Center for Nanoscale Controls on Geologic CO_2

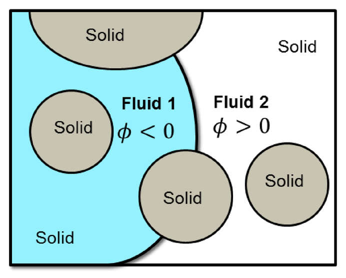
Pore-Scale Simulation of the Processes Associated with the Injection and Sequestration of CO_2 in the Subsurface

C. Soulaine[1], M. Abu AlSaud[1], S. Roman[1], M. Graveleau[1], S. Molins[2], C. Steefel[2], J. Wan[2], T. Tokunaga[2], H. A. Tchelepi[1]

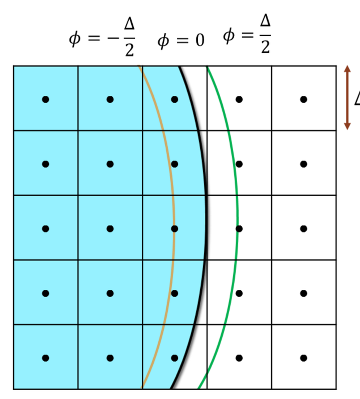
[1]Stanford University, [2]Lawrence Berkeley National Laboratory

Simulation of trapping mechanisms[2,3]

- Once the supercritical CO_2 is injected into the Earth's subsurface, it flows as a separate phase forming an immiscible interface with the brine already in place. The phases distribution in the domain is process-dependent involving complex configurations such as the entrapment of one of the phase by the flowing phase or the formation of thin films.



- Complex capillary mechanisms, mostly governed by the wettability of the mineral surface, lead to the trapping of CO_2 ganglia in the pore space.



- Development of a simulation framework to solve two-phase Navier-Stokes with a Level-Set approach,

Conservation of mass: $\nabla \cdot \mathbf{u} = 0,$

Transport of the Level-Set function : $\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0,$

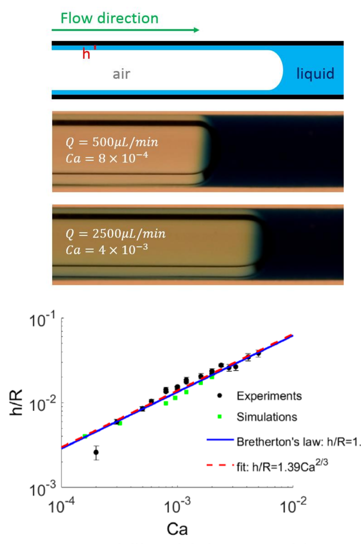
Momentum equation: $\rho \left[\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right] = -\nabla p + \nabla \cdot \left(\mu (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \right) + \sigma \kappa \mathbf{n} \delta_s + \rho \mathbf{g},$

Curvature of the interface: $\kappa = \nabla \cdot \frac{\nabla \phi}{|\nabla \phi|}$

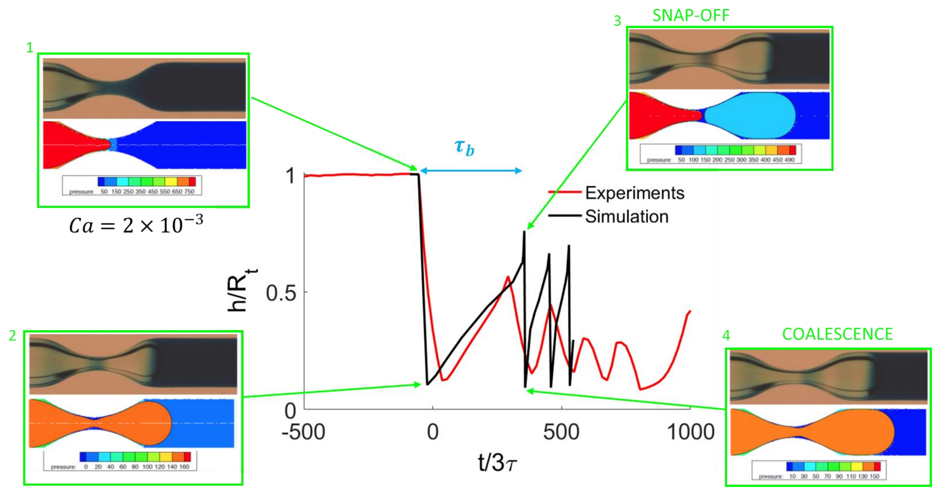
- Minimization of the spurious velocities that appear at the vicinity of the interface because of numerical errors in the computation of the curvature.
- Multi-scale formulation based on the lubrication theory to accurately model thin films deposited at the solid surface due to surface force (Van der Waals, Coulombic, etc.),

