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Modeling contaminant plumes in fractured limestone in 3-D: comparison of modeling approaches

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Understanding the fate and transport of contaminant plumes from contaminated sites in limestone aquifers is important because they are a major drinking water resource. This is challenging because they are often heavily fractured and contain chert layers and nodules, resulting in a complex transport behavior. Several modeling approaches have been developed to describe contaminant transport in fractured media, such as discrete fracture, equivalent porous media, and dual continuum models. However, these modeling concepts are not well tested for contaminant plume migration in real limestone geologies. Our goal is to develop and evaluate approaches for modeling the transport of dissolved contaminant plumes in fractured limestone aquifers in 3D and to determine the required flow and transport parameters.

Several fracture flow and transport models of different complexity are available. These include the established approaches of the equivalent porous medium model, discrete fracture model and dual continuum model. In addition to these, we present a new nested modelling approach, where a discrete-fracture model is embedded in an equivalent porous medium model to reduce computational efforts while accounting for the interplay between fractures and matrix. We also test a new hybrid dual porosity – discrete fracture model that resolves major flow features as discrete fractures and describes smaller-scale fractures and fissures as a matrix with the dual porosity approach.

The models were compared for a contaminated site in Denmark, where a plume of dissolved PCE has migrated through a fractured limestone aquifer. Field data includes information on spill history, distribution of the contaminant (multilevel sampling), geology and hydrogeology. To describe the geology and fracture system, data from borehole logs, packer tests, optical televiewers and cores was combined with an analysis of local heterogeneities and data from analogue sites. A pump and tracer test with contaminant sampling was performed at the site to determine flow and transport parameters of the fractures and matrix and to quantify the contaminant distribution in the aquifer.

The models were evaluated by examining their ability to describe the collected field data. Model parameters were determined using the shuffled complex evolution algorithm to optimize model fit. Fitting diagnostics were examined to determine parameter identifiability and to evaluate the appropriate level of model complexity.

The comparison with data showed that the models have substantially different representations of the contaminant behavior, with different consequences for evaluation of contaminant risk and potential remediation strategies. On the plume scale, the equivalent porous medium model and the dual-porosity model can reproduce the main transport features. However, small scale fracture-matrix interaction, such as diffusion of contaminant into the matrix, cannot be represented with an equivalent-porous medium model and require a more complex model. The paper concludes with recommendations on how to identify a suitable modeling approach for simulation of contaminant plumes.

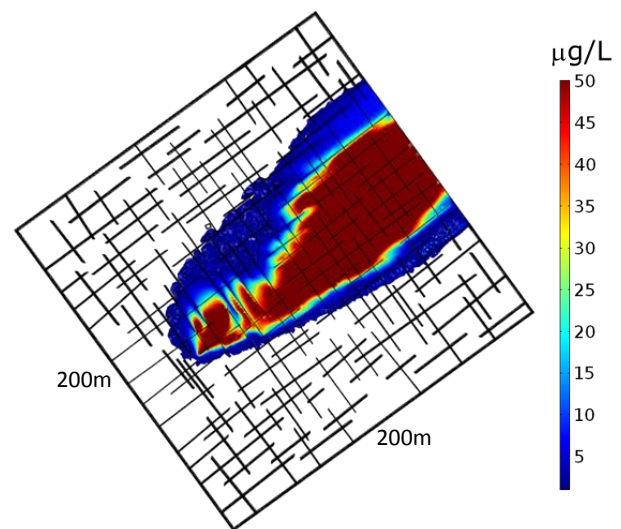


Figure 1: Dissolved PCE plume propagation in a fractured limestone using a 3D discrete-fracture model.