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Quantification of temperature impacts on the dissolution of chlorinated hydrocarbons into groundwater

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Shallow thermal energy storage has great potential for heat storage especially in urban and industrial areas. However, frequently existing organic groundwater contaminations in such areas were currently seen as exclusion criteria for thermal use of the shallow subsurface, since increased contaminant discharge is feared as consequence of heating. Contaminant discharge is influenced by a complex interaction of processes and boundary conditions as e.g. solubility, dispersion, viscosity and degradation, where there is still a lack of experimental evidence of the temperature dependent interaction. Even existing studies on basic influencing factors as e.g. temperature dependent solubilities show contradictory results. Such knowledge gaps should be reduced to improve the basis and liability of numerical model simulations and the knowledge base to enable a more differentiated and optimized use of resources. For this purpose batch as well as 1- and 2-dimensional experimental studies concerning the temperature dependent release of TCE (trichloroethylene) from a NAPL (non aqueous phase liquid) source are presented and discussed. In addition, this experimental studies are accompanied by a numerical model verification, where extensions of existing numerical model approaches on basis of this obtained experimental results are developed.
Firstly, temperature dependent TCE solubility data were collected using batch experiments with significantly better temperature resolution compared to earlier studies, showing a distinct minimum at 35°C and increased solubility towards 5°C and 70°C. Secondly, heated 1-dimensional stainless steel columns homogenously filled with quartz sand were used to quantify source zone depletion and contaminant discharge at 10-70°C. Cumulative mass discharge curves indicated two blob categories with distinct differences in dissolution kinetics. Increasing the temperature showed here an increase of the amount of fast dissolving blobs indicating higher NAPL-water contact areas. Thirdly, heatable 2D-tanks (40 cm x 25 cm x 10 cm) homogenously filled with quartz sand and percolated by distilled H_2O were used to investigate the dissolution behavior and plume development of TCE from a residual source zone (5 cm x 5 cm x 10 cm) at 10-70°C. Using NAPL source zone saturation of 5% (Case A) and 20% (Case B) two exemplary cases of a depleted and a fresh source zone were investigated. TCE outflow concentrations in case A increased continuously with increasing temperature, but were controlled by the temperature-dependent solubility in Case B. The experimental results showed that the TCE mass transfer rate has a minimum at about 40°C, if dissolution is non-rate limited and a continuous increase with increasing temperature for rate-limited systems. Implementation of temperature dependent NAPL dissolution and two different blob categories with different mass transfer rate coefficients in the OpenGeoSys code proved successful in reproducing the experimental results.

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