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Effects of fracture aperture statistics and boundary characteristics on DNAPL entrapment, dissolution and source depletion behavior

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Prediction of the dissolved mass flux generation from dense non-aqueous phase liquids (DNAPLs) entrapped in fractured rocks is important for many cleanup scenarios, yet challenging due to the high level of heterogeneity of the medium. As fracture networks are formed by fractures intersecting with each other, both individual single fractures and intersecting fractures are considered here. Log-normally distributed aperture fields with local fracture transmissivities following the cubic law are assumed and DNAPL migration, entrapment and dissolution are modeled. The effect of different hydraulic characteristics at fracture intersections is also examined. Multiple realizations with different sets of aperture statistics and fracture dip angles are considered. T2VOC/TMVOC/iTOUGH2 codes are used for the modeling. For the purpose of upscaling, the temporal evolution of the simulated solute outflow concentration is fitted to a simplified source depletion Damkohler number model. This is done for the different sets of fracture aperture statistics, intersection and boundary characteristics.

The results suggest that the entrapment volume and geometry of DNAPL in a heterogeneous fracture are highly sensitive to the aperture statistics. A more heterogeneous aperture field (larger standard deviation or smaller correlation length) results in more DNAPL trapping and slower aqueous phase velocity, and thus a longer removal time. The observed outflow concentrations are fitted to the simplified source depletion model to quantify the effective, upscaled source depletion behavior. Modeling of different fracture dip angles reveals that gravity plays an important role as well. The presence of a highly permeable pathway at fracture intersection also influences dissolution, producing lower outflow concentrations, indicative of lower mass transfer rates. The results provide insight as of how fracture aperture and fracture intersection characteristics should be taken into account when upscaling DNAPL migration, entrapment and dissolution behavior from single fracture scale to the scale of fracture networks. In the light of the modeling results, laboratory work has also been initiated to experimentally investigate the issue of DNAPL entrapment and dissolution in fractures.