$$\frac{\partial h}{\partial t} + \frac{1}{\mu} \nabla \cdot \left[\left(\frac{h^3}{3} \right) \nabla (\sigma \kappa - \Pi(h)) + \frac{h^2 \tau}{2} \right] = 0$$

- The liquid film dynamics in constricted capillary tubes is investigated both numerically and experimentally with an optical technique that has been developed to measure the film thickness. Experiments and simulations are in good agreement.



Measurement of film thickness with an optical technique

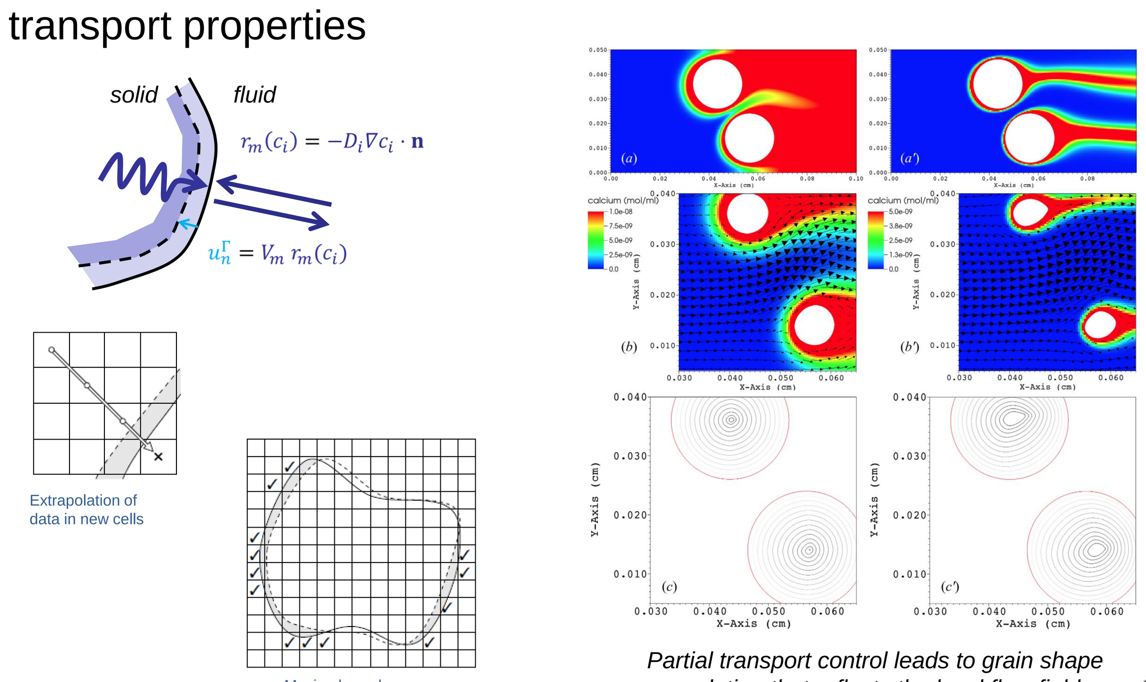


Cycles of snap-off and coalescence

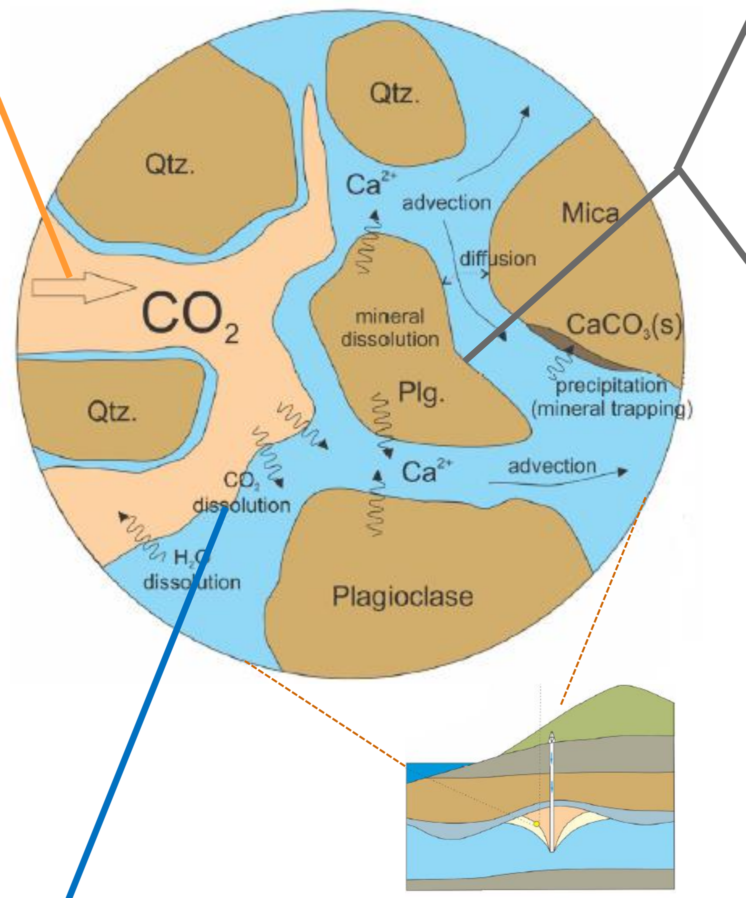
- In a constricted capillary, we observed cycles of snap-off/coalescence and that no bubbles are disconnected from the main flow during the drainage of water. These cycles are due to instabilities of the wetting liquid lens because of local fluctuations in capillary pressure. These results suggest that snap-off might not be the preferred mechanism for residual trapping of CO_2.

Reactive interfaces with moving embedded boundary conditions[5]

- Reactive processes associated with CO_2 sequestration scenarios such mineral dissolution-precipitation take place at interfaces between the fluid and the solid phases. These processes may change the properties of the rock, including porosity, permeability, and specific surface area.
