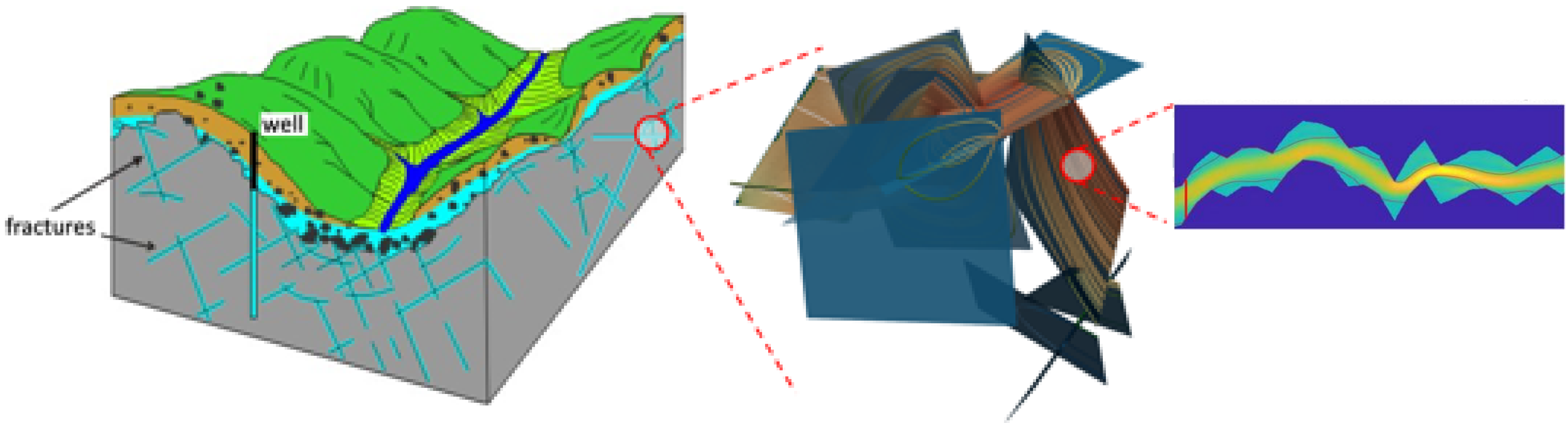
Characterization, modeling, and remediation of fractured aquifers through cutting-edge research tools



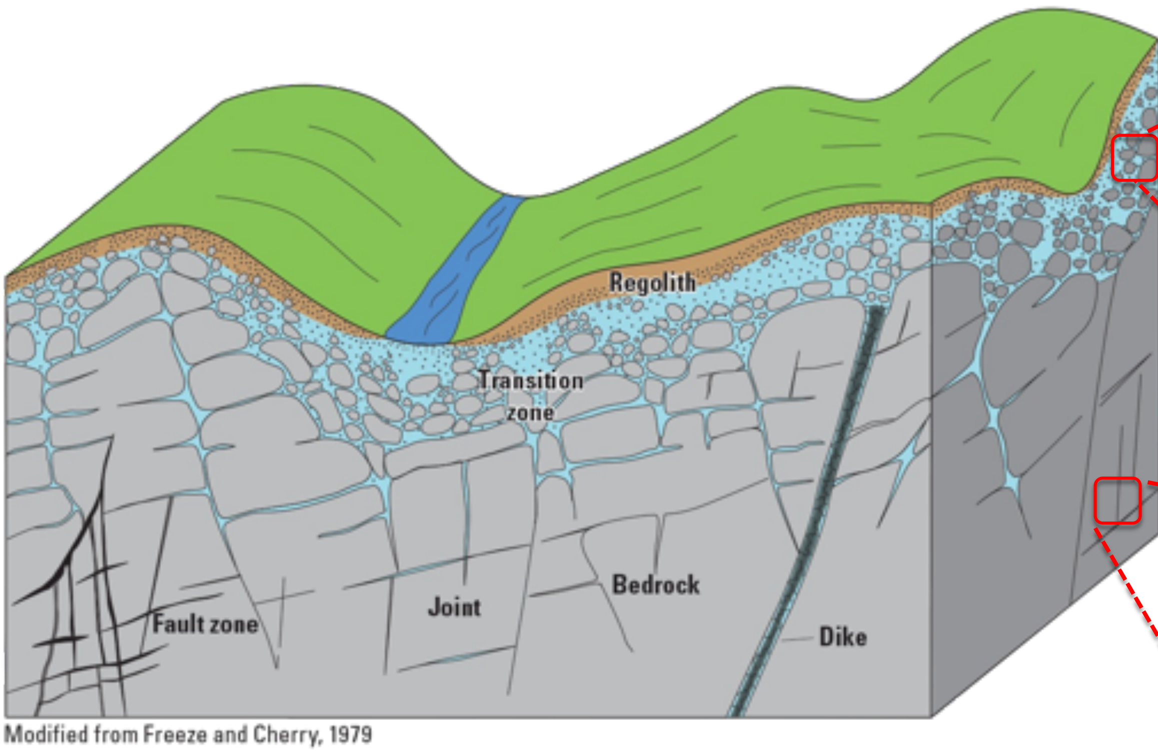
Peter K. Kang

University of Minnesota, Twin Cities

Department of Earth & Environmental Sciences

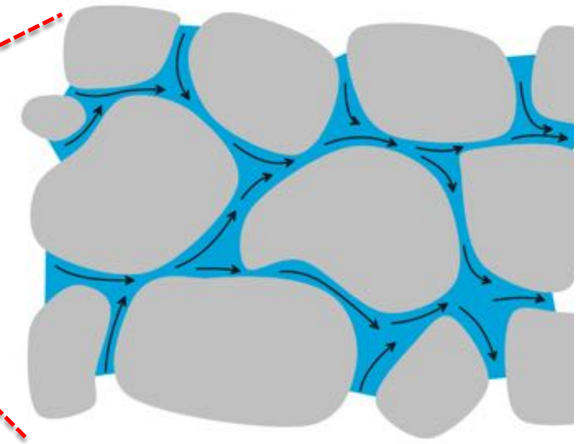
MGWA 2022

Groundwater flow is fundamentally porous and fractured media flow!

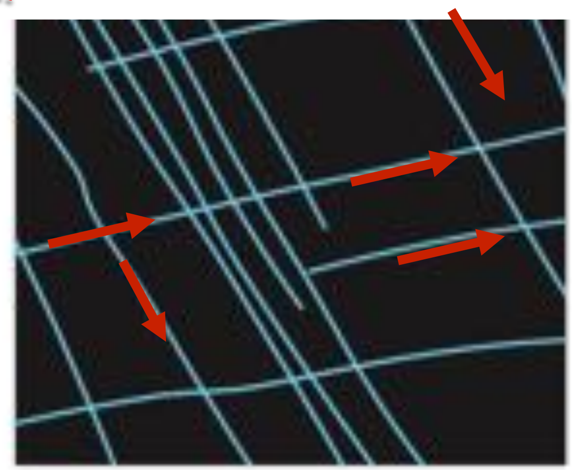


https://pubs.er.usgs.gov/publication/sir20225041

Unconsolidated porous media



Fractured media



My research group studies fractured rock hydrogeology and coupled processes in fractured rock.

Why should we care about flow and transport through <u>fractures</u>?

: key to addressing global energy, climate change, and water issues

Energy

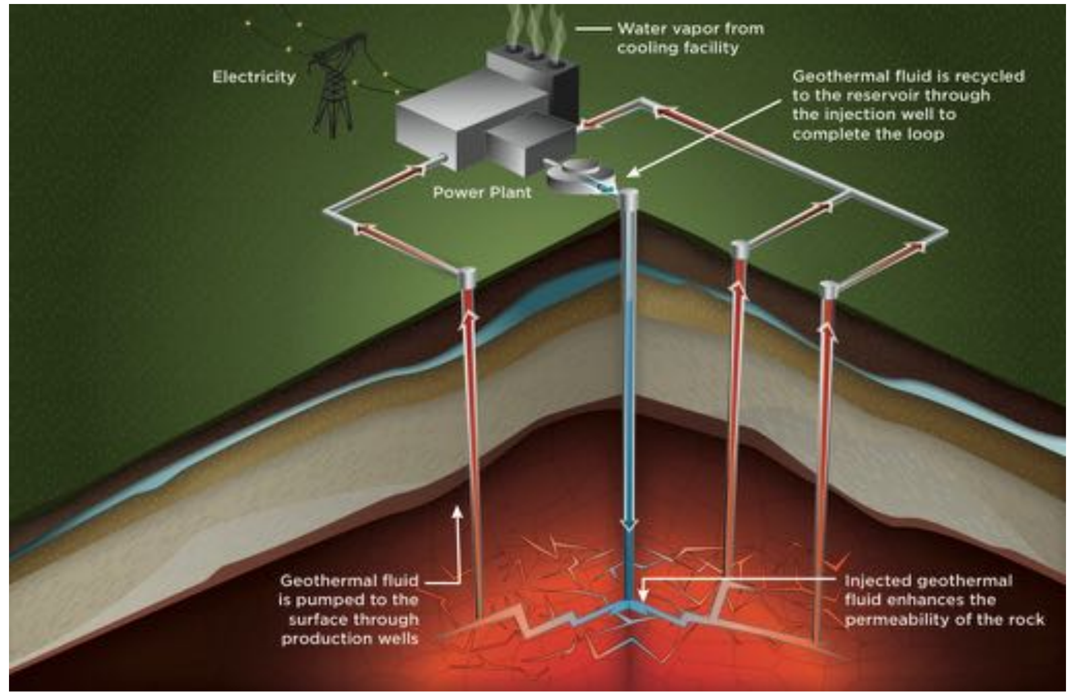
- Mining, oil and gas recovery
- Geothermal energy production
- Hydraulic fracturing
- Geologic nuclear waste disposal

Climate Change

- Geologic carbon sequestration
- Methane release from aquatic sediments
- Sea water intrusion

Water

- Groundwater management / remediation
- Managed aquifer recharge



Retrieved from cleanenergyaction.org

Geothermal energy is expected to have 26-fold increase by 2050 (DOE).

Why should we care about flow and transport through <u>fractures</u>?

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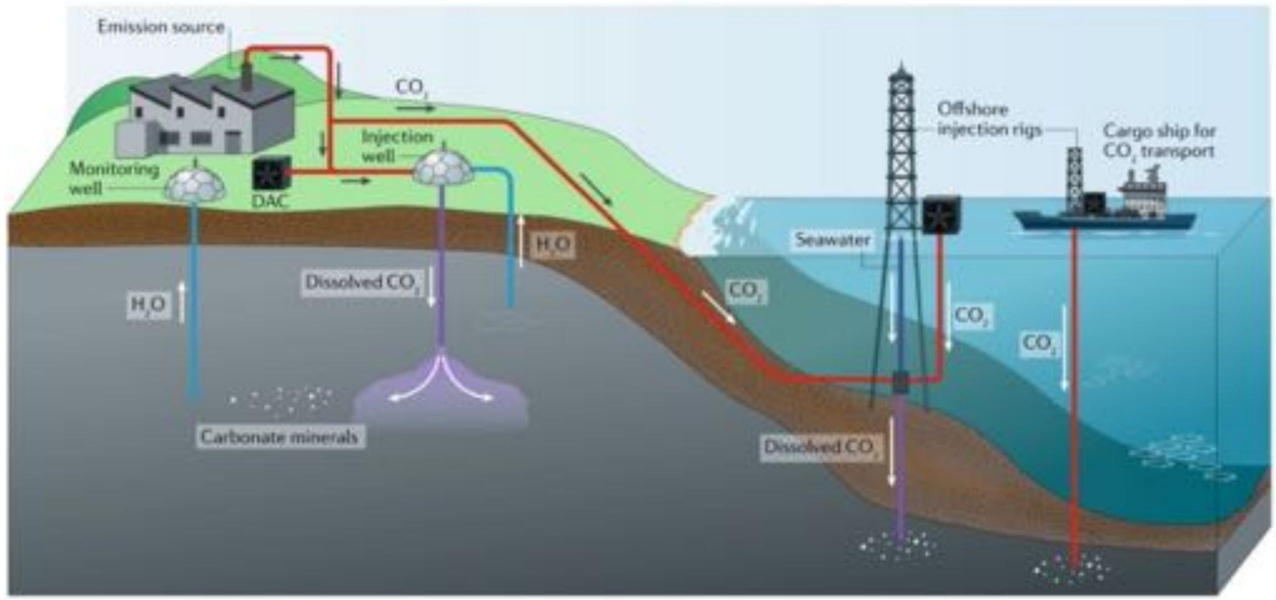
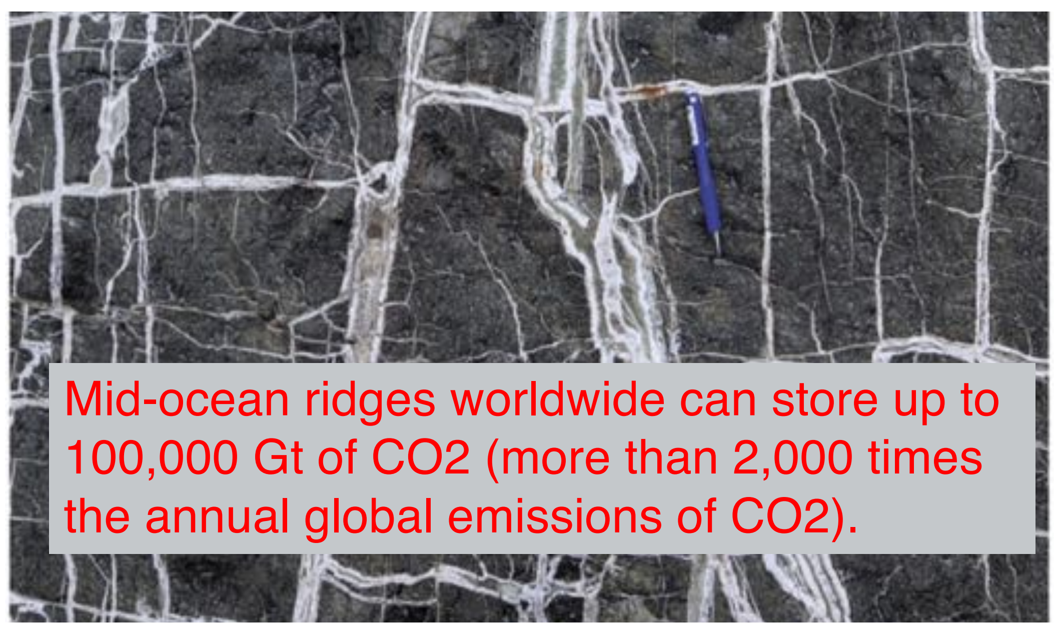


Snæbjörnsdóttir et al., *Nature Reviews Earth & Environment*



Why should we care about flow and transport through **fractures**?

