition using combinations of lithological class and geological formation as strata. The statistical data are subsequently coupled with a geological voxel model of the subsurface to stochastically parameterise the geological units on reaction capacity. This combined approach will be illustrated for the Dutch province Zeeland.

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. A statistical investigation of several hunderds of sediment analyses is performed that provides the geochemical properties of the sediments. Here, classification based on sedimentary facies may provide additional insight on spatial heterogeneity within lithological classes.

A two-step stochastic algoritm is established for parameterisation of a geological voxel model. First, the cumulative frequency distribution (cfd) functions are calculated for the geochemical strata. Next, all voxels are classified into the geochemical strata and the cfd functions are used to put random reaction capacity variables into the geological voxel model. The result is a heterogeneous geochemical reaction capacity model of the subsurface having grid cells of 100x100x0.5 m. This model can be used in e.g. groundwater transport models or other instruments for groundwater quality management.