- Discrepancies between laboratory and field rates suggest that according to hydrodynamics conditions, some of the mineral surface areas is not reached by the reactants.
- A numerical framework is developed to investigate at the pore-scale the evolution of the pore structure of the media due to mineral dissolution-precipitation, and to upscale reaction rates at larger scale under various flow conditions.
- Flow and reactive transport in the pore space are described with the incompressible Navier-Stokes equations (conservation of momentum and mass) and an advection-diffusion equation (includes aqueous complexation reactions), respectively.
- Dissolution-precipitation reactions change the shape and position of the interface, which stays a sharp boundary. The reactive interface is represented on the Cartesian grid by moving embedded boundary conditions.
- The grain shape evolution depends strongly depends on transport properties



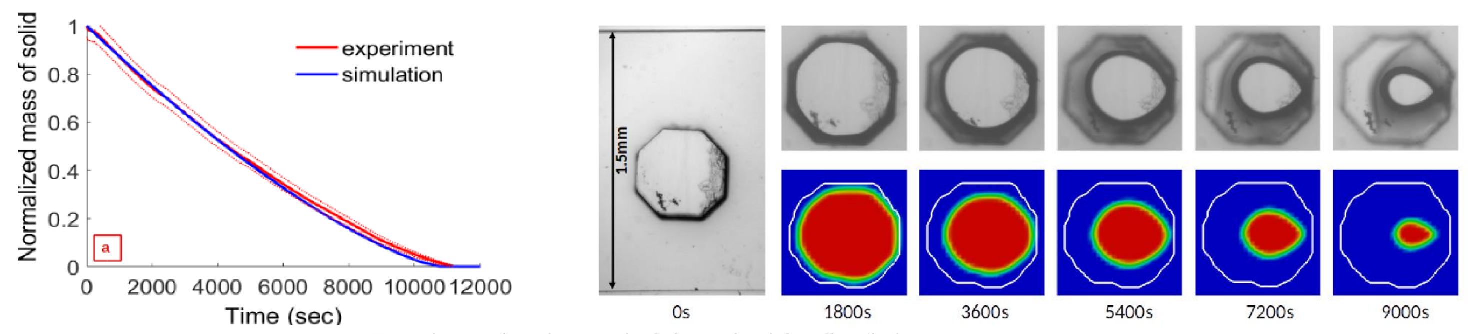
Partial transport control leads to grain shape evolution that reflects the local flow field