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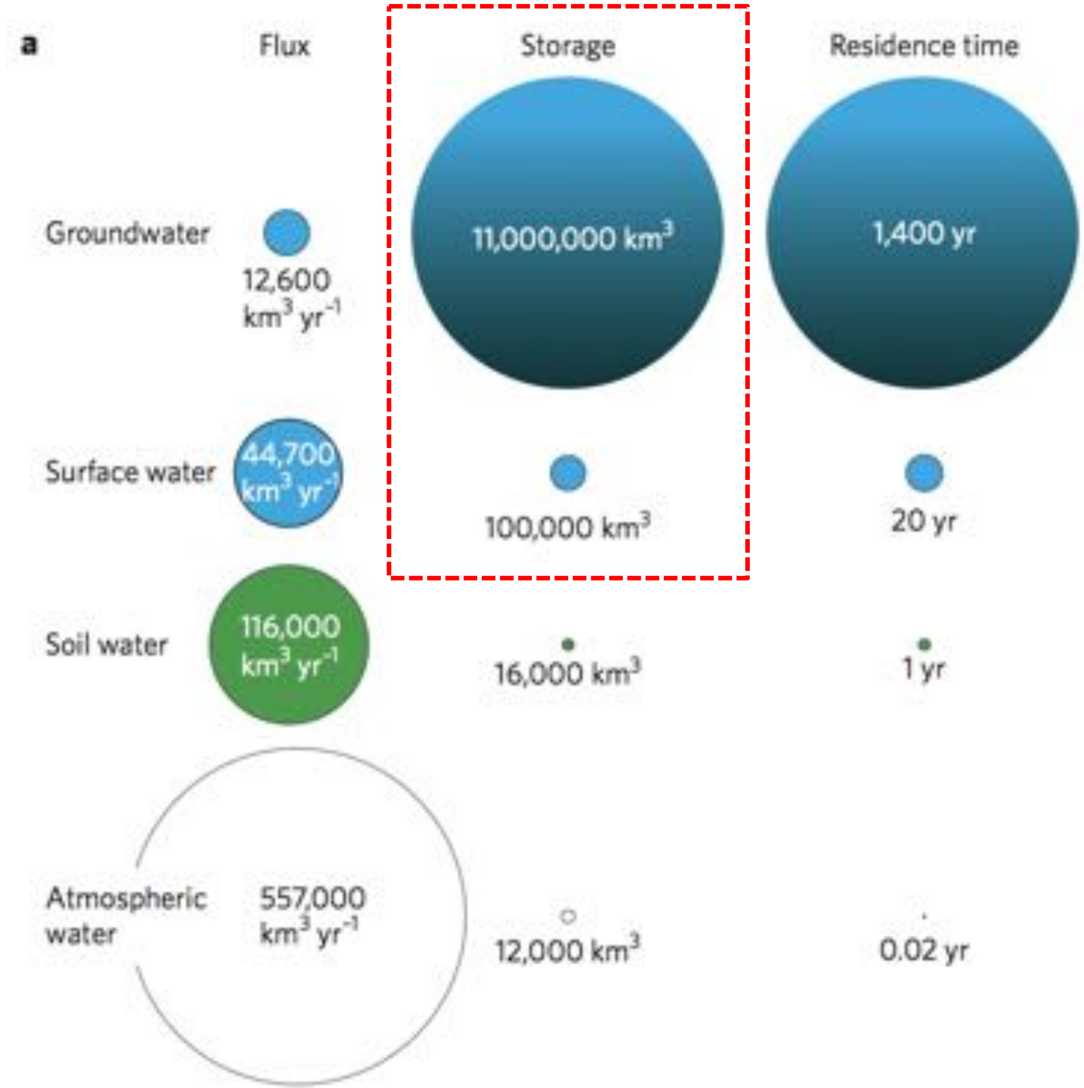


Aeschbach-Hertig and Gleeson, Nature Geosci. (2012)

Importance of fractured rock aquifers: Global scale

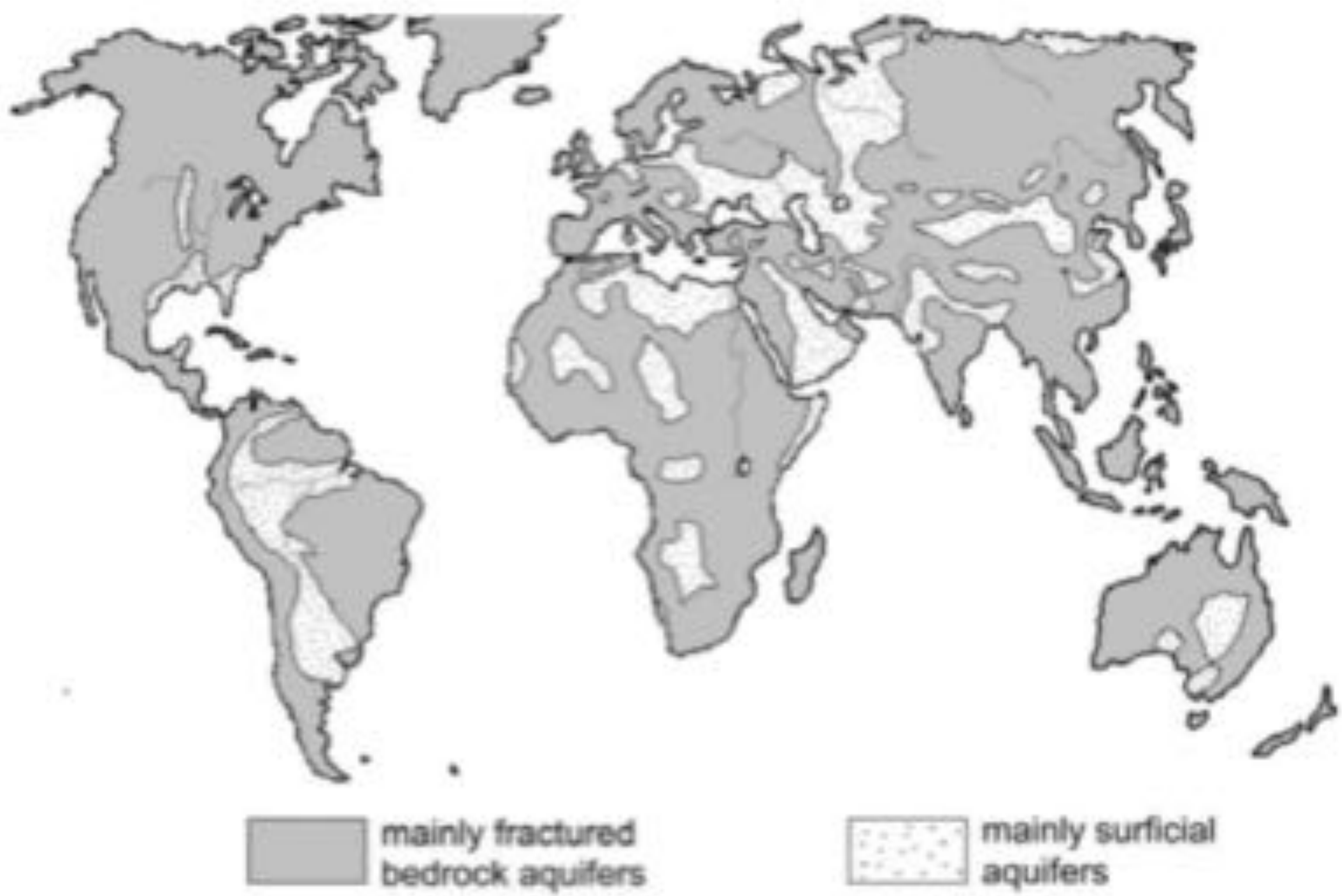
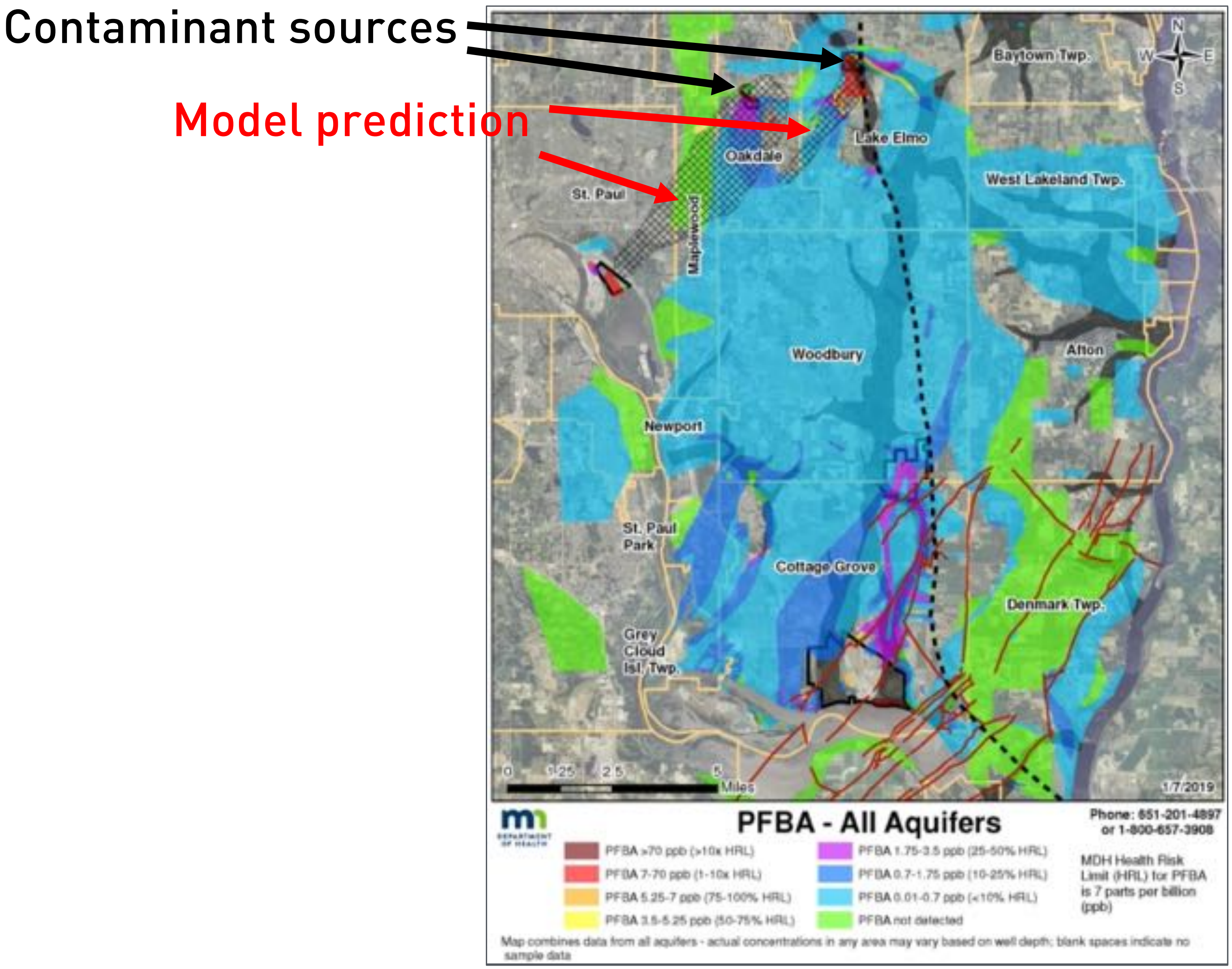


Fig. 1.1. Sketch-map of worldwide fractured rock aquifer distribution (interpreted after Plummer *et al.* (2002)).

75 % of the earth's surface consist of fractured or karstic fractured rock aquifers

Despite the critical importance, predicting subsurface transport is challenging and unresolved problem



$850 million settlement between the 3M company and the state of Minnesota

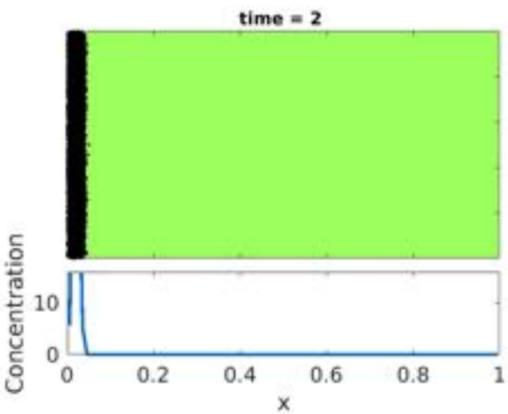
Source: Minnesota Department of Health

Flow channeling in fractured media leads to anomalous transport

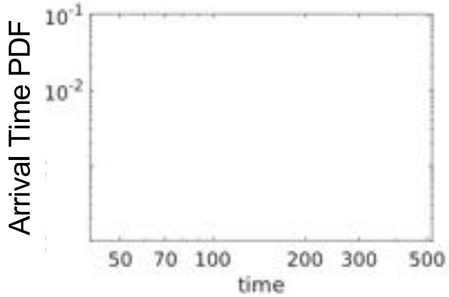
Traditional groundwater modeling frameworks are based on porous media flow

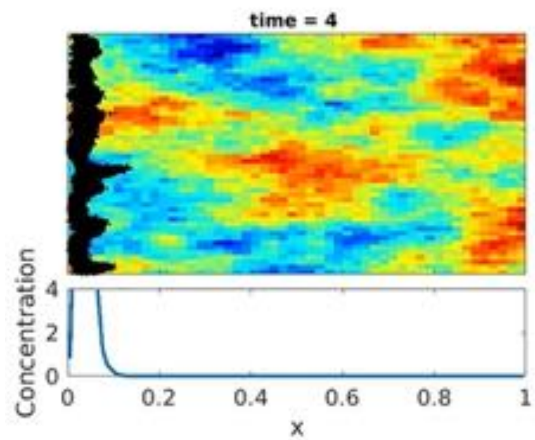
Flow channeling in fractured media leads to anomalous transport

