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FELLOWSHIP FINAL REPORT

Multi-scale observation and simulation of mineral reactions in subsurface energy systems

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REPORT INFO

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ABSTRACT

Mineral reactions in subsurface energy systems result in deviations from local equilibriums and can impact critical engineering properties of the system, including storage capacity (porosity) and injectivity (permeability). Accurate understanding and prediction of reaction rates and impacts on formation properties is needed for safe and efficient design and implementation of these engineered systems. Precise simulation of mineral reaction rates is limited by a poor understanding of the mineral reactive surface area in porous media. Here, pore scale numerical simulations are leveraged to simulate mineral reactions for varied flow and reaction conditions and the effective surface area analyzed. Numerical simulations of reactions in a porous media mesh are carried out in OpenFOAM® and a new scaling factor, relating the effective surface area to the accessible surface area, determined.

1- Introduction

Subsurface geologic formations play a critical role in the energy transition to net zero, serving as a host for anthropogenically produced CO_2 or flexible means of H_2 storage to increase reliance on production of renewable energy, for example. As gases are injected, local geochemical equilibriums may be altered, creating conditions favorable for dissolution of formation minerals[1–7] Reactions can occur over a wide range of spatial (nm to km) and temporal (s to 100s of years) scales, impacting formation properties and the efficiency, risk, and environmental impact of such systems.

Reactive transport simulations are a powerful means of simulating fate and transport in natural and engineered systems[8–11]. Accurate simulation of mineral reaction rates requires precise model parameterization, where mineral reactive surface area is the most poorly constrained parameter in terms of reaction rate simulations[12]. Prior work has shown use of accessible mineral surface areas, the surface areas of minerals in contact with the reactive fluid, provides improved simulation of mineral reaction rates in multi-mineral consolidated samples[13]. Such surface area can be quantified from a multi-scale imaging analysis of the desired sample[6,13,14].

While mineral accessible surface area has notably improved simulation of reaction rates in multi-mineral porous media, the additional impact of hydrodynamics on the surfaces participating in the reactions has yet to be considered. Pore scale numerical simulations of calcite dissolution under varied flow and reaction conditions have shown reaction rates and reaction patterns may not be uniform [15]. As such, the effective surface area, that which participates in the reaction, may be further reduced. This work aims to understand the impact of hydrodynamics on mineral effective surface area in porous media. Here, pore scale numerical simulations of a multi-pore body system are carried out for varied flow and

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reaction conditions and effective surface areas quantified. A scaling factor between the effective and accessible mineral surface area is proposed as a means of upscaling the observed restriction in reactive surface area to continuum scale reactive transport simulations.

2- Experimental details

Simulations are carried out on a simple porous media geometry (Fig. 1) based on exo5.stl [16] using snappyHexMesh. The mesh has a uniform thickness of 6.0x10^{-5} m, width of 1x10^{-3} m and length 1.1x10^{-3} m. No flow boundaries were applied to the grain surfaces and four sides of the bounding box. The grid refinement was chosen to capture the diffusive and reactive boundary layers.

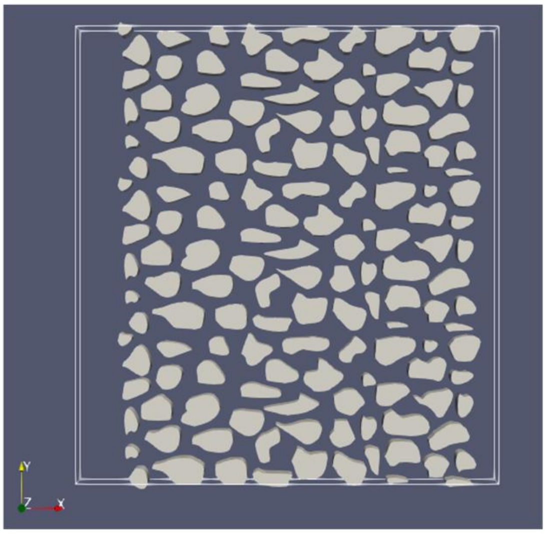

Figure 1: Porous media mesh for pore scale numerical simulations, based on exo5.stl from C. Soulaine.

