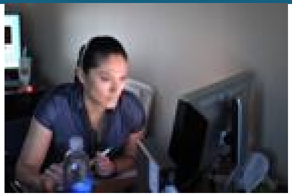
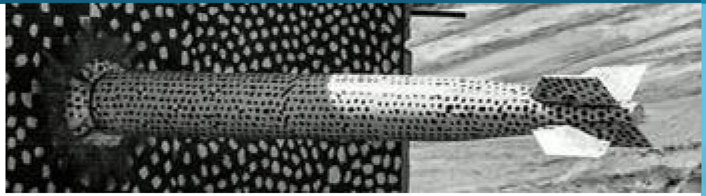
SAND2021-15748C

Experimental and numerical study of pore-scale flow and reactive transport





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AGU 2021 Fall Meeting

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This work was supported by the Laboratory Directed Research and Development program at Sandia National Labora

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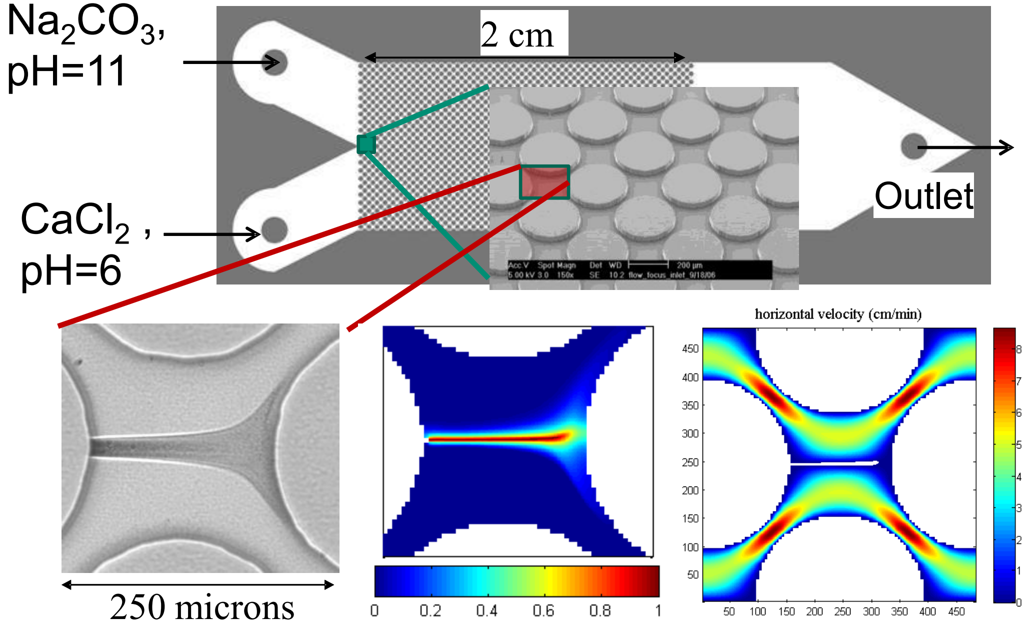
Motivations

- Pore scale physics has been significantly improved over the past ~15+ years
- Various studies on hydrodynamics, reactive transport, and coupled processes (e.g., chemo-mechanical coupling) are motivated with many subsurface applications (geologic carbon storage, unconventional resources recovery, nuclear waste repository, geothermal energy, etc) and Multiphysics in porous media (contaminant transport, fuelcells, flow& transport in varying saturated media, membrane filter systems, etc)
- Both experimental and numerical capabilities have been improved with both sensing and experimental apparatus and computational hardware & algorithms
- A few new emerging techniques can be utilized to improve these continuing efforts
- One overarching question is what fundamental knowledges need to be improved and how micro- and macro-processes are meaningfully integrated depending on our scientific and practical interests