Fickian Transport vs Non-Fickian (Anomalous) Transport

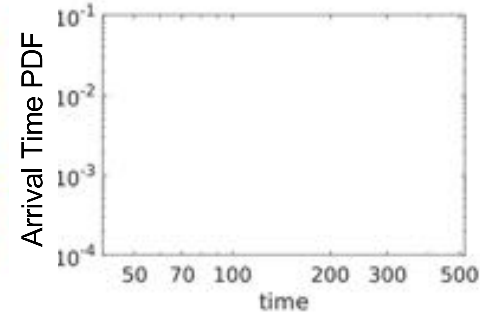


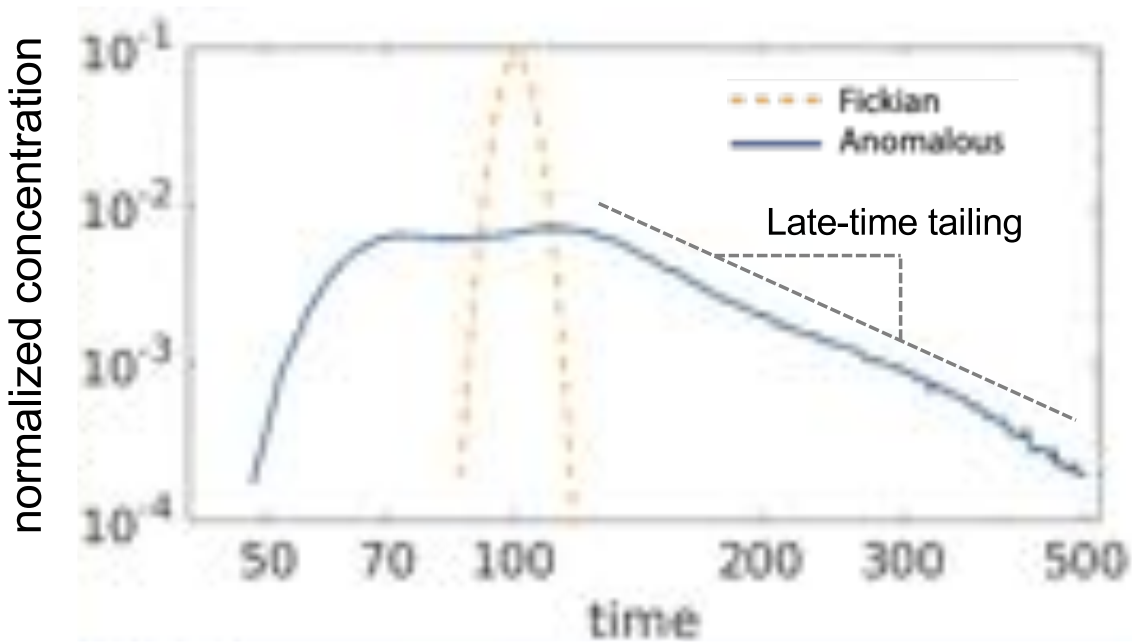
Breakthrough Curve





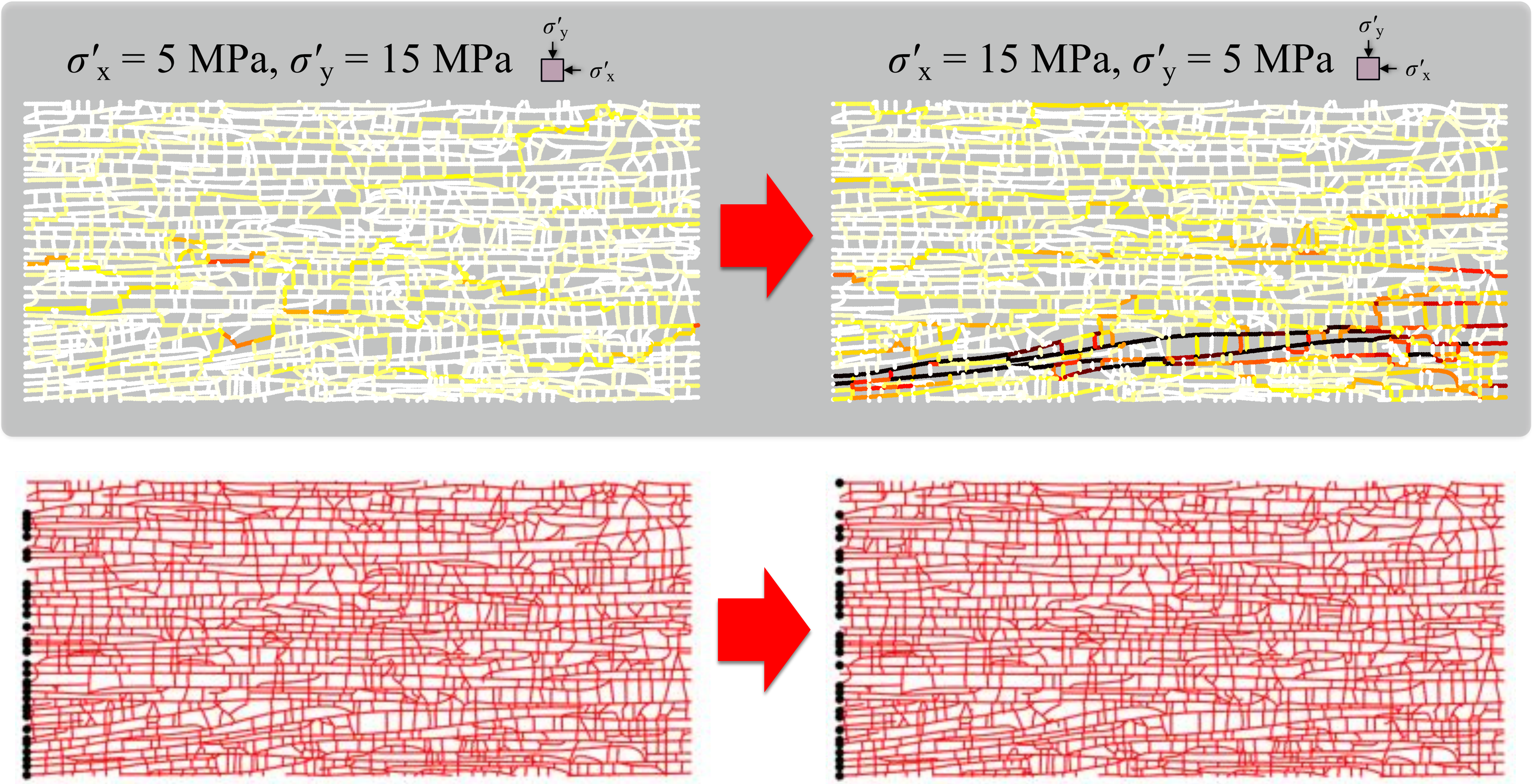
Breakthrough Curve





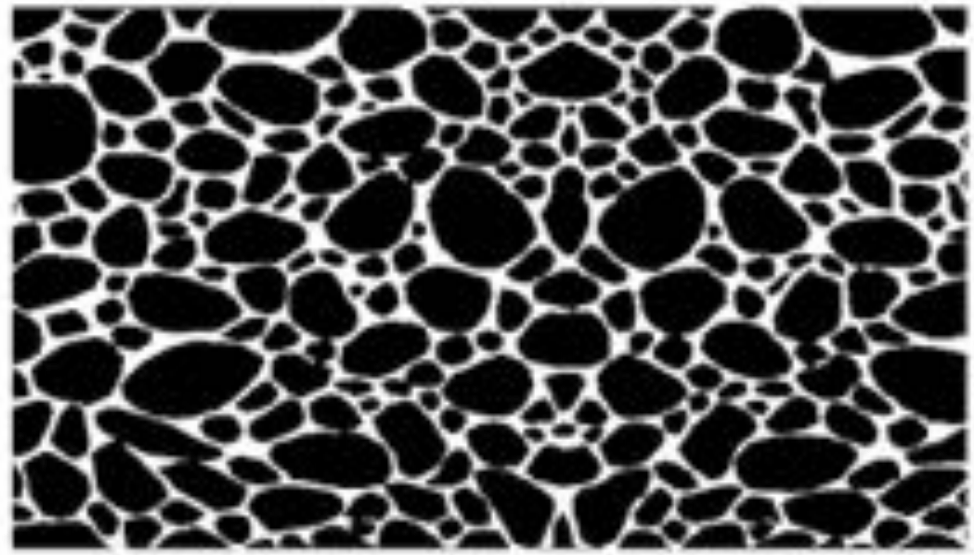
Anomalous Transport (late-time tailing): extremely long retention of contaminants

Flow channeling and anomalous transport in fracture networks

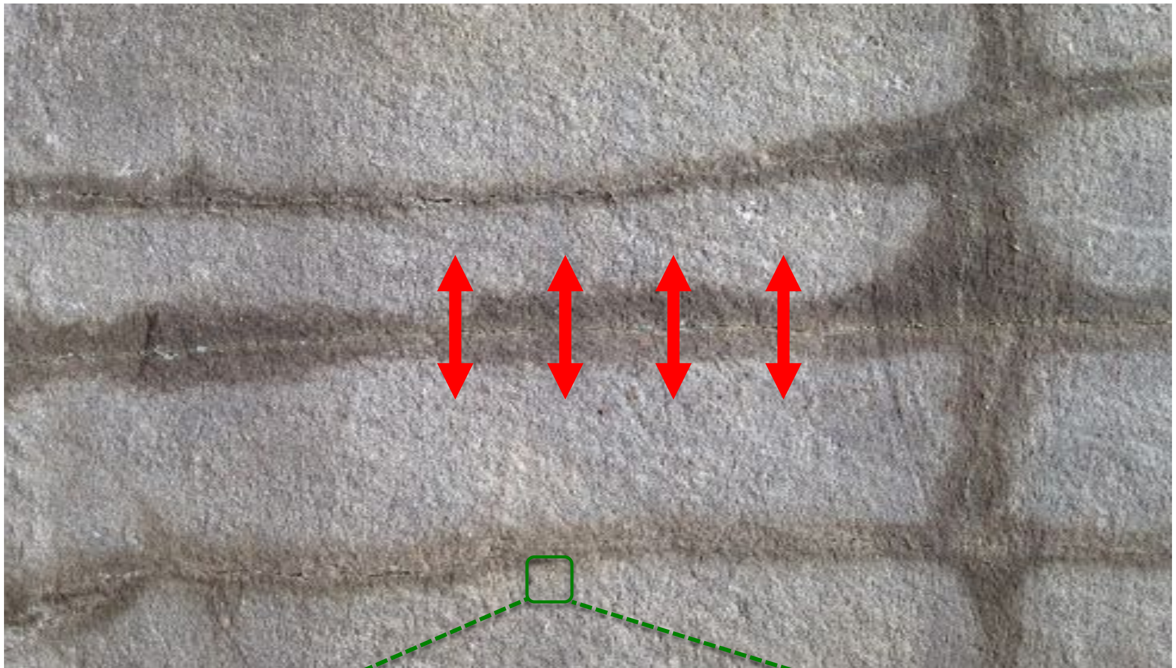


P. K. Kang, Q. Lei, M. Dentz, and R. Juanes. *Water Resources Research.* (2019)

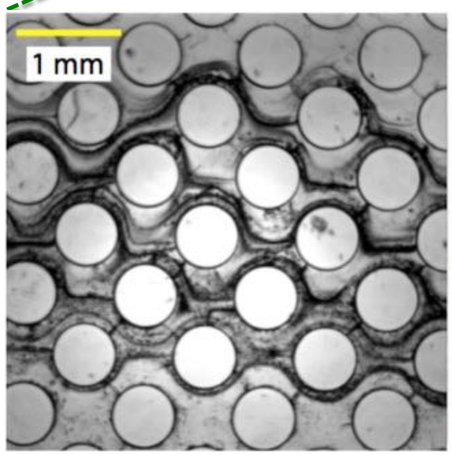
Key Challenge 1: Flow channeling & inertia effect



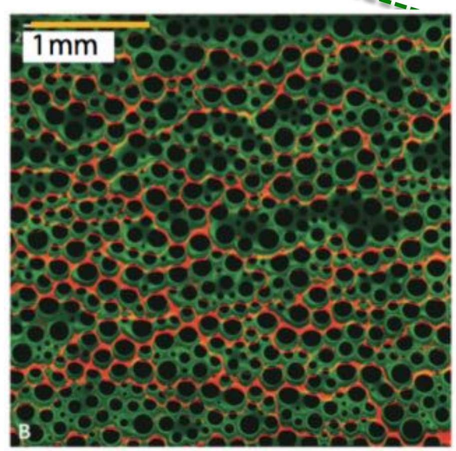
Key challenge 2: Multi-scale heterogeneity + Biogeochemical processes



Pore scale



Geochemical reactions

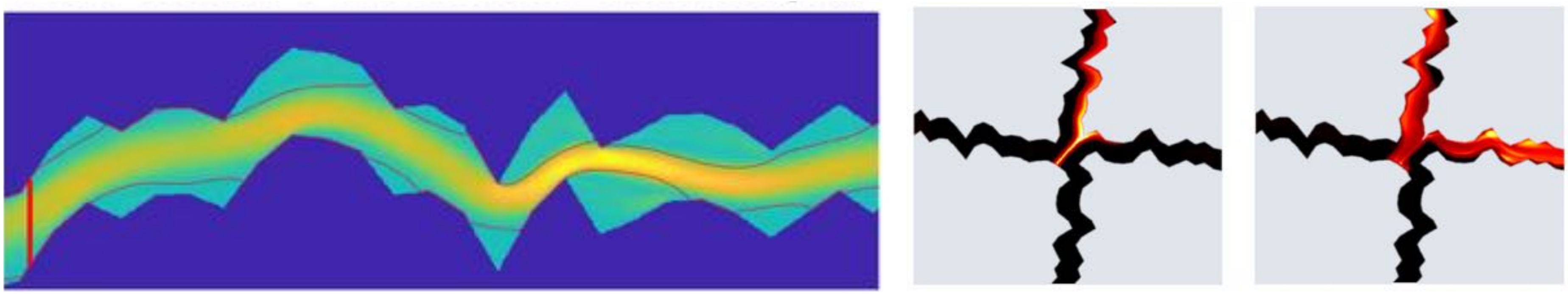


Biological activities

Durham et al., 2012

Presentation Overview

Part 1: Inertia effects on transport, mixing, & reaction in fractured media

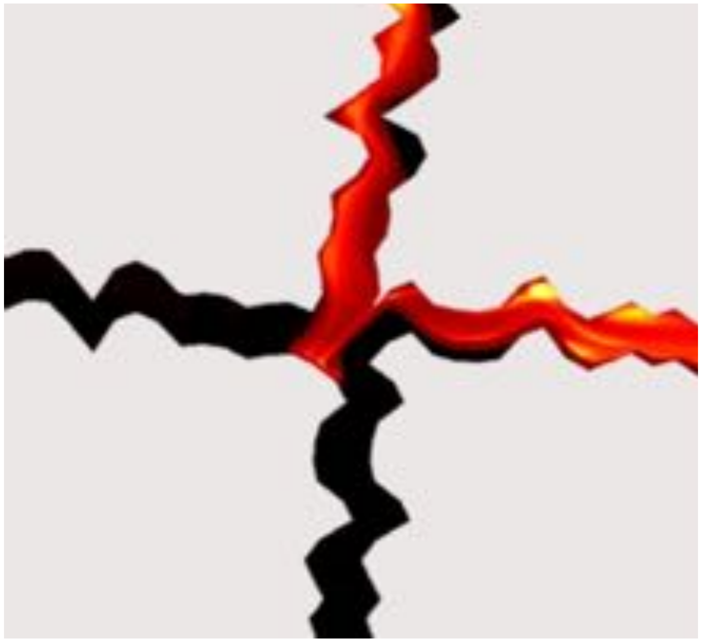


Part 2: Machine Learning to upscale transport processes from structural info.

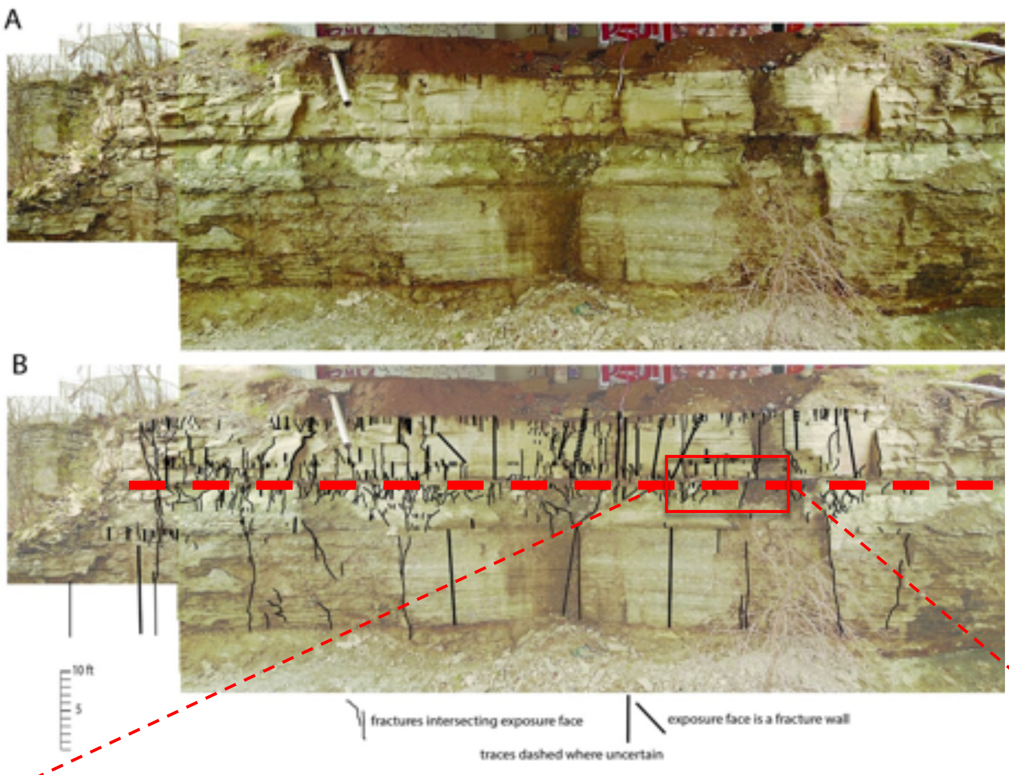
Part 3: Predicting transport processes in a fractured aquifer site

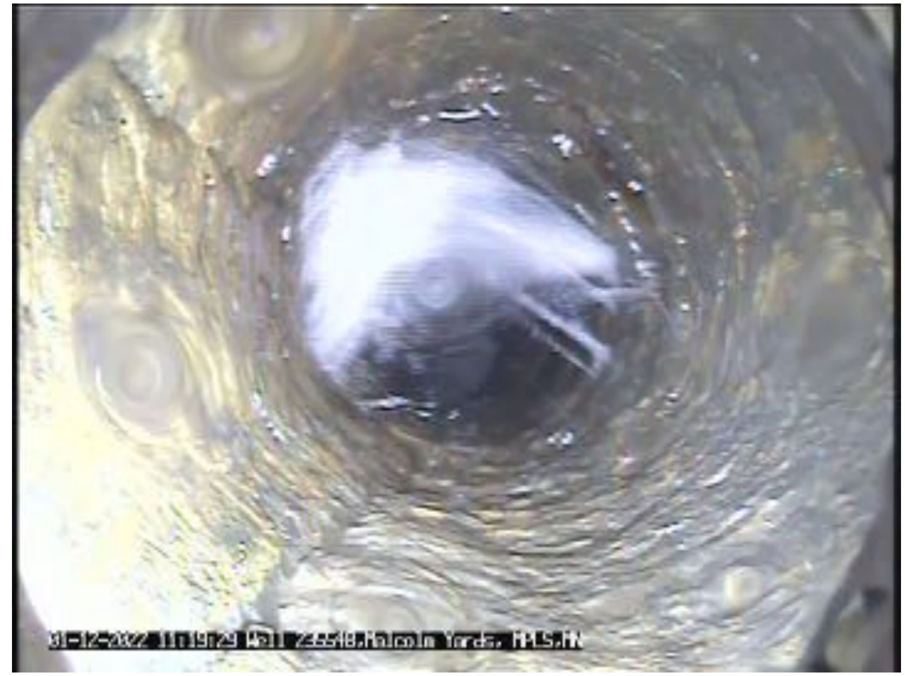
Part 1:

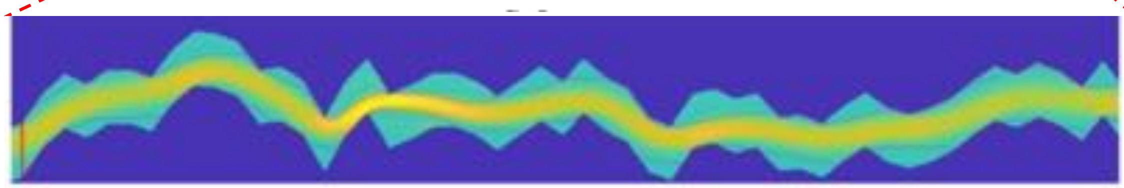
3D & Inertia Effects on Transport, Mixing and Chemical Reaction



