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A phase field method pore-scale model for simulating kinetic interface sensitive tracers reactive transport in porous media two-phase flow systems

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Over the last few years, our understanding of the processes involved in the application of Kinetic Interfacial Sensitive (KIS) tracers in two-phase flow as a means to quantify the fluid-fluid interfacial area has been enhanced with the use of controlled column experiments (Tatomir et al. 2015,2018). However, there are still some open questions regarding the effect of immobile water, either as capillary and dead-end trapped water or as a film, and the measured by product concentration at the outflow.

In this study, a new pore-scale reactive transport model is presented, based on the phase-field method, which is able to deal with the KIS tracer interfacial reaction and selective distribution of the by-production into the water phase. The model is validated by comparing the analytical solutions for a diffusion process across the interface and a reaction-diffusion process, and is tested for a drainage process in a capillary tube for different Péclet numbers. The applicability of the model is demonstrated in a realistic 2D porous medium NAPL/water drainage scenario used in the literature. Four case studies are investigated in detail to obtain macroscopic parameters, like saturation, capillary pressure, specific interfacial area, and concentration, for a number of combinations between the inflow rate, the contact angle and diffusivity. We derive a relation between the by-product mass at the outflow and the mobile part of the interfacial area, which is formulated by adding a residual factor. This term relates to the part of the by-product produced by mobile interface that becomes residual in the immobile zones.