Reactive transport modeling of CO_2 in carbonate rocks:Single pore model

PRIYANKA AGRAWAL[*1], JANOU KOSKAMP[1], AMIR RAOOF[1] AND MARIETTE WOLTHERS[1]

1 Department of Earth Sciences-Geochemistry, Utrecht University, 3508TA, The Netherlands
 (*correspondence: p.agrawal@uu.nl)

Reactive transport modeling of CO_2-saturated water in a single pore of carbonate rock is a complex problem which includes several processes such as fluid flow, chemistry, transport of solution species and dissolving solid boundary. Evolving pore structure and size is controlled by reaction kinetics and flow properties. We would like to include impact of solution stoichiometry and surface roughness in reaction kinetics which have already been observed on molecular scale [1]. In the model, solid pore walls move due to the surface reactions because of calcite dissolution.
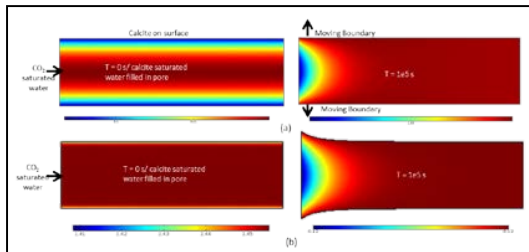

Figure 1: Ca concentration profile for flow velocity (a) 1e-8 m/s (b) 1e-6 m/s

We observe that the regime of flow is a key factor controling dissolution. For fluid velocity around 1×10^{-8} m/s there is no significant dissolution (Figure 1). By increasing velocity with two orders of magnitude, drastic changes in dissolution pattern and subsequent pore geometry evolution is seen mostly near the inlet, because of saturation with respect to calcite along the flow path. The same obesrvations are noted for curved pore walls. Higher velocity is expected to have more penetration of reaction front and to bring out more characteristric difference in pore shape evolution pattern for rough pore walls. Our objective is to relate pore volume change with macroscopic properties such as porosity and permeability for different peclet numbers which will be used as an input for pore scale simulation in PoreFlow[2].

References
 [1] Wolthers et al. (2013) CrystEngComm 15, 5506. [2] Raoof et al. (2013) Computers & Geosciences, 61, 160-174.