Inertia effects are common and important in fractured rocks

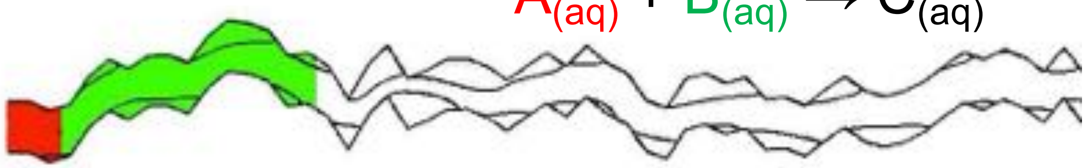




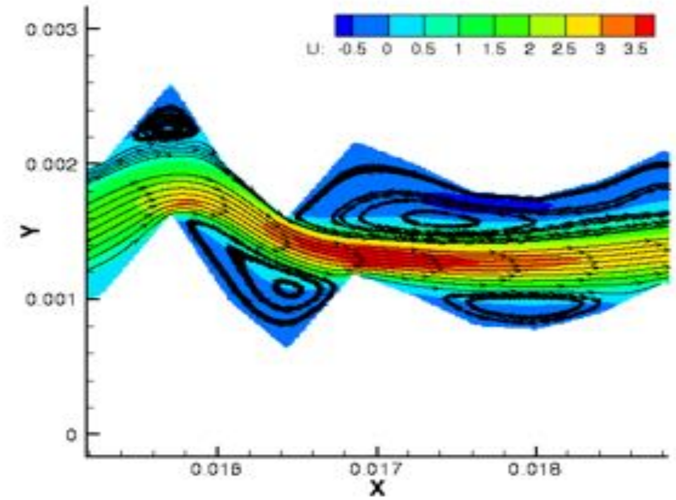


Yoon and Kang, *Physical Review Fluids, 2021*

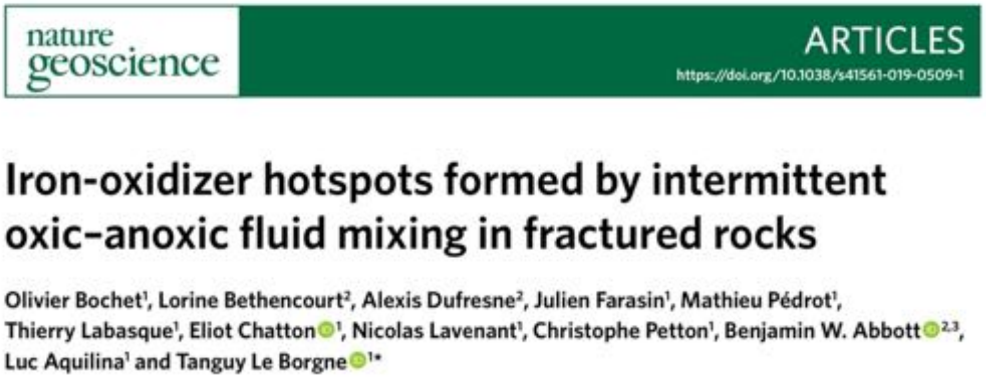
$A_{(aq)} + B_{(aq)} \rightarrow C_{(aq)}$



S. Yoon and P. K. Kang, *Transport in Porous Media*, 2021



Fracture intersections are mixing and reaction hotspots

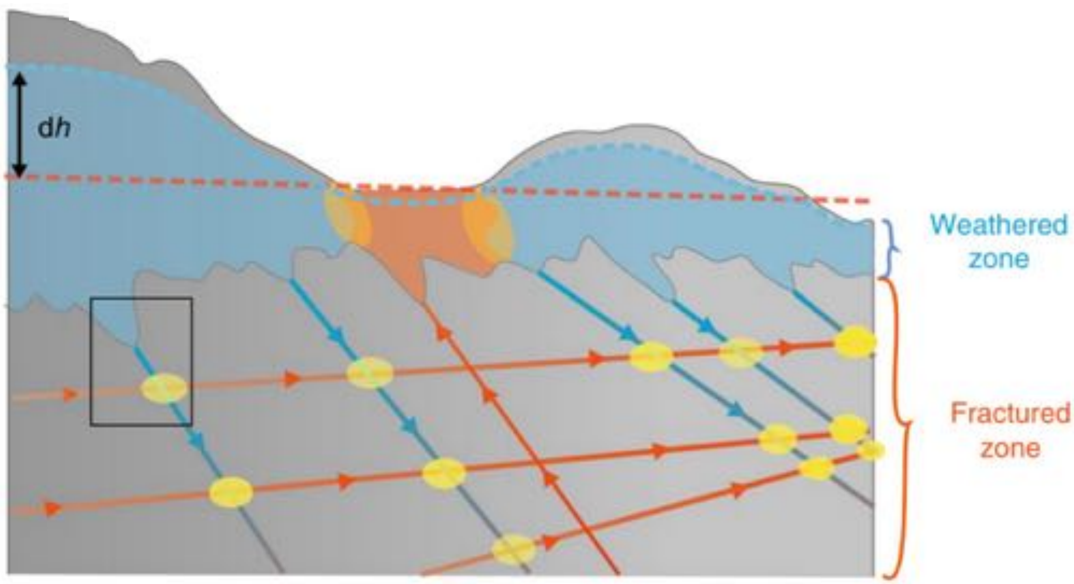

nature geoscience

ARTICLES

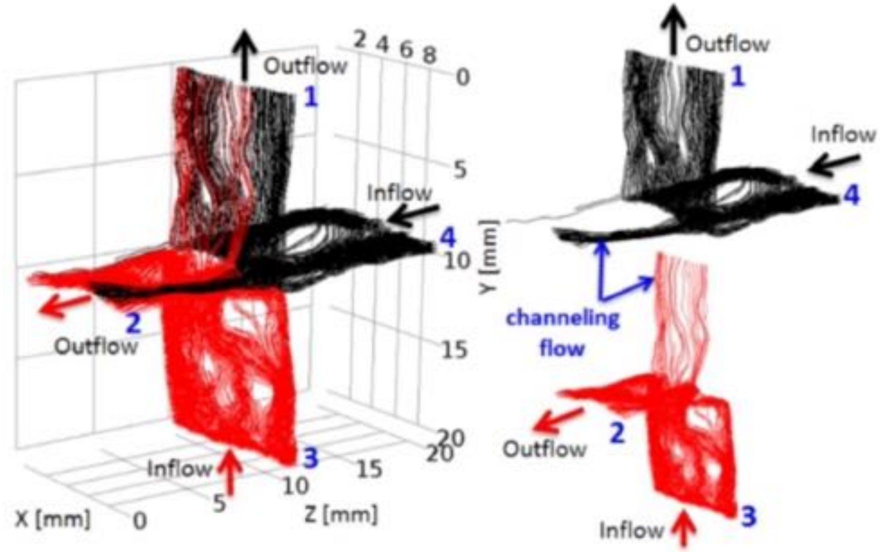
https://doi.org/10.1038/s41561-019-0509-1

Iron-oxidizer hotspots formed by intermittent oxic–anoxic fluid mixing in fractured rocks

Olivier Bochet[1], Lorine Bethencourt[2], Alexis Dufresne[2], Julien Farasin[1], Mathieu Pédrot[1], Thierry Labasque[1], Eliot Chatton[1], Nicolas Lavenant[1], Christophe Petton[1], Benjamin W. Abbott[2,3], Luc Aquilina[1] and Tanguy Le Borgne[1*]



Rock fracture intersections

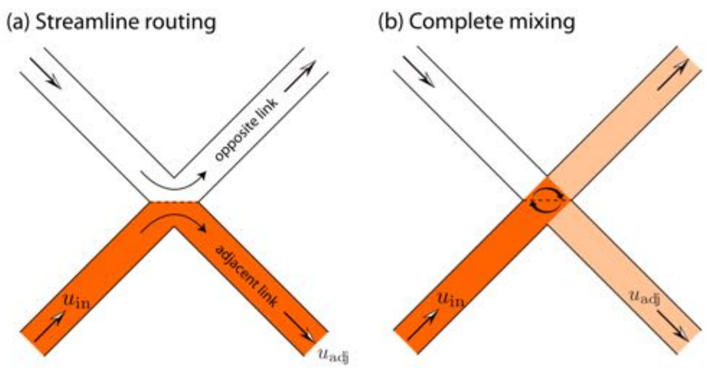


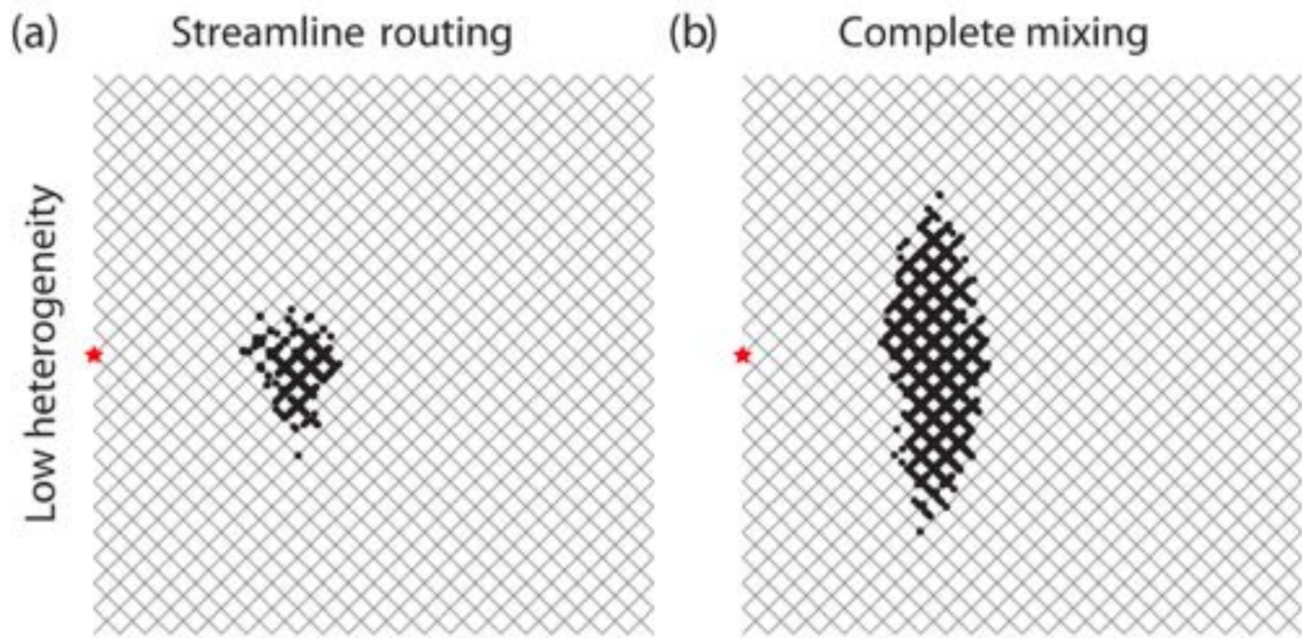
L. Zou, L. Jing, and V. Cvetkovic, 2017. *ADWR.*

Inertia effects on reaction at 3D fracture intersections are poorly understood

Mixing at intersections can have macroscopic impacts on spreading and dissolution patterns.

Pe >> 1 Pe << 1





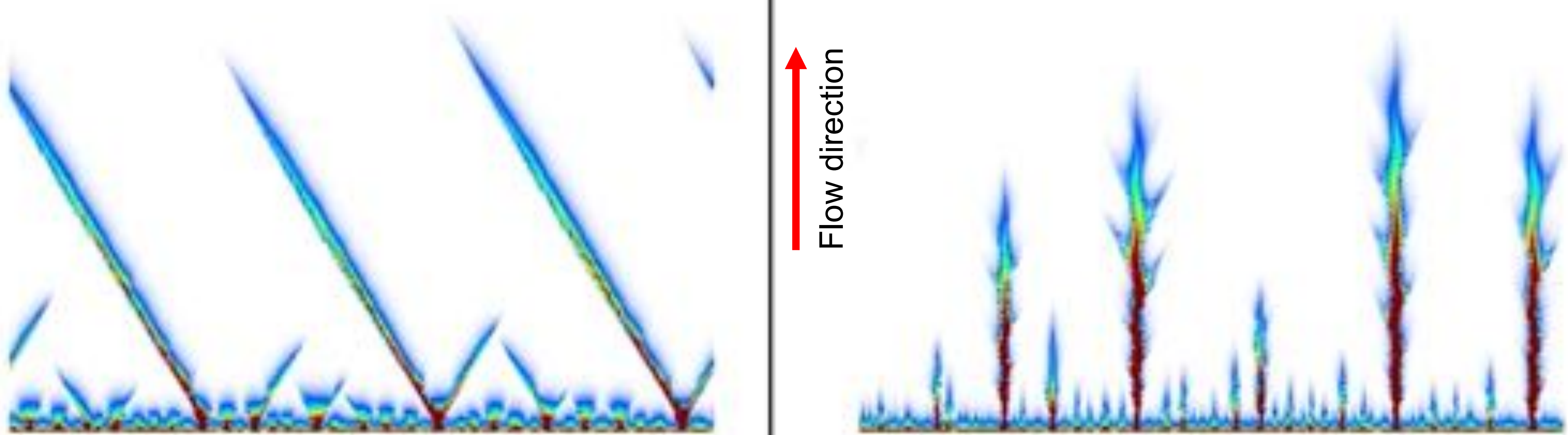
Flow direction Flow direction

P. K. Kang et al., *Physical Review E, 2015*

Mixing at intersections can have macroscopic impacts on spreading and dissolution patterns.

Complete mixing

No mixing
(streamline routing)



R. Sharma, P. Szymczak, P. K. Kang, *in preparation.*

Key hypothesis of this study

- Inertia and 3D flow effects can dramatically change mixing and reaction dynamics at fracture intersections.

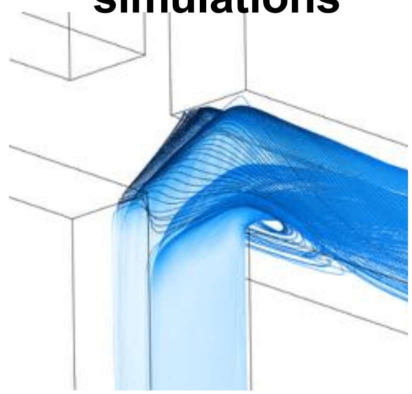
- To test the hypothesis, we combine:

Microfluidics experiment

Pore-scale intersection (microfluidics chip)

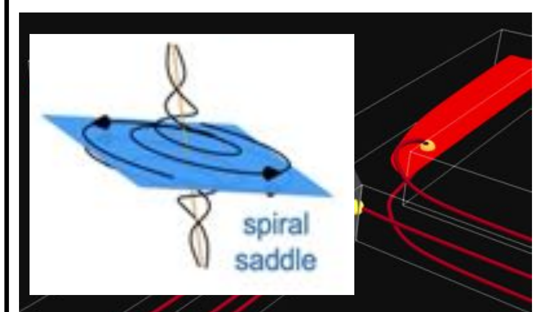
+

3D direct numerical simulations



+

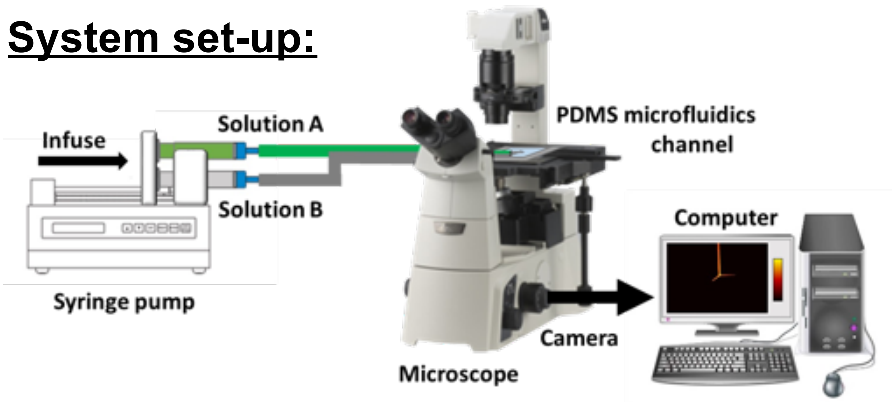
Flow topology analysis



S. H. Lee and P. K. Kang, 2020, *Phys. Rev. Lett.* (Editors' Suggestion)

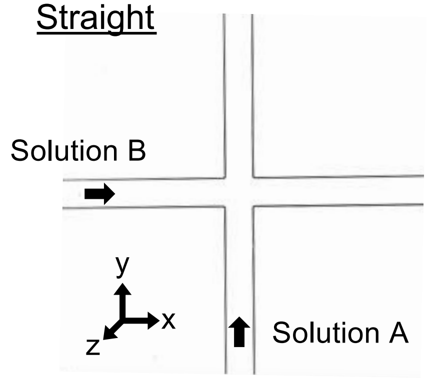
Microfluidics experiments

System set-up:



Microfluidics chips:

Straight



Channel dimension

aperture = 100 μm

depth = 70 μm

length = 20 mm

Flow condition

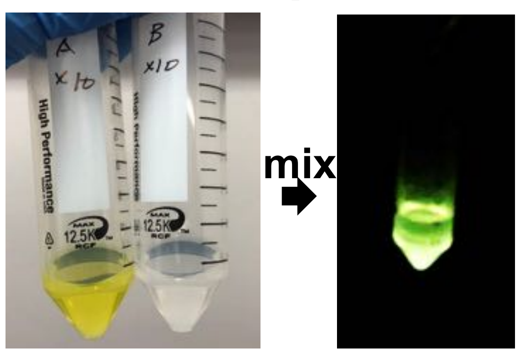
Re = 1 – 300

Q = 2 – 570 μl/min

Pe = $10^4 – 10^6$ Da = $10^{-2} – 10^{-5}$

Chemiluminescence reaction (A + B → C)