A few representative examples

Microfluidic device/ideal geometry

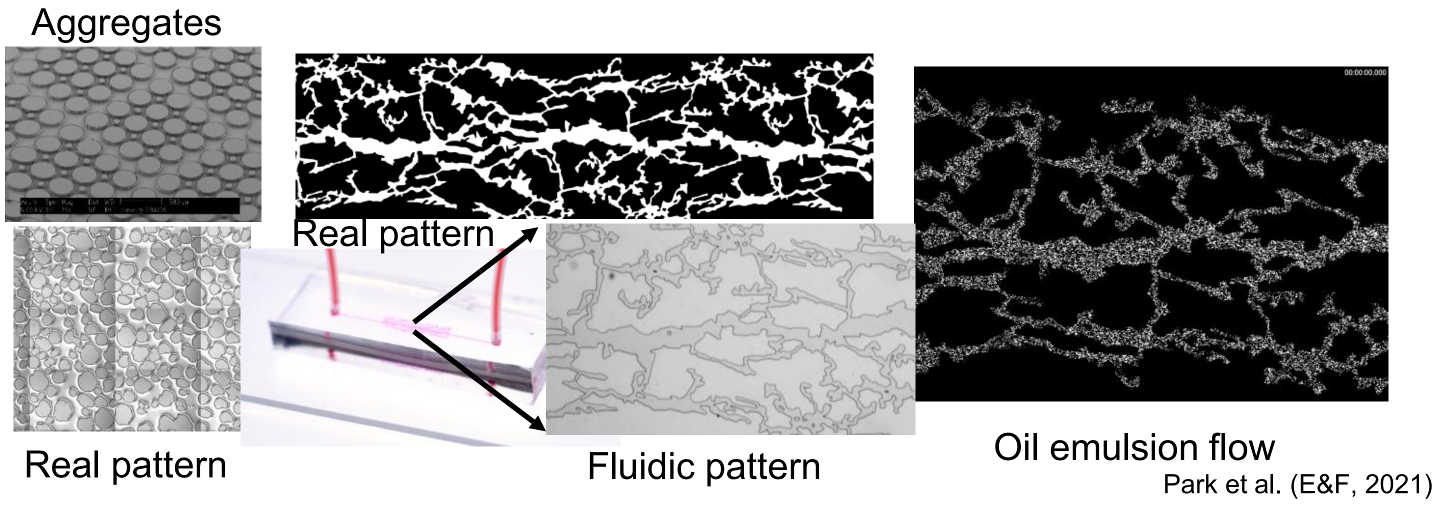


Optical mage of calcium carbonate ($CaCO_3$) precipitates (left), lattice Boltzmann flow field (middle), calcite precipitation (right)

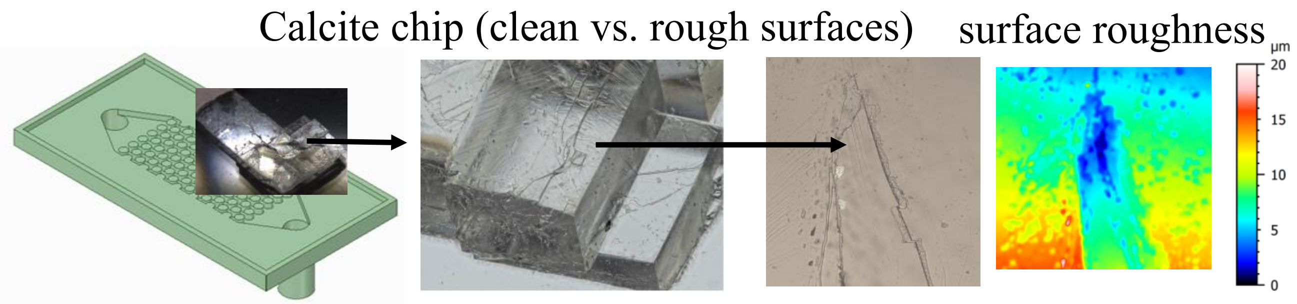
- Fabricated fluidic device (with silicon wafer & surface treatment) with theoretical/synthetic geometry
- Fast optical (4-10 fps) and confocal 3D imaging at ~0.1-10 um
- Pore scale modeling/detailed continuum modeling have been validated
- Expensive and some artifacts in data analysis