Chemical and physical processes associated with CO_2 injection and sequestration at the pore-scale[1]

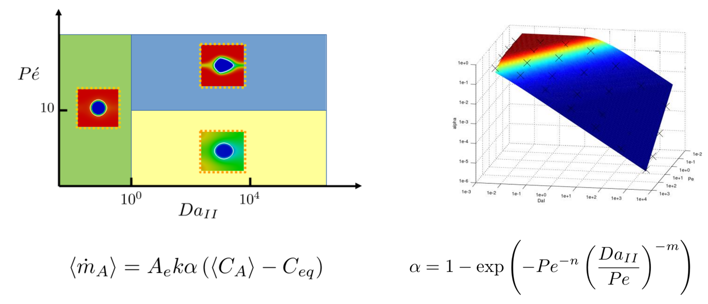
Mineral dissolution and wormholing[6,7]

- A micro-continuum model is proposed to simulate the dissolution of solid minerals at the pore-scale. The approach employs the Darcy-Brinkman-Stokes formulation and locally averaged conservation laws combined with immersed boundary conditions for the chemical reaction at the solid surface.

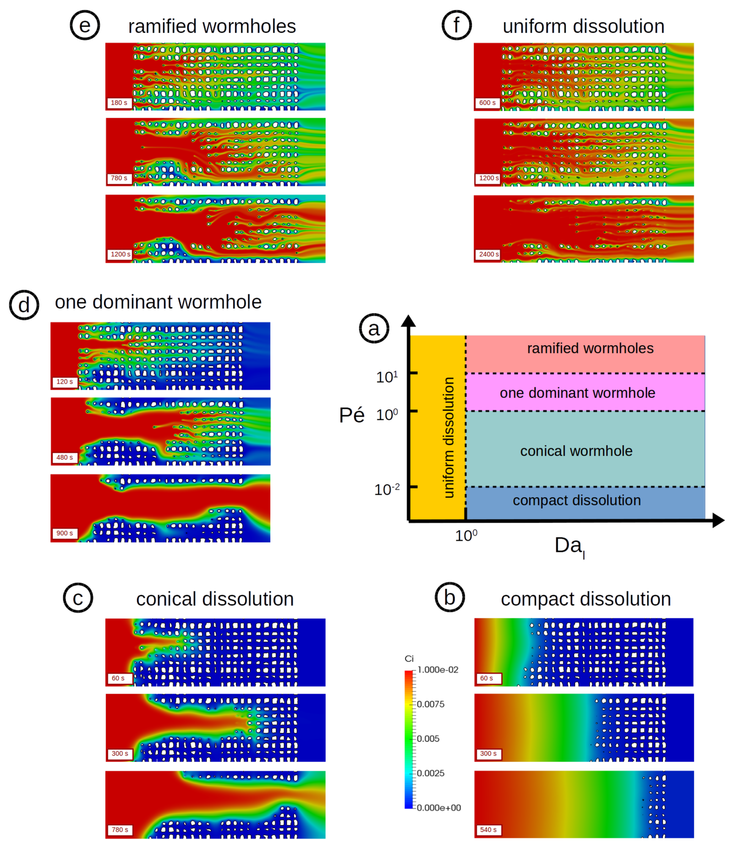


Experimental and numerical data of calcite dissolution process

- The simulation framework is validated using an experimental microfluidic device to image the dissolution of a single calcite crystal. The evolution of the calcite crystal during the acidizing process is analyzed and related to flow conditions, i.e., Péclet and Damköhler numbers.
- Macroscopic laws for the dissolution rate are proposed by upscaling the pore-scale simulations.