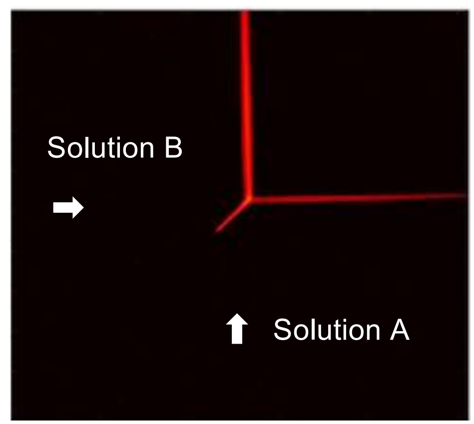
A + B → C



Jonsson and Irgum, 1999, Anal. Chim. Acta;
de Anna et al., 2014, ES&T

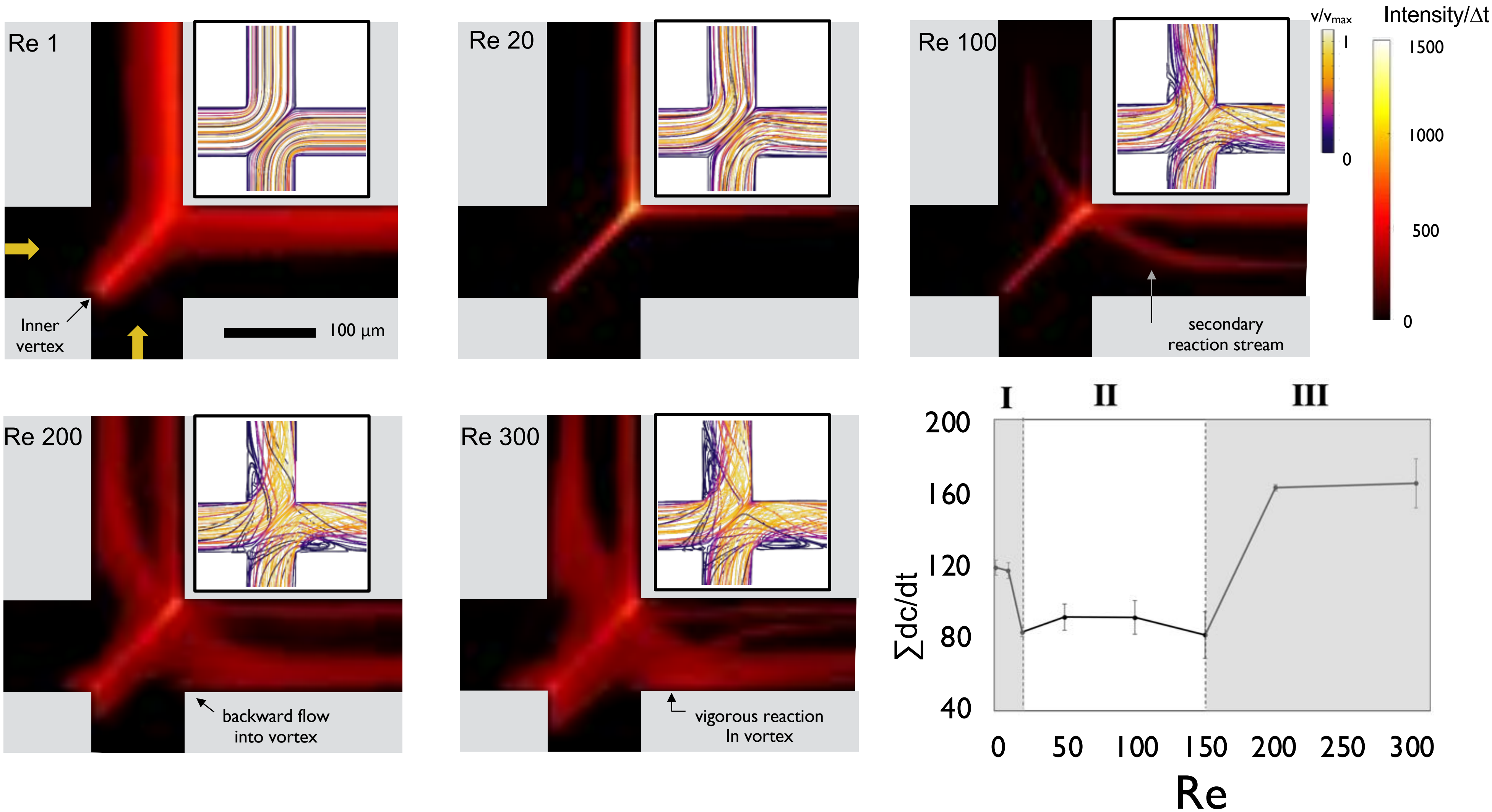
Reaction produces Luminescence

Example image:

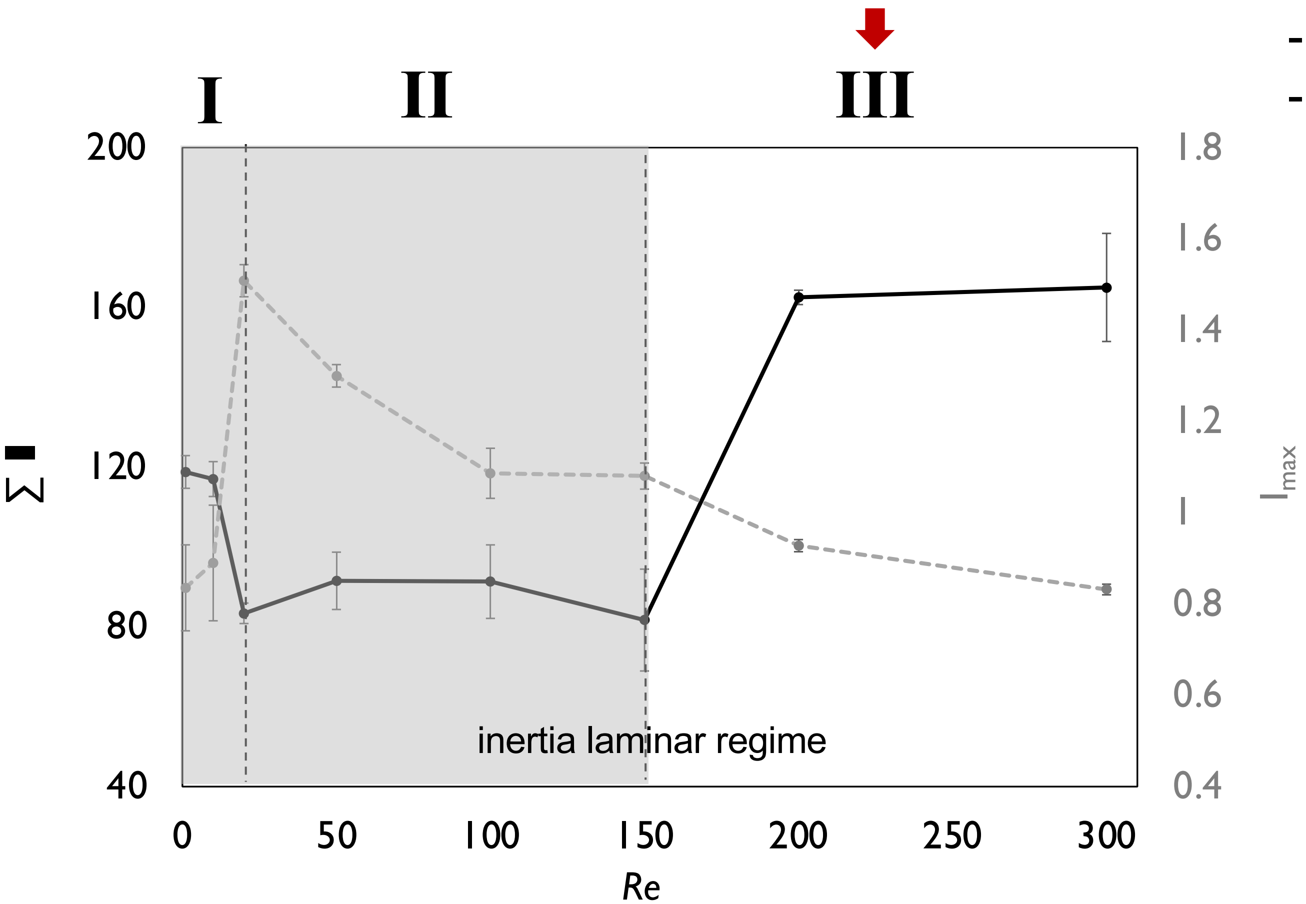


Intensity is proportional to the reaction rate, dC/dt

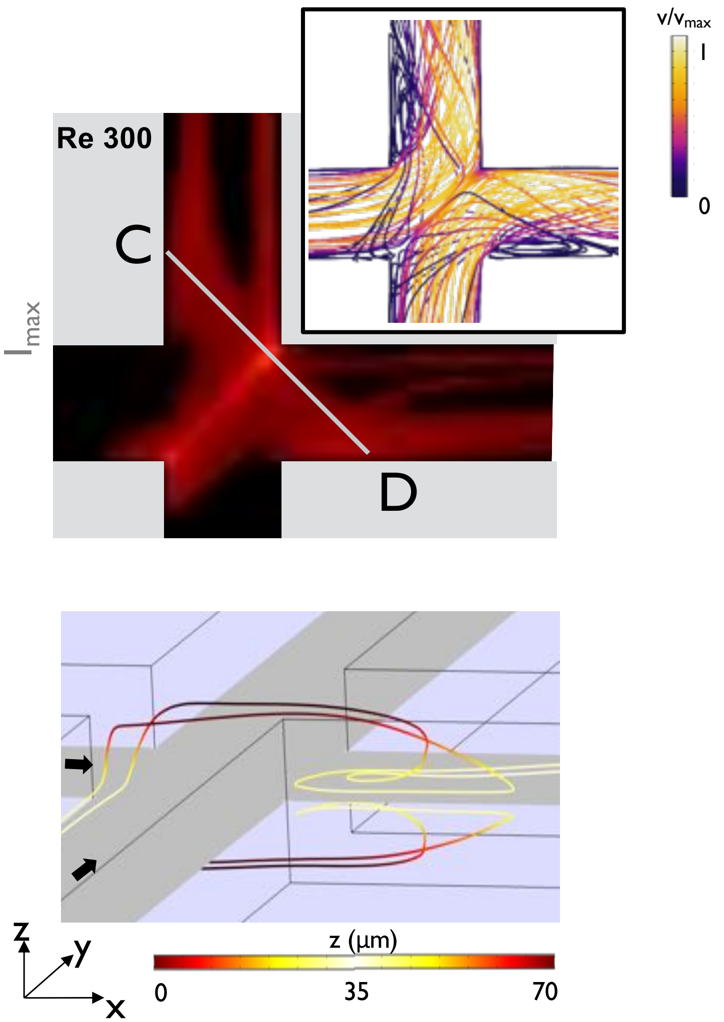
Three distinctive reaction regimes are observed



Vortices lead to dramatic increase in reaction rate

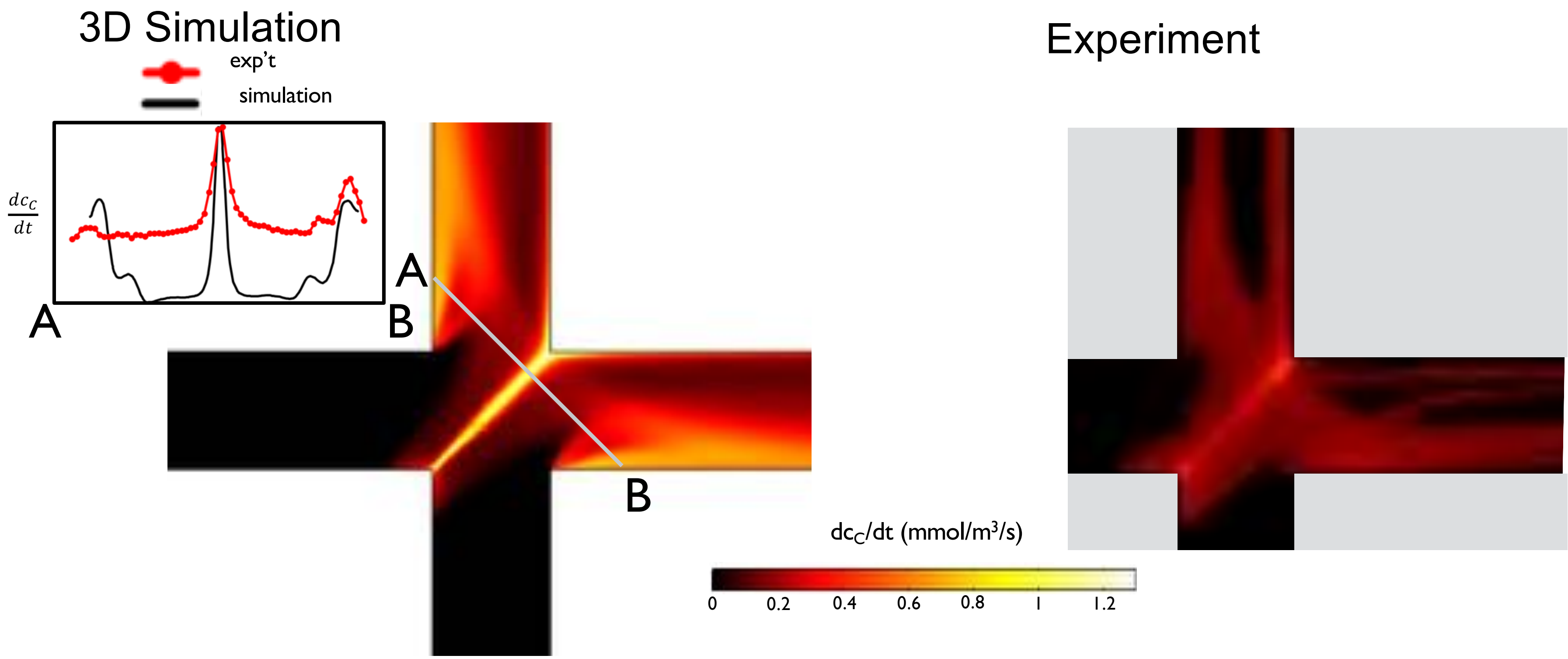


Regime III: Re > 150
Characterized by
- Intense 3D flow and vortex
- Enhanced overall reaction rate

