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Modelling approach to account for competitive sorption of PFAS in MODFLOW-based solute transport simulations

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Per- and polyfluoroalkyl substances (PFAS) are extremely persistent contaminants that constitute an increasing problem for drinking water resources worldwide. Modelling tools to predict the subsurface transport of PFAS are important both for risk assessment and for design and evaluation of in-situ PFAS stabilization using activated carbon (AC) or other sorbent amendments. At highly contaminated hotspots, such as fire-fighting training sites, a mixture of many PFAS are typically present in the contaminated groundwater. The different PFAS can interact in the sorption process and e.g. compete for sorption sites, which may affect both the risks associated with PFAS transport and the efficacy of remediation strategies such as sorbent amendments.

The aim of this study was to develop a user-friendly modelling approach to account for competitive sorption of PFAS in a solute transport package that can be applied in combination with groundwater flow modelling with MODFLOW, and to illustrate the effect of competition on the transport of different PFAS for a field site scenario. A competitive sorption model for PFAS was implemented in MODFLOW/MT3DMS and can be run in combination with a graphical user interface for MODFLOW such as GMS. The new model is aimed for practical applications of site modelling and PFAS risk assessment when competition effects may be important. Modelling of a field site scenario based on a fire-fighting training site at a Swedish airport illustrates that competitive sorption affects the transport of PFAS in the groundwater and can provide valuable site-specific insight for remediation efforts.