## Geochemical transport modeling of a phreatic drinking water pumping station

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We developed a regional scale 3-dimensional multicomponent reactive transport model to predict the groundwater quality at a phreatic drinking water production site. PHT3D (Prommer et al., 2003) was used as model code. PHT3D couples the 3-dimensional transport simulator MT3DMS with the goechemical model PHREEQC-2. The study examined the influence of various land use functions on the quality of the abstracted groundwater as well as the occurrence of various type of geochemical processes. The following processes were incoporated in the model: nitrate reduction, aqueous complexation, cation exchange, dissolution and precipitation of minerals (carbonates, hydroxides and pyrite). The model is filled with local determined geochemical and hydrochemical data. The redox reactivity of the sediments is derived from sensitive respiration experiments. Time series of groundwater quality data were available for validation.

Figure 1 shows the modeled and measured  $NO_3$  concentration of the abstracted groundwater. The scenarios predicts the concentration with and without measures taken in 1990 to reduce the manure use after a period of almost 2 decades of intensive manure spreading.



Figure 1: modeled and measured NO<sub>3</sub> concentration of abstracted groundwater

## Reference

Prommer, H., Barry, D.A. & Zheng, C., [2003]. MODFLOW/MT3DMS based reactive multi-component transport modeling. Ground Water 42 (2).

## A model for calculating the solubility of gases (CO<sub>2</sub>, H<sub>2</sub>S,...) used for the sequestration of global warming gases

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A thermodynamic model for calculating the solubility of gases (CO<sub>2</sub>, H<sub>2</sub>S, N<sub>2</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>) in pure water and in salt solutions in a wide temperature, pressure and ionic solutions is presented. Although parameterized from the gas-H<sub>2</sub>O-NaCl systems, the model accurately predicts gas solubilities in many other aqueous salt systems, such as seawater, without fitting data from these systems. This model finds wide applications, such as in the study of gas sequestration, and in rock-fluid interactions.