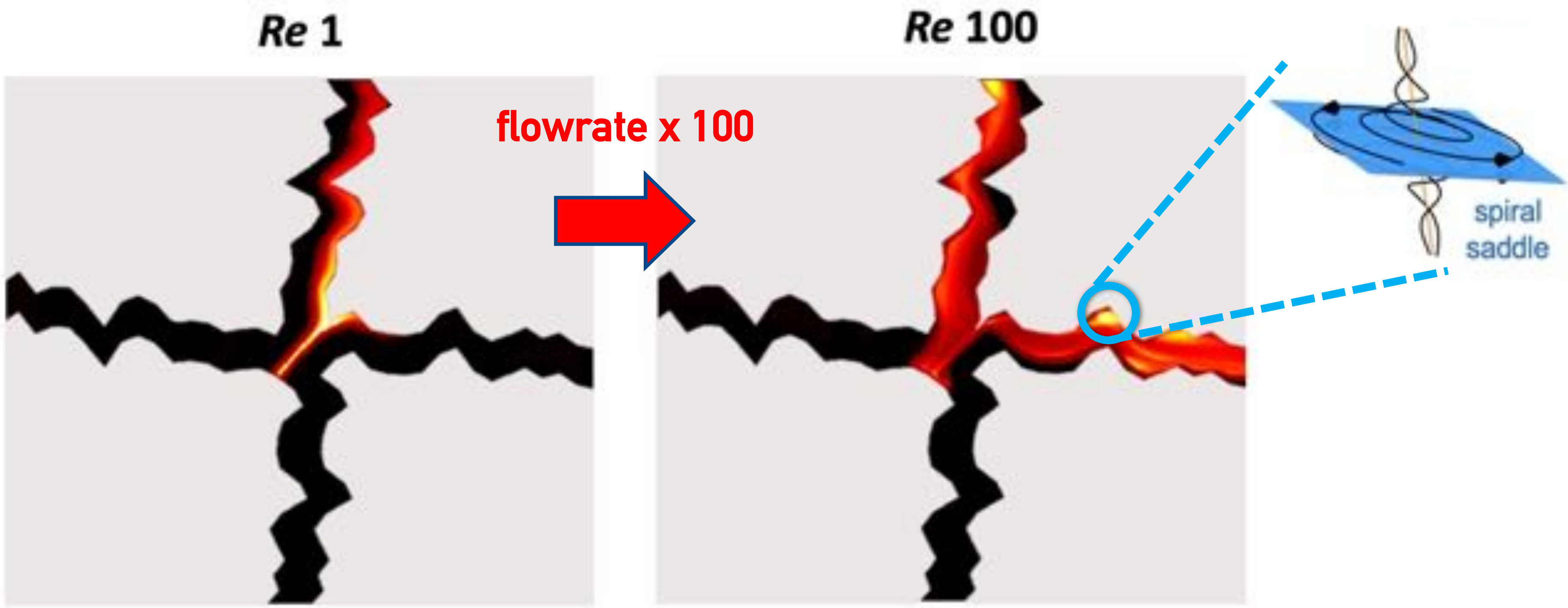


3D vortex topology leads to mixing & reaction hotspots

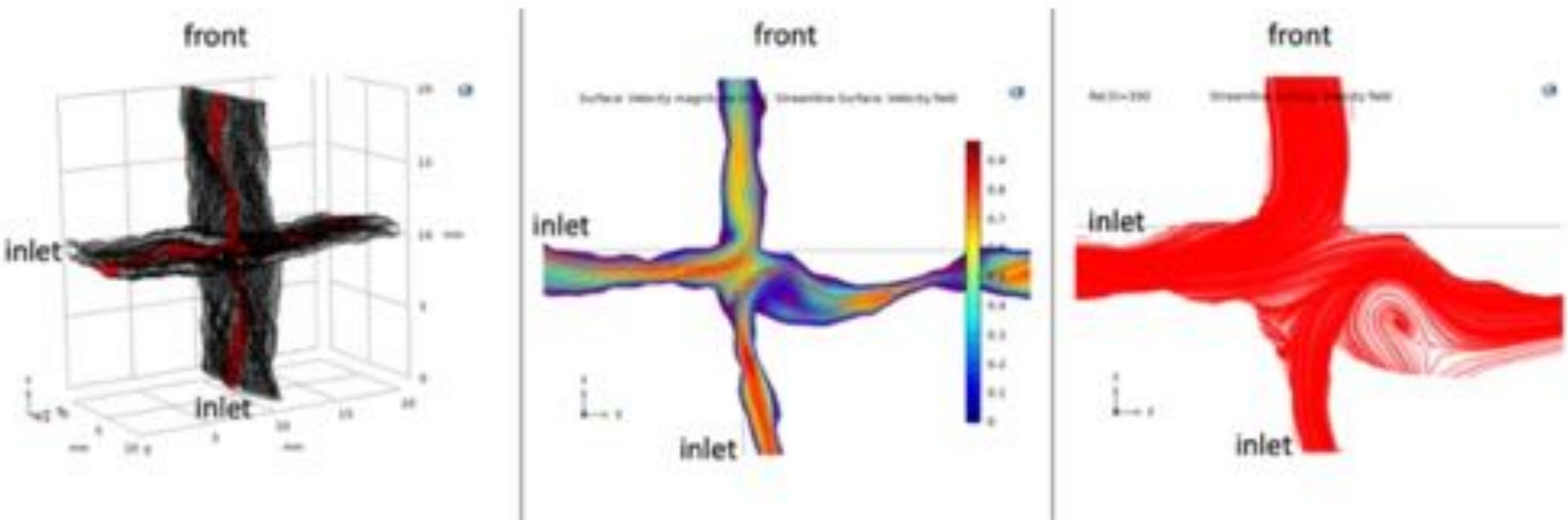
Reaction rate, dc/dt, map @ Re = 300



Inertia & channeling effects fundamentally change mixing and reaction

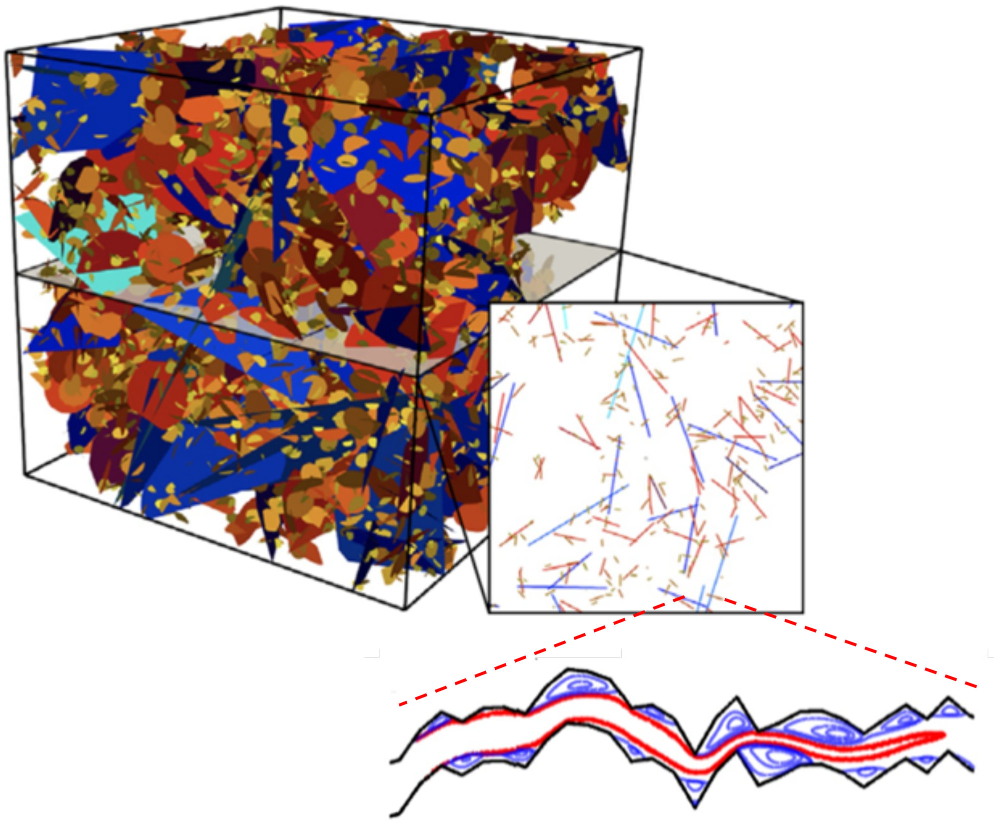


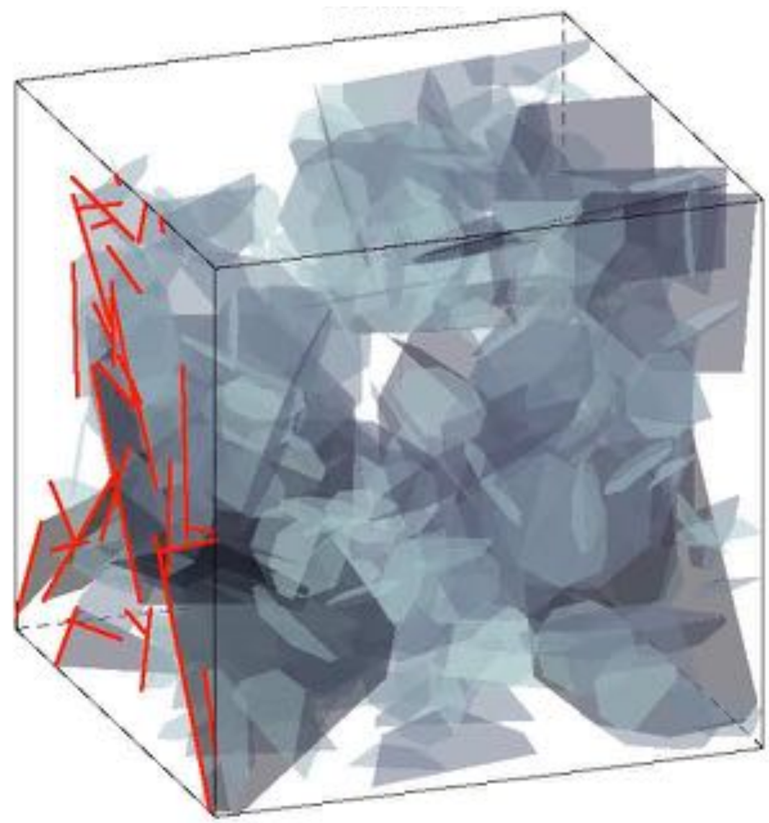
S. Lee and P. K. Kang, 2020, *Phys. Rev. Lett.*



Upscaling transport, mixing, and reaction in fracture networks

- **Incorporate 3D and inertia effects** into network scale models and properly upscale transport processes.





NSF CAREER: solute transport, mixing, and reaction in fractured media across scales

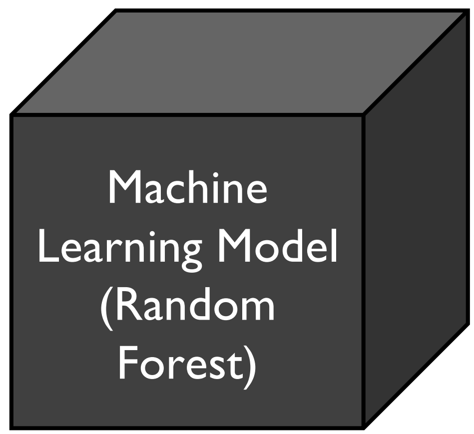
Part 2:

Machine learning to upscale transport processes

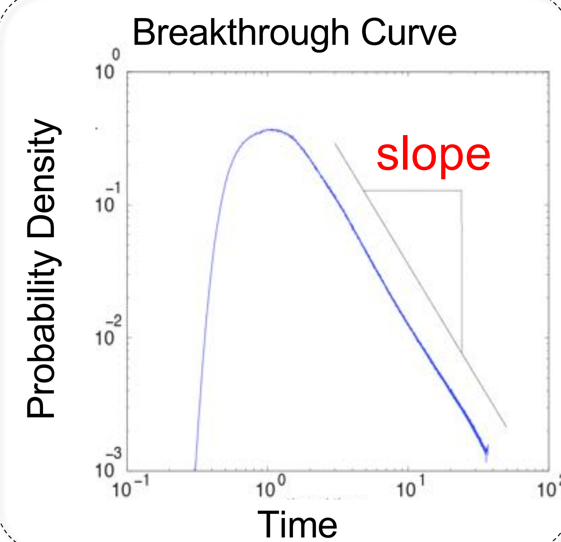
Machine learning-assisted identification of key structural properties governing transport processes

Input (structural properties)

- Percentage of Dead-end fractures
- Fracture density
- Shortest path length
- Node connectivity
- Network Entropy …



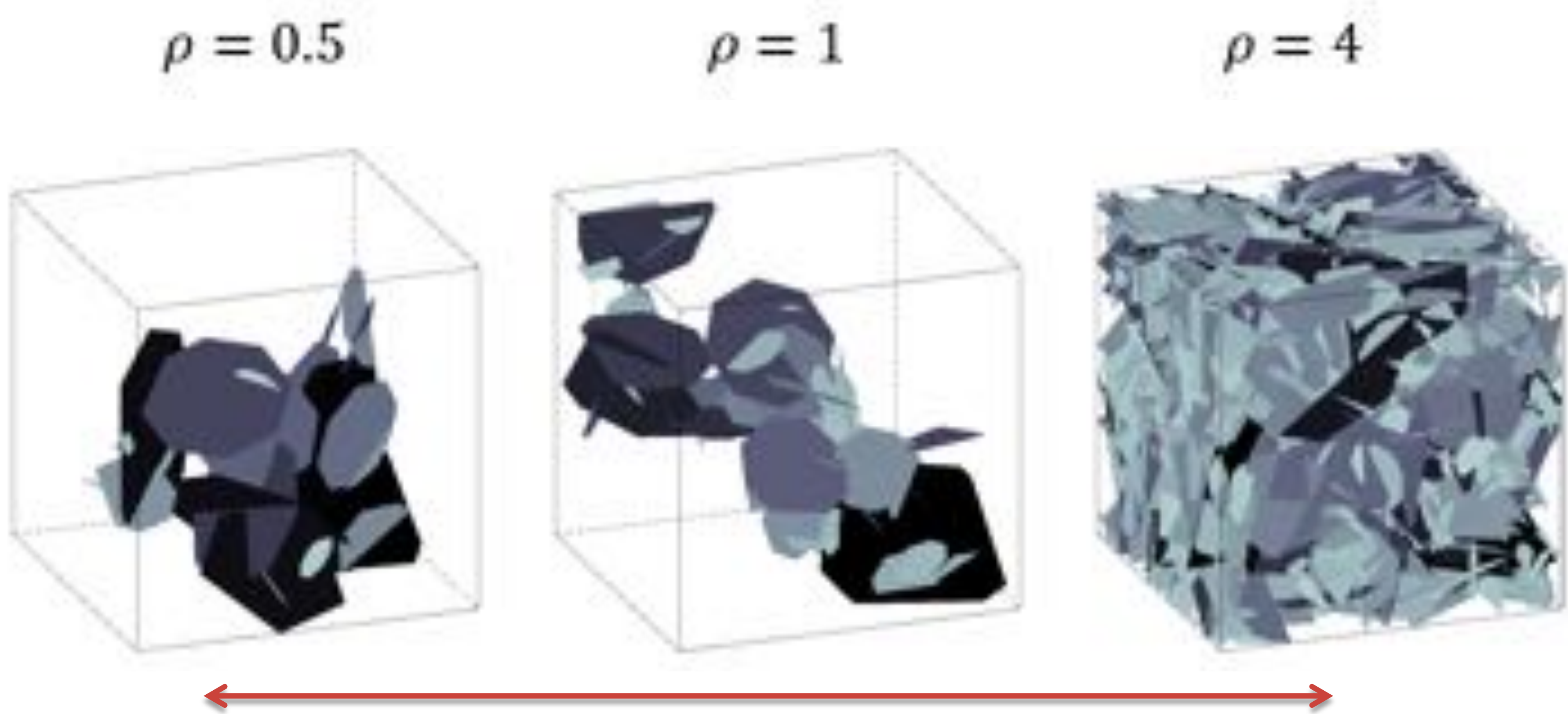
Output (transport processes)



Can we predict transport processes directly from key properties of fracture networks?

Machine learning application to fracture networks

What are the key structural properties inducing anomalous transport?



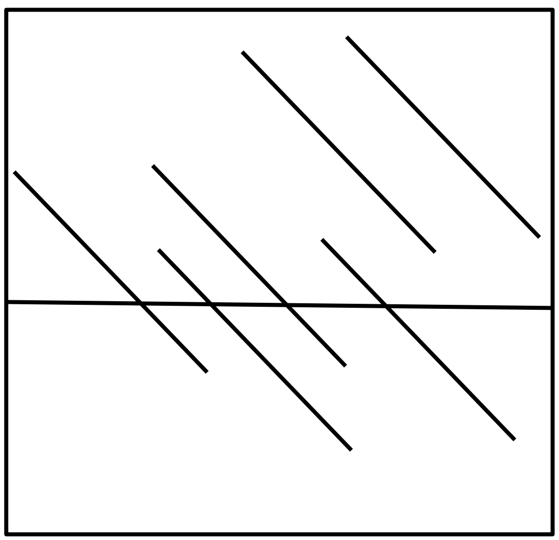
A wide range of structural complexity of fracture networks

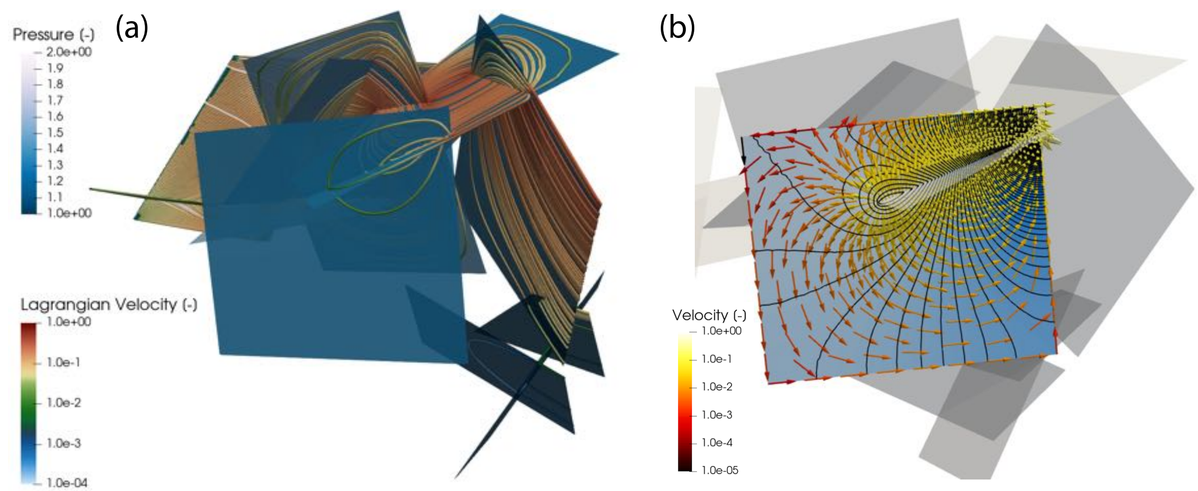
dfnWorks DISCRETE FRACTURE NETWORK

What are the key structural properties inducing anomalous transport?

Dead-end fractures?