Flow of an impressible fluid was simulated in OpenFOAM® by application of constant pressure conditions at the inlet and outlet of the system. The steady-state velocity field was then simulated (Fig. 2). The average velocity of the network was 2.86x10^{-5} m/s and permeability 3.08x10^{-11} m^2.

Reactions in the network were simulated by application of a first order reactive boundary condition to the grain surfaces. A constant concentration of a reactive component, C, was then introduced to the inlet of the network. The change in concentration of T was simulated until steady state was reached.

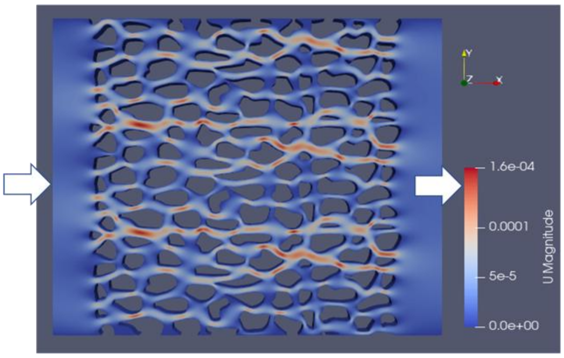

Figure 2: Simulated steady state velocity field indicating inlet (left) and outlet (right) flow directions.

Dimensionless Peclet and Damkohler numbers can be used to describe flow and reaction conditions. The Peclet number, *Pe*, describes the rate of advection over diffusion of a component and is defined as

$$Pe = \frac{v_0\sqrt{K}}{D} \qquad (1)$$

where v_o is the velocity, K is the permeability, and D is the diffusion coefficient. The Damkohler number, Da_{II}, is a ratio of the rate of reaction over diffusion and is given by,

$$Da_{II} = \frac{kl\prime}{D} \qquad (2)$$

where k is the reaction rate constant and l' is the characteristic length. The ratio of Pe and Da_{II} also provides useful means of characterizing the relative importance of flow and reaction conditions and defined as,

$$Da_I = \frac{Da_{II}}{Pe} \qquad (3)$$

Here, various flow and reaction conditions are considered by varying the reaction rate constant and diffusion coefficient. A large range of Peclect and Damkohler numbers were probed to gain understanding of variations of impacts of hydrodynamics on effective surface area.

For each simulation, the effective surface area, A_e, was calculated from

$$A_e = \frac{\Phi D \int_r n\cdot\nabla C\, dA}{k\int_V C dV} \qquad (4)$$

where Φ is the porosity, n the normal vector at r surface mesh. A scaling factor, alpha, for each simulation condition was then computed by dividing the effective surface area by the total surface area of the mesh.

3- Results and discussion

Simulated concentrations of C for varied flow and reaction conditions are given in Fig. 3. The reaction pattern can vary widely depending on the Peclet and Damkohler number.

