

# **Estimating the spatial distribution of surface reaction sites from the breakthrough curves of a dual tracer test: a pore-scale reactive transport model study**

SUNWONG LIM AND HEEWON JUNG

Chungnam National University

Presenting Author: [sunwong@g.cnu.ac.kr](mailto:sunwong@g.cnu.ac.kr)

Accurately estimating subsurface geochemical reactions is challenging due to the complex pore geometries and flow of fluids and chemicals at small scales. While recent advances in analytical techniques have improved access to pore scale information, large scale characterizations of subsurface environments often rely on tracer tests, which provide limited information and obscure pore scale processes. To overcome this limitation, we utilize a pore scale reactive transport model to connect tracer breakthrough curves with pore scale hydrogeochemical processes, specifically those involving 1st-order consumption reactions at reactive surfaces. The simulations were conducted in three domains with distinct pore geometries but the same porosity, under a range of average flow velocities (i.e., Péclet numbers  $\in \{1, 5, 10\}$ ) and system reactivity conditions (i.e., Damköhler numbers  $\in \{0, 100\}$ ). Heterogeneous spatial distribution of reactive surfaces was quantitatively described by calculating the local sum of reactivities distributed along the main flow channel ( $F_{Da} \in \{0.167, 0.333, 0.5, 0.667, 0.833, 1\}$ ). The time derivatives of reaction rate breakthrough curves, calculated using the difference in flux-weighted concentrations of conservative and reactive tracers, show type I and type II peaks that correspond to advection- and diffusion-dominated surface reactions, respectively. The reaction rate at the type I peak displays a perfect linear correlation with  $F_{Da}$ , suggesting that the distribution of reactive surfaces along the main channel can be estimated from BTCs without directly accessing the pore scale information.