Dissolution of a single mineral grain: comparison of microfluidic experiments with pore-scale simulations

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Dissolution at the pore scale

$$\nabla \cdot (\mathbf{uu}) - \nu \nabla^2 \mathbf{u} = -\nabla p$$

$$\nabla \cdot (\mathbf{u}c) = D \nabla^2 c$$

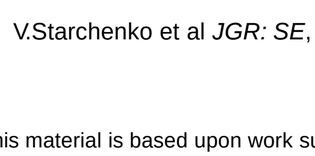
$$-D\mathbf{n} \cdot \nabla c = R(c)$$

$$\frac{d\mathbf{r}}{dt} = -\frac{D}{c_{sol}} (\mathbf{n} \cdot \nabla c)\mathbf{n}$$

u	fluid velocity
ν	kinematic viscosity
c	reactant concentration
D	molecular diffusion coefficient
$R(c)$	reaction rate
c_{sol}	mineral concentration
c_{in}	inlet reactant concentration
r	surface point position

Why pore-scale modeling?

Cannot apply spatial averaging when gradients are large



Concentration field (blue to red)
Highly non-uniform dissolution
Exposed surface area does not predict dissolution rate

flow

Pore-scale simulations can provide data for upscaling
Large-scale DNS - crossing scales by brute force

Questions:

- Are dissolution rate constants really constant?
- Can we predict evolution of pore space from first principles?

Simulation: Reactive transport with OpenFOAM

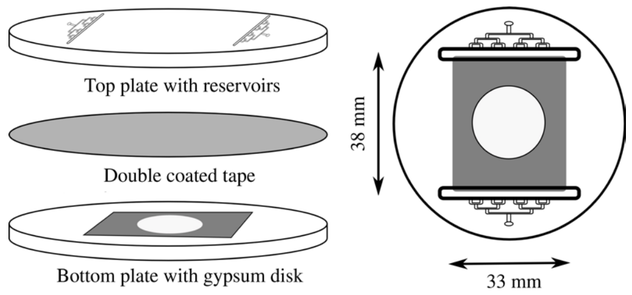
Flow and reactive transport from dissolFoam

https://github.com/vitst/dissolFoam/

2nd-order conservative finite volume scheme Mesh of polyhedral cells, created with SnappyHexMesh utility
Mesh points lie on the boundaries - no interpolation

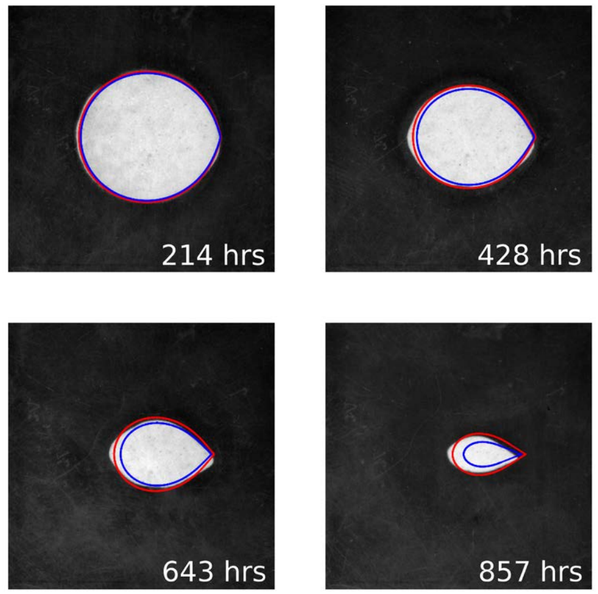
V.Starchenko et al *JGR: SE*, **2016**, 121, p. 6421

Experiment: Dissolving a single grain



Microfluidic experiments designed to observe changes in size and shape as cylindrical disks (radius 10 mm) of gypsum dissolved for periods of up to 40 days.

Comparison of experiment and simulations

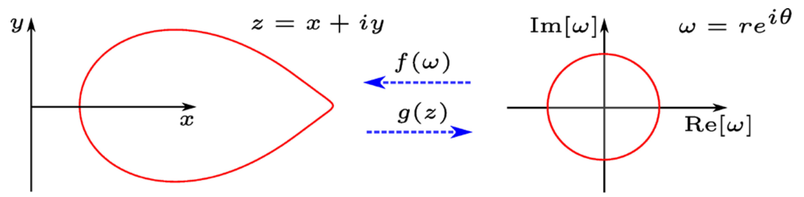


Comparisons without any fitting parameters
Blue lines - simulations with constant diffusion coefficient
Red lines - simulations with activity correction to *D*

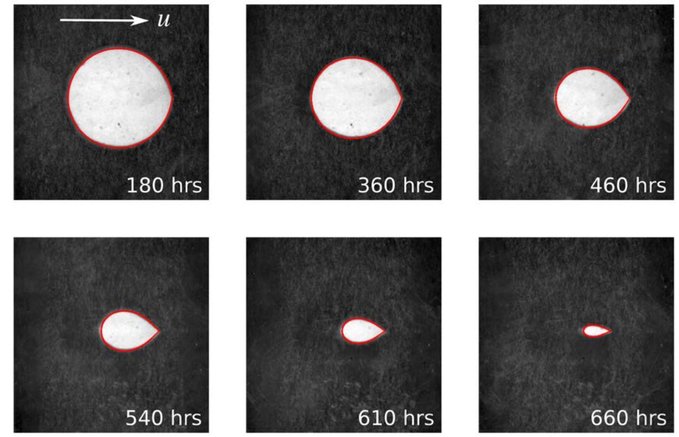
F. Dutka et al Chem. Geol., **540,** 119459, 2020

Analytical approach: evolving conformal mappings

Closely related problem can be solved by conformal mapping
Assume potential flow (in a Hele-Shaw cell) and $c = 0$ on the boundary (infinite reaction rate)



One derives a differential equation for the evolution of the mapping f(ω) (Polubarinova-Galin equation), the solution of which gives the evolving shapes of the disk



Images from microfluidic experiments together with the shapes from the conformal mapping (red) selected at times when the enclosed area matched that of the undissolved solid (white)

Applications of conformal mapping:

Upscaling theories for dissolution of porous rocks
Theory for a disk shows that dissolution rate is not proportional to exposed area:

$$S_R \sim \sqrt{S_E}$$

This material is based upon work supported by the National Science Center (Poland) under research Grant No. 2012/07/E/ST3/01734 and by the U.S. Department of Energy Office of Basic Energy Sciences,