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Numerical investigations of front morphology in two-phase flow in porous media using reactive interface sensitive tracers

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CO_2 storage into saline porous geological formations is one of the most promising technologies to reduce anthropogenic greenhouse gas emissions to the atmosphere. The effectivity of CO_2 residual and solubility trapping mechanisms are highly influenced by the magnitude of the interface separating the two fluid phases (i.e. brine and supercritical CO_2). Therefore, knowledge of the magnitude and the shape of the injected CO_2 plume is important to provide more information on trapping effectiveness in the formation. Kinetic interface sensitive (KIS)tracers (Tatomir et al. 2018) have the potential to provide information about the time-dependent development of the fluid-fluid interfacial area. KIS-Tracers, injected with the CO_2-phase, are characterized by being subjected to an irreversible chemical reaction at the CO_2-brine interface that results into two products in the brine phase, highly soluble in the wetting phase, i.e. an acid and an alcohol. The size of the interfacial area can be quantified based on the concentration of the acid in the brine phase.

The numerical model developed in Tatomir et al. 2018 is applied to replicate laboratory experimental results reported in Heiss et al. (2011). The calibration of the numerical model is accomplished with regard to porosity, permeability, entry pressure, capillary number, and viscosity ratio affecting the front morphology. A periodic geometrical pattern of heterogeneities and a random pattern are considered in a two-dimensional sandbox with the dimensions of 40 cm x 30 cm x 1.2 cm. The role of this type of hydraulic heterogeneities is to induce changes in front pattern and to implicitly increase the fluid-fluid interfacial area. The first step to calibrate the models is the comparison of the modelled and experimental non-wetting front morphologies for the two cases. The next step is to investigate the relationship between fluid-fluid interfacial area and concentration of acid on the calibrated models. The concentration and saturation breakthrough curves (BTC) are measured at different point-observation locations positioned on a vertical line. Implementing a linear regression over the BTC acid concentration and non-wetting saturation data the macro-scale length (in 2D) of the front is calculated. The main assumption is that the concentration can be calculated as time integral of the product between the reaction rate constant and fluid-fluid interfacial area.

We propose a Monte-Carlo based inverse method for estimating the parameters defining the polynomial relationship between the specific fluid-fluid interfacial area capillary pressure and saturation. The simulation results show that the numerical model can reproduce accurately the laboratory experiment of Heiss et al. 2011. A relation between the interfacial area and acid concentration is proposed. The results show that KIS tracers can be used in two-dimensional experimental setup and can provide information about the size and dynamic evolution of the interfacial area. These are relevant for designing the sampling procedure in future laboratory experiments.