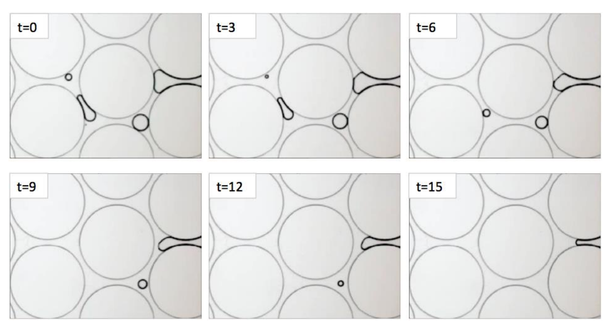
- Finally, the emergence of wormholes during the injection of acid in a two-dimensional domain of calcite grains is discussed based on pore-scale simulations.



Simulation of dissolution instabilities

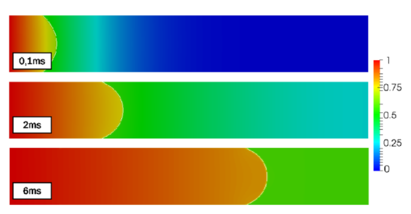
Simulation of CO_2/brine dissolution[4]

- The CO_2 from the supercritical phase dissolves in the aqueous phase to form carbonic acid which lowers the pH of the brine as the carbonic acid dissociates to the bicarbonate ions.



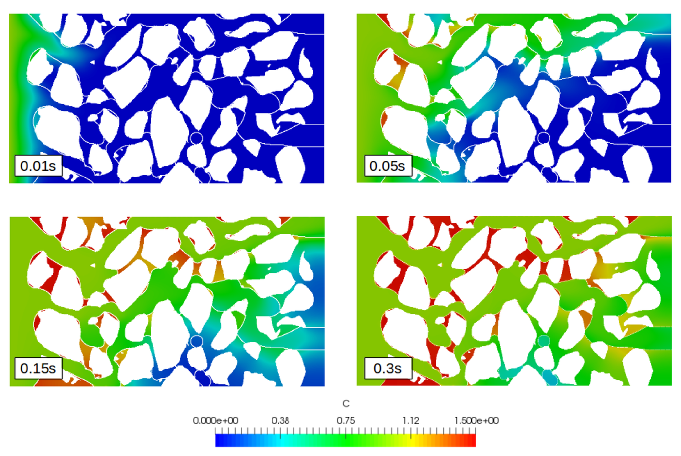
Micromodel experiments of CO_2/brine dissolution

- Estimation of the rate of interphase mass transfer of CO_2 at large scale is challenging because the dependency of the exchange coefficient, k, on flow conditions is still unclear. $F_A = a_f k \left(H_A \langle C_{g,A} \rangle^g - \langle C_{l,A} \rangle^l \right)$
- A simulation framework is proposed to investigate multicomponent multiphase flow in porous media at the pore-scale. It solves equations for the species concentrations in the framework of the Volume of Fluid approach including thermodynamics equilibrium at the fluid/fluid interface.
- The framework is used to simulate interphase mass transfer in static and dynamic conditions in complex pore space.

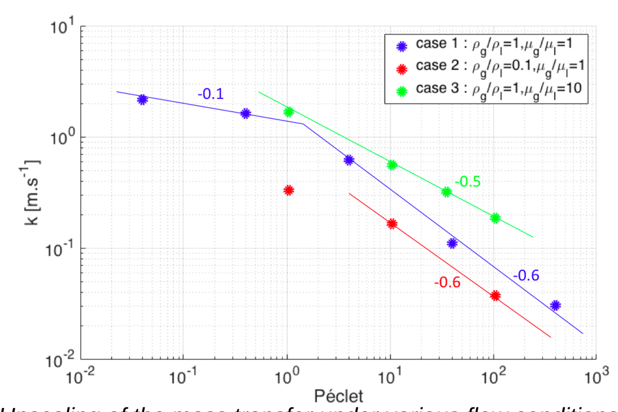


Mass transfer during drainage in a capillary tube

- Simulation results are then upscaled to Darcy's scale (residual saturation interfacial area, mass exchange coefficient k…)



Simulation of the accumulation of CO_2 in the residual water



Upscaling of the mass transfer under various flow conditions

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