Zhang et al. (EST, 2010), Yoon et al. (WRR, 2012), Fanizza et al. (WRR, 2013), Boyd et al. (GCA, 2014), Singh et al. (EST, 2015), Yoon et al. (RiMG, 2016, EST 2019)

Fluidic device with complex/realistic geometry & surface properties



Park et al. (E&F, 2021)



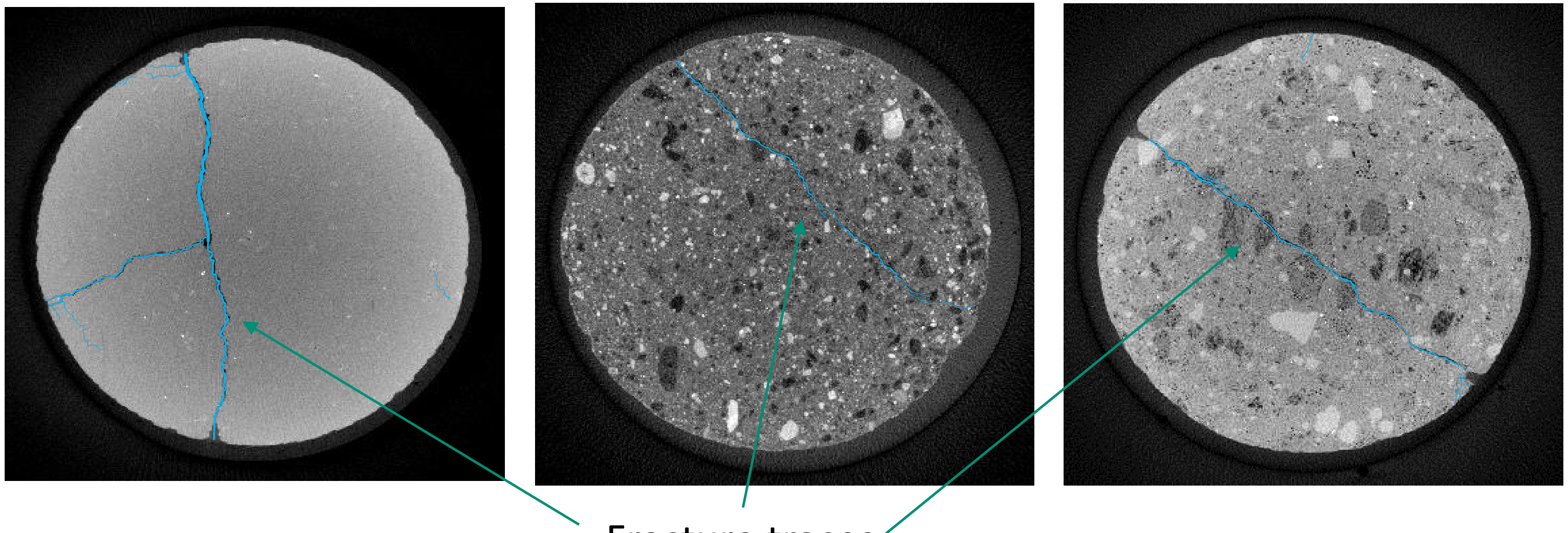
Testing bed of precipitation/dissolution of calcium carbonate in real-rock mock-up

- Real-time imaging of change of $CaCO_3$ morphology with precipitation/dissolution
- Measurement of effluent concentrations with known surface geometry and media structure

Oosrom et al. (Com.Geo. 2016), Park et al. (E&F, 2021), Martinez et al. (SAND, 2018))

