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Comparison of different modeling approaches to simulate contaminant transport in a fractured limestone aquifer

K. Mosthaf, L. Rosenberg, N. Balbarini, M.M. Broholm, P.L. Bjerg and P.J. Binning

It is important to understand the fate and transport of contaminants in limestone aquifers because they are a major drinking water resource. This is challenging because they are highly heterogeneous; with micro-porous grains, flint inclusions, and being heavily fractured. Several modeling approaches have been developed to describe contaminant transport in fractured media, such as the discrete fracture (with various fracture geometries), equivalent porous media (with and without anisotropy), and dual porosity models. However, these modeling concepts are not well tested for limestone geologies. Given available field data and model purpose, this paper therefore aims to develop, examine and compare modeling approaches for transport of contaminants in fractured limestone aquifers.

The model comparison was conducted for a contaminated site in Denmark, where a plume of a dissolved contaminant (PCE) has migrated through a fractured limestone aquifer. Multilevel monitoring wells have been installed at the site and available data includes information on spill history, extent of contamination, geology and hydrogeology. To describe the geology and fracture network, data from borehole logs was combined with an analysis of heterogeneities and fractures from a nearby excavation (analog site). Methods for translating the geological information and fracture mapping into each of the model concepts were examined. Each model was compared with available field data, considering both model fit and measures of model suitability. An analysis of model parameter identifiability and sensitivity is presented.

Results show that there is considerable difference between modeling approaches, and that it is important to identify the right one for the actual scale and model purpose. A challenge in the use of field data is the determination of relevant hydraulic properties and interpretation of aqueous and solid phase contaminant concentration sampling data. Traditional water sampling has a bias towards fracture sampling, however concentrations in the limestone matrix are needed for assessing contaminant rebound. The comparison with data showed how much information is required to discriminate between models, and recommendations on how to identify the best modeling approach are presented.

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