2D vs 3D

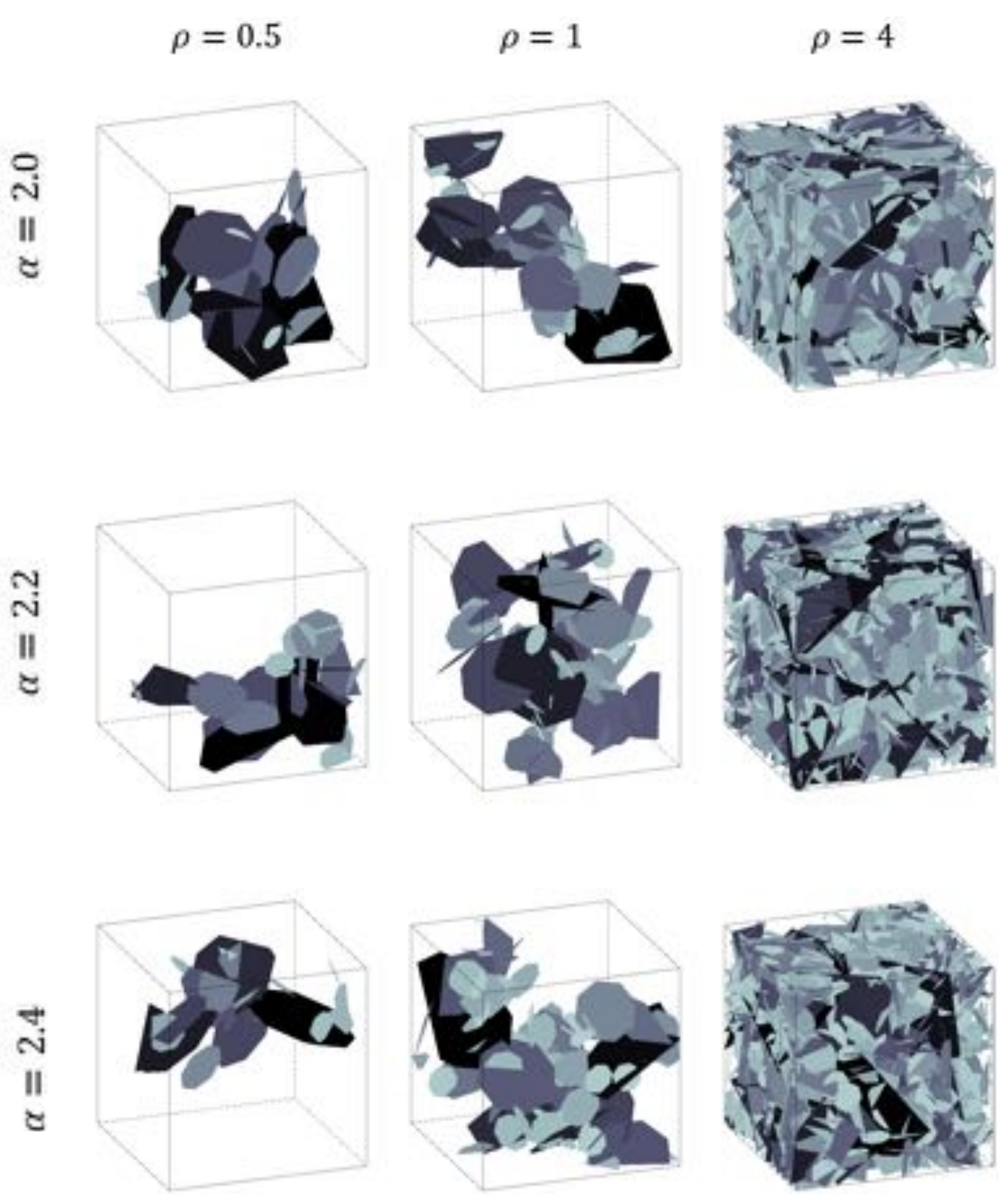




- Dead-end fractures are considered to play a key role in 3D DFN.
- No direct evidence of dead-end fracture effects on anomalous transport.

Kang et al., *Water Resour. Res.* (2020).

Big data generation for machine learning application



- Fracture density:

  $$\rho = \frac{N_{frac}}{\overline{N}_{frac}}$$

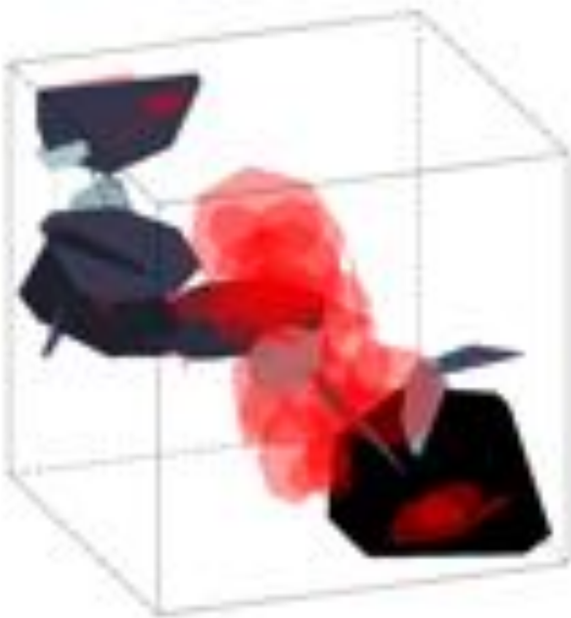
  ($\overline{N}_{frac}$: mean required number of fractures to percolate)

- Fracture length distribution:

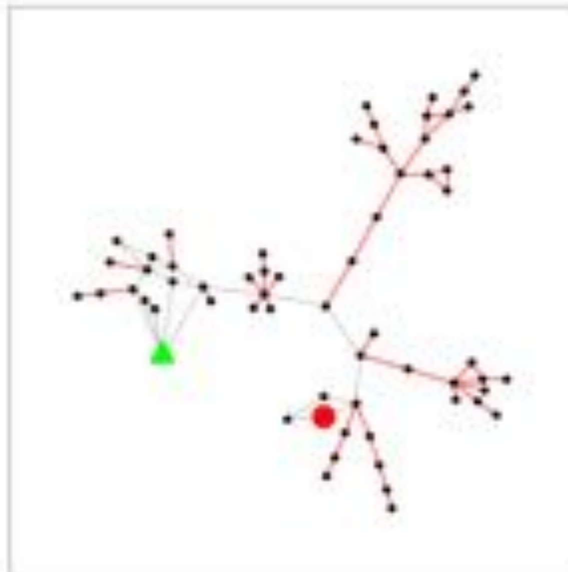
  $$p_r(r) = \frac{\alpha}{r_0} \frac{(r/r_0)^{-1-\alpha}}{1-(r_u/r_0)^{-\alpha}}$$

- We generate > 20 fracture networks for each combination (1568 realizations)

Quantifying structural properties (Feature Extraction) using Graph Theory



Discrete Fracture Network (DFN)



Graph Representation

Extracted structural features:

1. Percentage of Dead-end fractures
2. Mean & Variance of node degree
3. Shortest path length
4. Node connectivity
5. Assortativity
6. Network Entropy

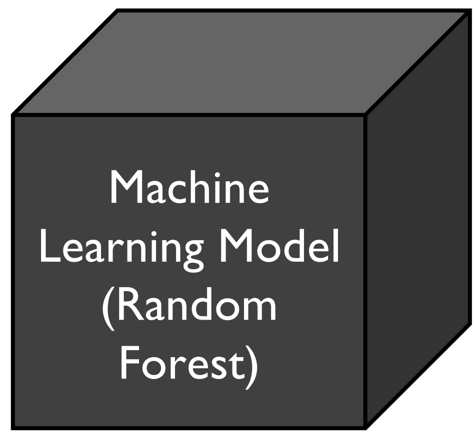
.
.
.

Graph theory is applied to extract structural (topological) properties of fracture networks.

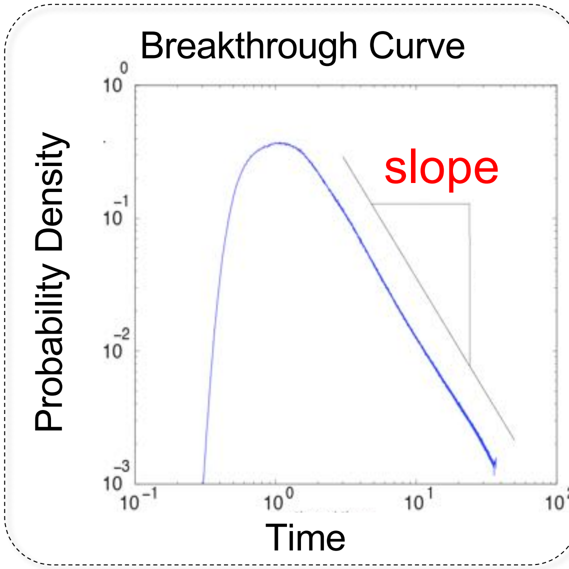
Machine learning-assisted identification of key structural properties governing transport processes

Input
(structural properties)

- Percentage of Dead-end fractures
- Fracture density
- Shortest path length
- Node connectivity
- Network Entropy …

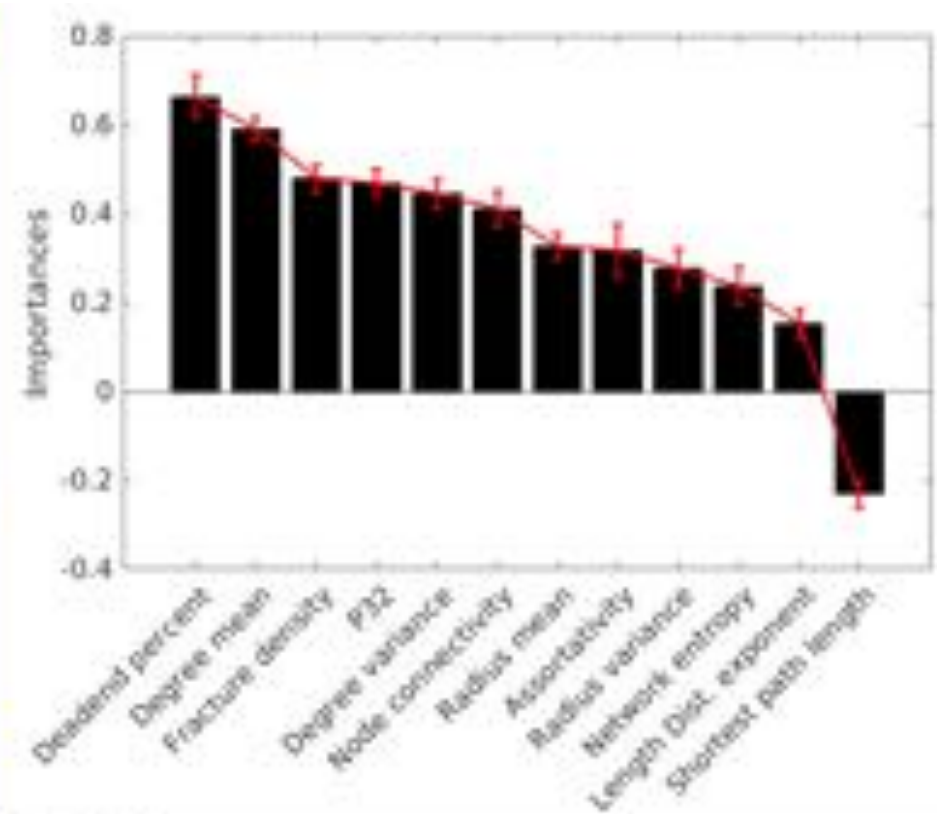


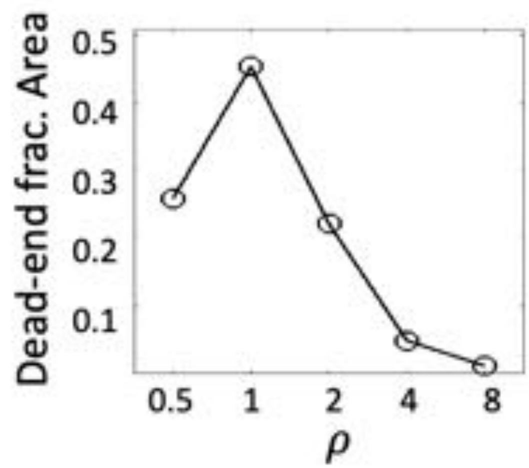
Output
(transport processes)

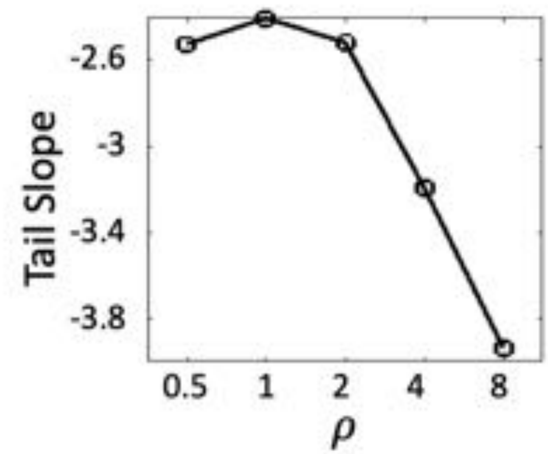


Quantifying importance of input properties using machine learning

Importance ranking using Random Forest





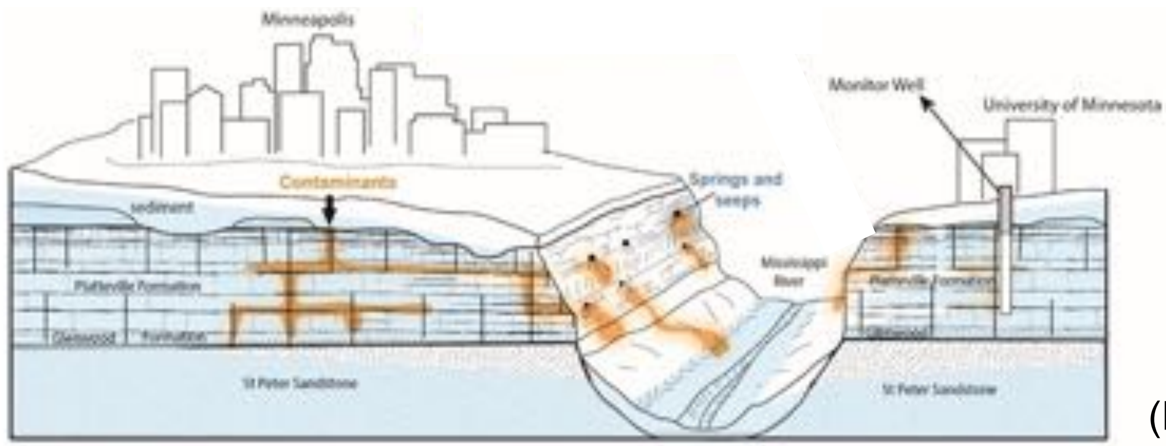


S. Yoon, J.D. Hyman, W. S. Han, and **P. K. Kang**, under review

Dead-end fracture is identified as the key structural property for predicting late-time tailing.