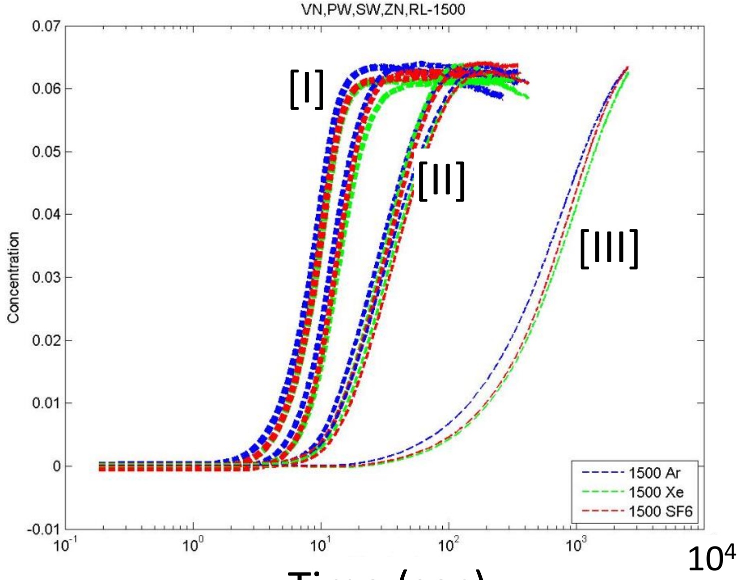
Chemo-mechanical Coupling

[I] Fracture dominant flow [II] Fracture-Matrix flow [III] Matrix-Fracture flow



Fracture traces

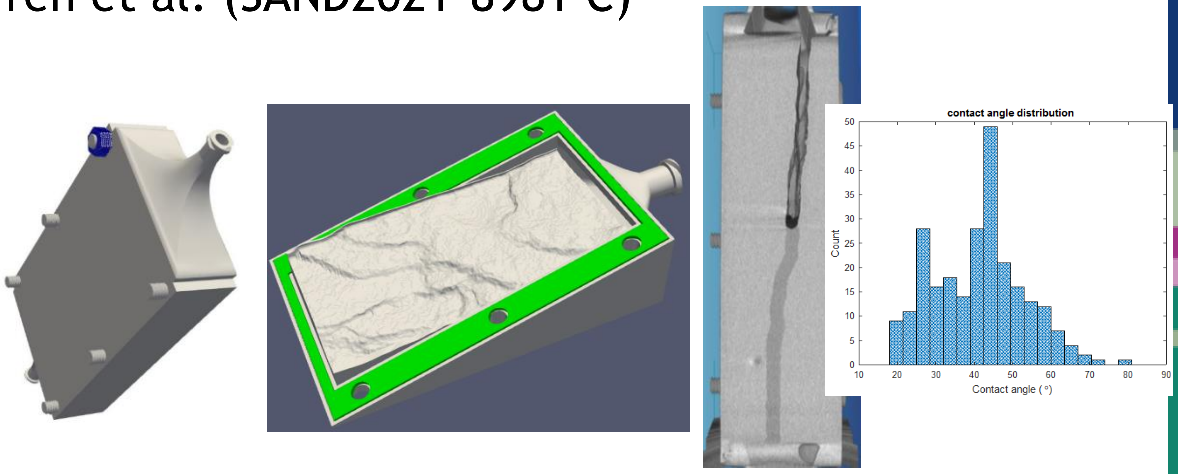
Breakthrough Curves of Tracer Gases



Time (sec)

From Warren et al. (SAND2021-8981 C)

- Variations in fracture, microfracture, matrix porosity, and compositions affect
  - Aperture and connectivity of fracture network
  - Interaction between fracture and matrix
  - Permeability response as a function of stress
  - Mechanical properties
  - Response of fracture varies, hence reactive transport



3D printed fractured media

Martinez et al. (SAND2017-10469)

Summary

- Scalable and predictive modeling for flow, transport, and mechanics through natural porous and fractured media is essential for a variety of engineering applications for many societal needs (energy, climate change, engineering materials, etc.)
- FAIR (findable, accessible, interpretable, reproducible) principles can be very powerful to achieve our overarching goals of predictive power of various reactive transport processes in porous/fracture media
- A few recent community initiatives (e.g., ML works, open data portals) can be benchmarked in reactive flow/transport community
- Digital rock physics/pore scale physical modeling augmented with new emerging techniques has a high potential to advance our understanding of coupled flow, transport, and (poro)mechanics