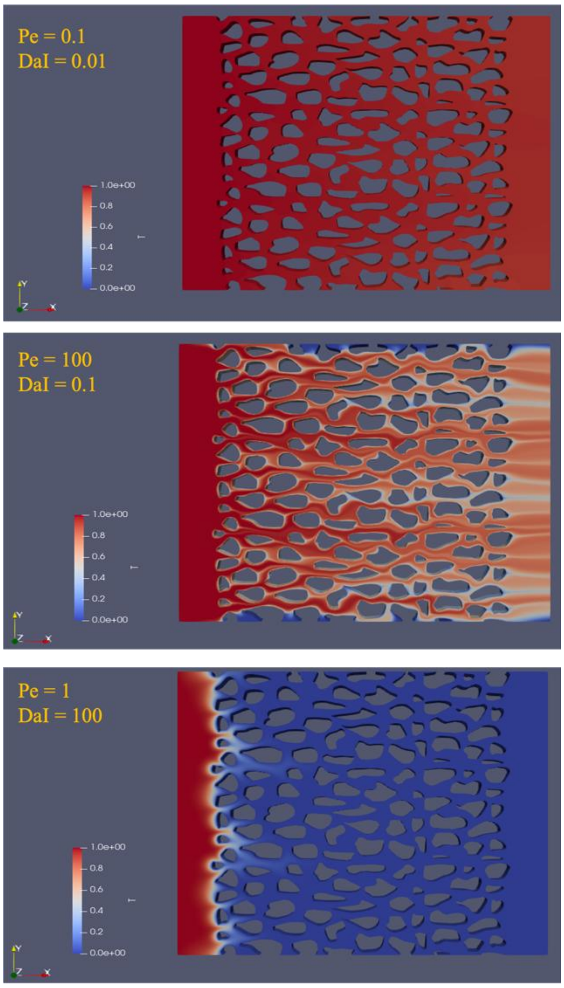

Figure 3: Simulated concentrations of C for varied flow and reaction conditions.

For small values of Peclet and Damkohler number, reactions proceed uniformly in the network with all surfaces participating in the reaction. This is demonstrated, for example, in Figure 3 (top) where the concentration of C at steady state is uniform throughout the network. For this simulation, the rate constant is 4 x 10^{-8} m/s and diffusion coefficient is 1.5 x 10^{-9} m^2/s. As reactions proceed uniformly, the effective surface area is equal to the accessible surface area and alpha is one.

As conditions change, some surfaces may not participate in the reactions. For larger Peclet number conditions, as demonstrated in Figure 3 (middle), for example, there is a heterogenous distribution of C in the network. In this system, the highest concentrations of C in the network occur in high velocity flow regions. Diffusion is small (D = 1.5 x 10^{-12} m^2/s) and advection is a more prominent mechanism for bringing the reactive ions to the mineral surfaces. As such, the effective surface area is reduced as compared to the total surface area and alpha is 0.58.

Further reductions in effective surface area are evident in high Da_I systems, as shown in Figure 3 (bottom). Here, the rate of reaction is relatively fast such that the reactant is consumed before reaching the rest of the network. As such, only a small proportion of the reactive surfaces participate in the reaction and alpha is 0.1273.

4- Conclusion

Mineral effective surface area has a noted dependence on hydrodynamics that can greatly impact the proportion of surfaces participating in the reaction. Depending on the conditions, reactions may only occur on a small proportion of the accessible mineral surfaces. The pore scale numerical simulations in this work provide a means of quantifying the effective mineral surface area and upscaling factor to integrate such impacts into continuum scale reactive transport simulations. Simulations can be expanded to consider a large range of flow and reaction conditions and robust fit to the calculated scaling factor (alpha). This has the potential to greatly improve simulation of mineral reaction rates in continuum scale reactive transport models in diverse environments.

5- Perspectives of future collaborations with the host laboratory

Collaboration on this work is ongoing. Simulation efforts have continued, and results presented at two of the premier international conferences in the field. Efforts to apply for additional funding to continue with and expand on these initial observations are ongoing. This includes hopeful funding to support graduate student or postdoctoral trainees to continue, and expand, simulations.

6- Articles published in the framework of the fellowship

This work is ongoing, but results have been presented at two international conferences:

1. Beckingham, L.E., Soulaine, C. Impact of hydrodynamics on accessible mineral surface area. Presentation at Interpore2025, May 19, 2025, Albuquerque, NM, USA.
2. Beckingham, L.E., Driba, D.L. Soulaine, C. Predicting mineral reaction rates in subsurface energy systems. Invited presentation at American Geophysical Union Fall Meeting, December 14-19, 2025, New Orleans, LA, USA.

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