Part 3:
Characterizing and predicting transport processes at a fractured aquifer site

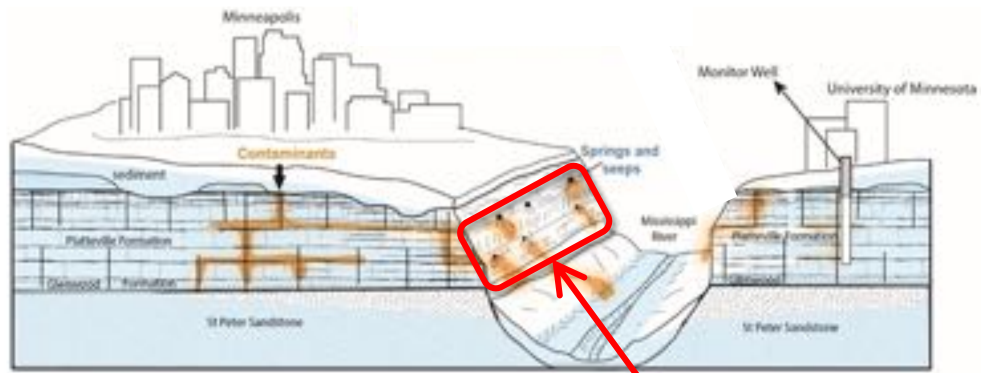
Contaminated Fractured Limestone Site on UMN campus



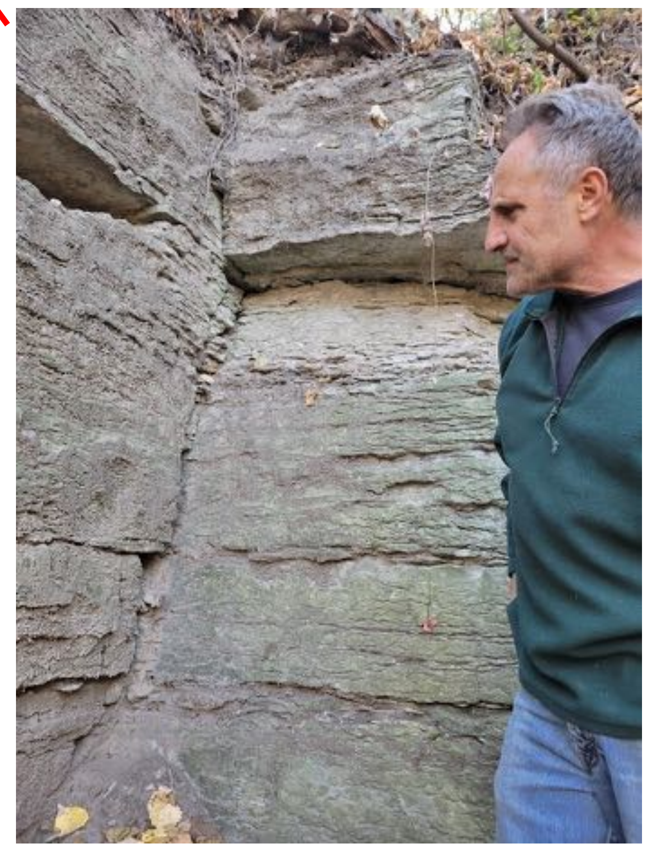
(Runkel et al., 2019)

15 min walking distance from Earth Sciences building

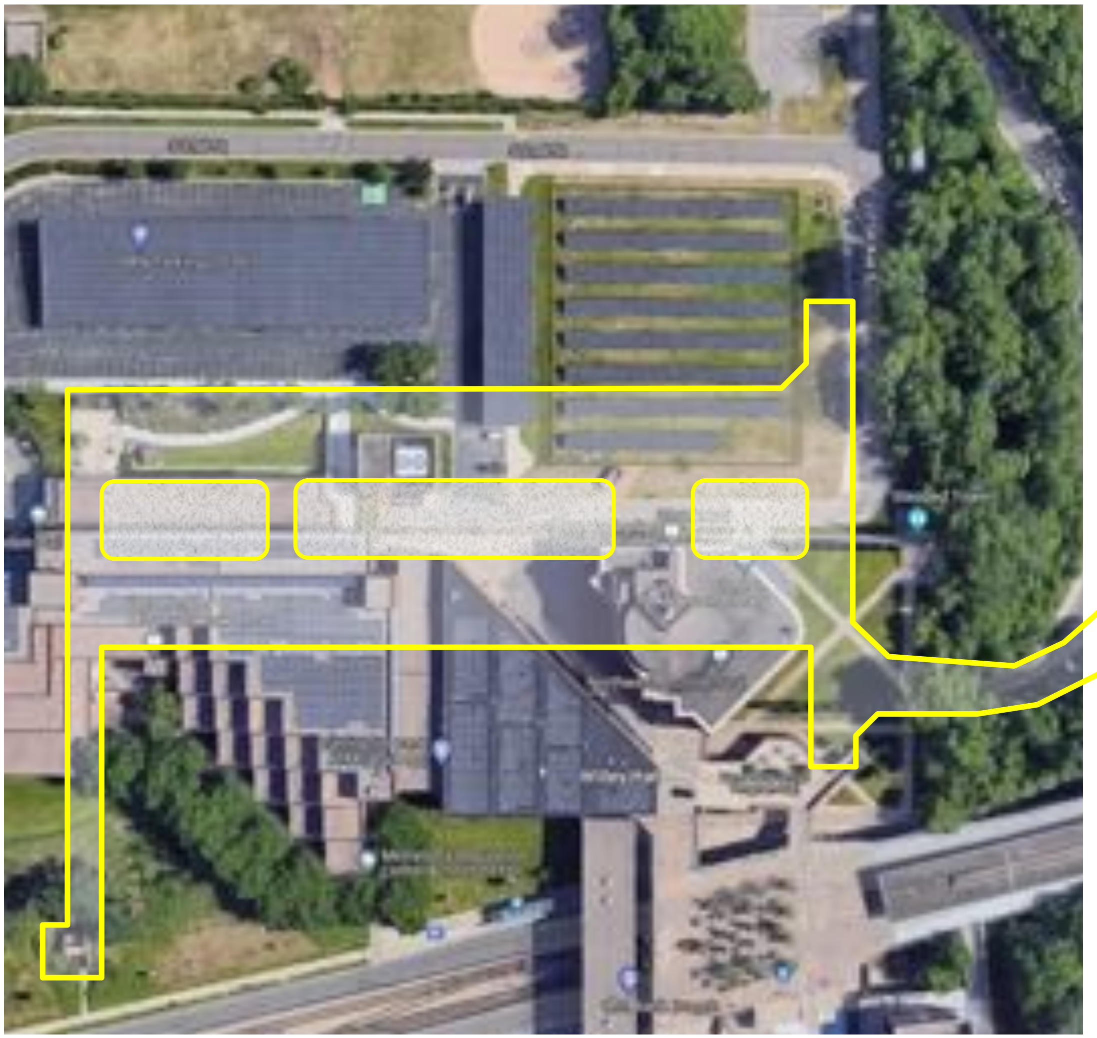
Fracture outcrop data is abundant near the site

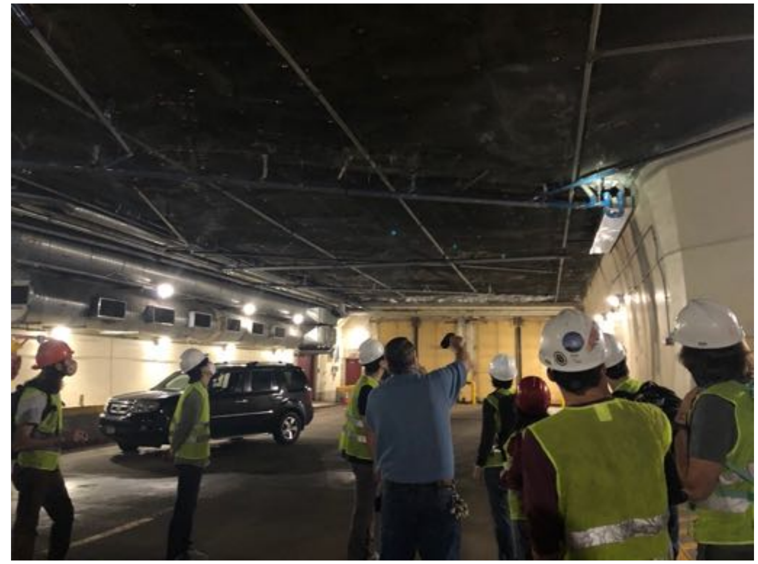


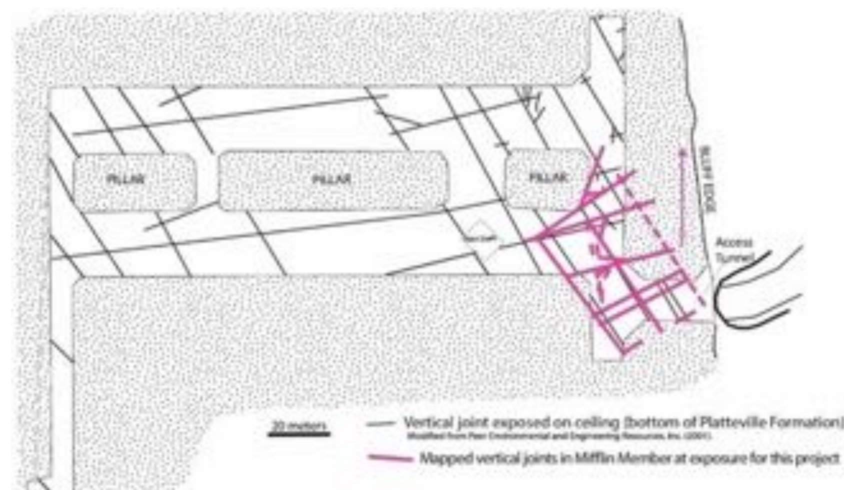
(Runkel et al., 2019)



Fracture outcrop data is available from multiple locations

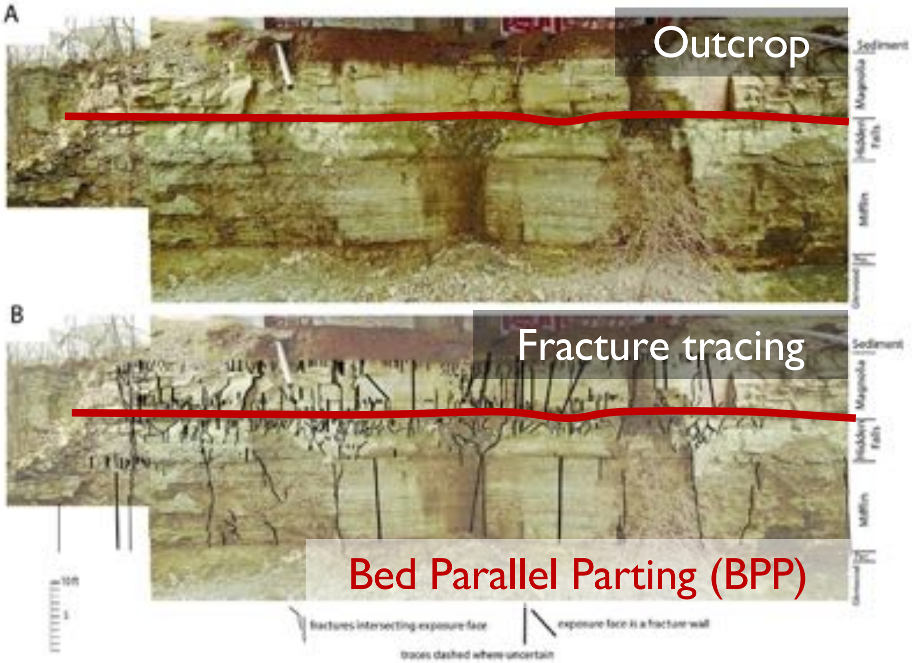




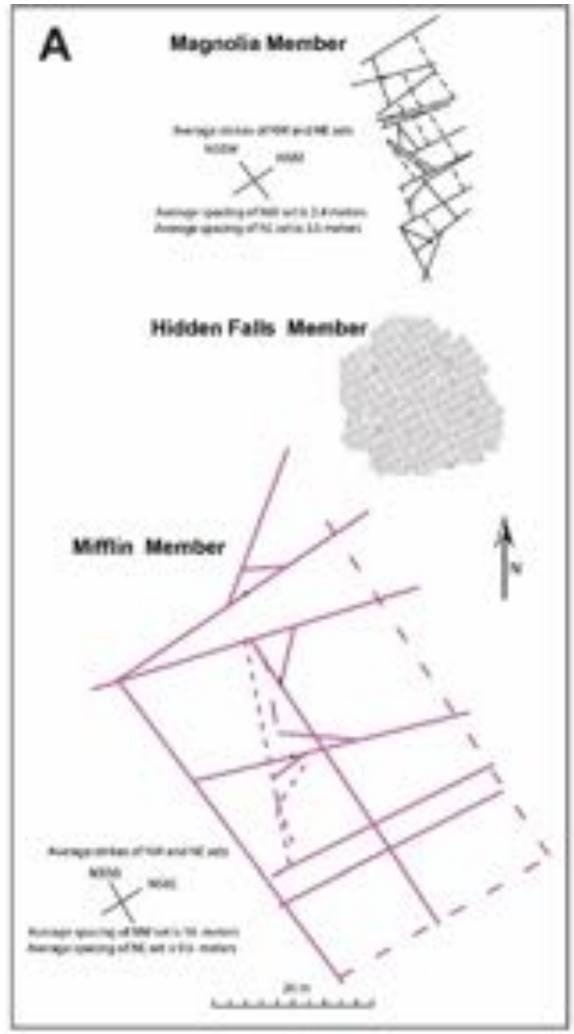


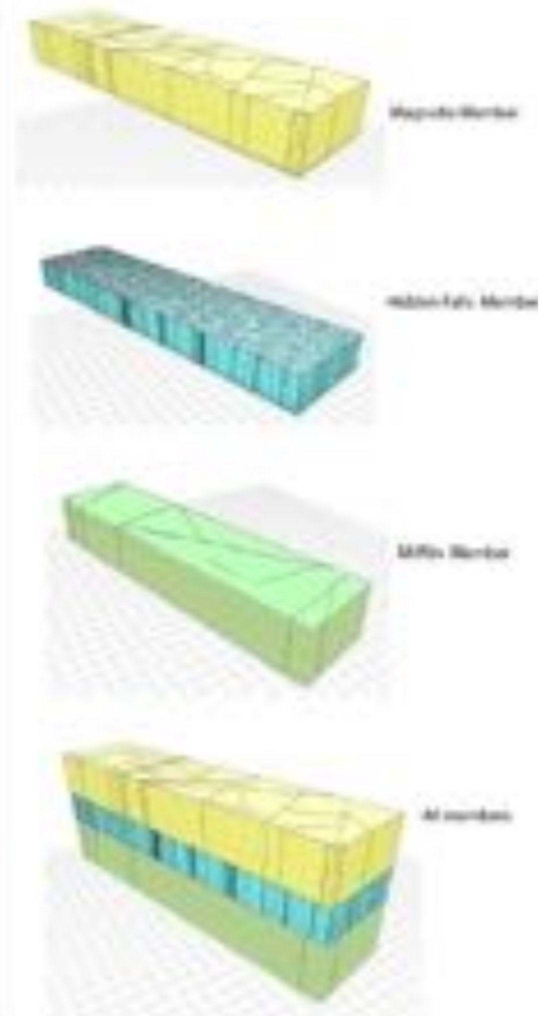
(Runkel et al., 2019)

Detailed fracture outcrop characterization in collaboration with MGS



(Runkel et al., 2019)

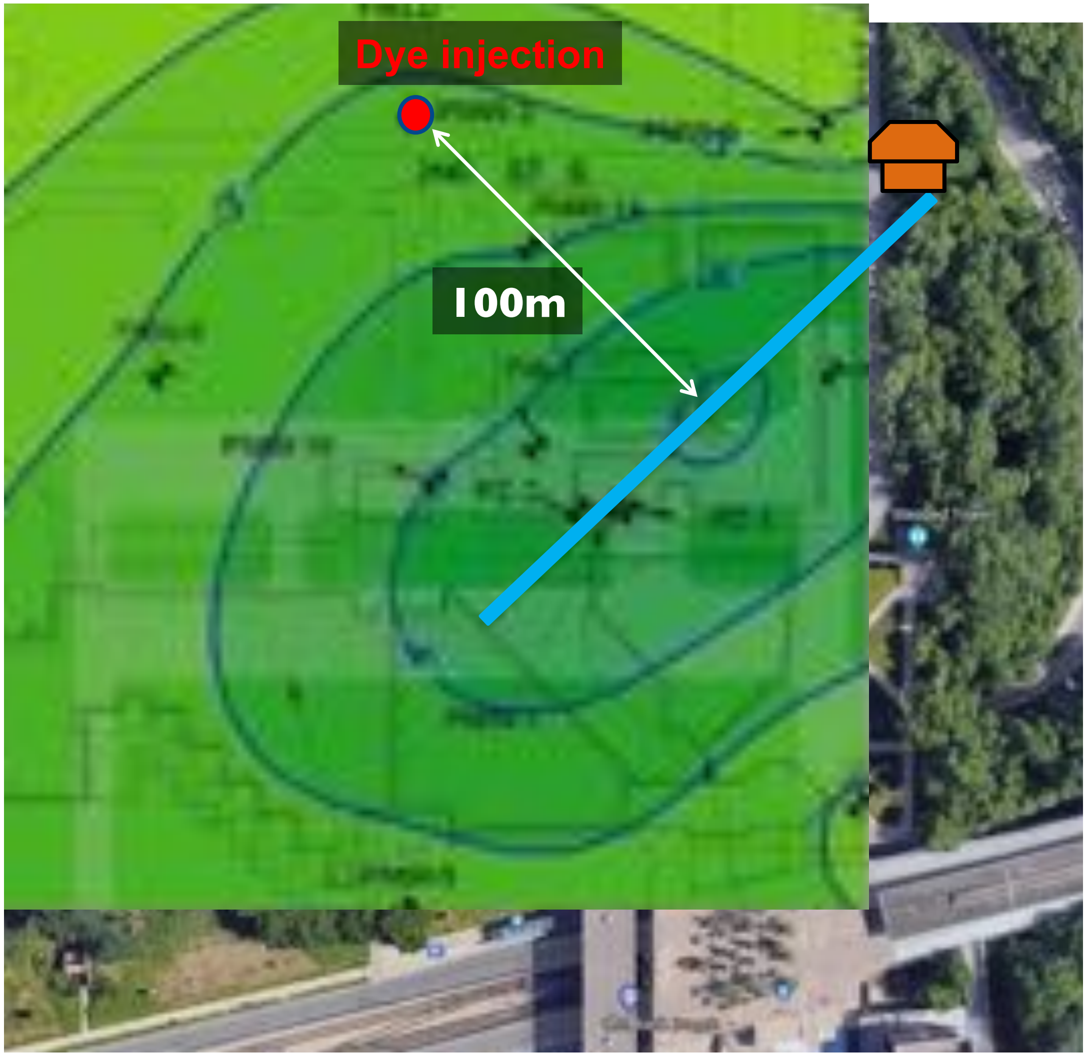




Horizontal well is under operation at the site

460-ft (140 m) long,
6–in (0.15 m) diameter

Tracer experiments are conducted at the site

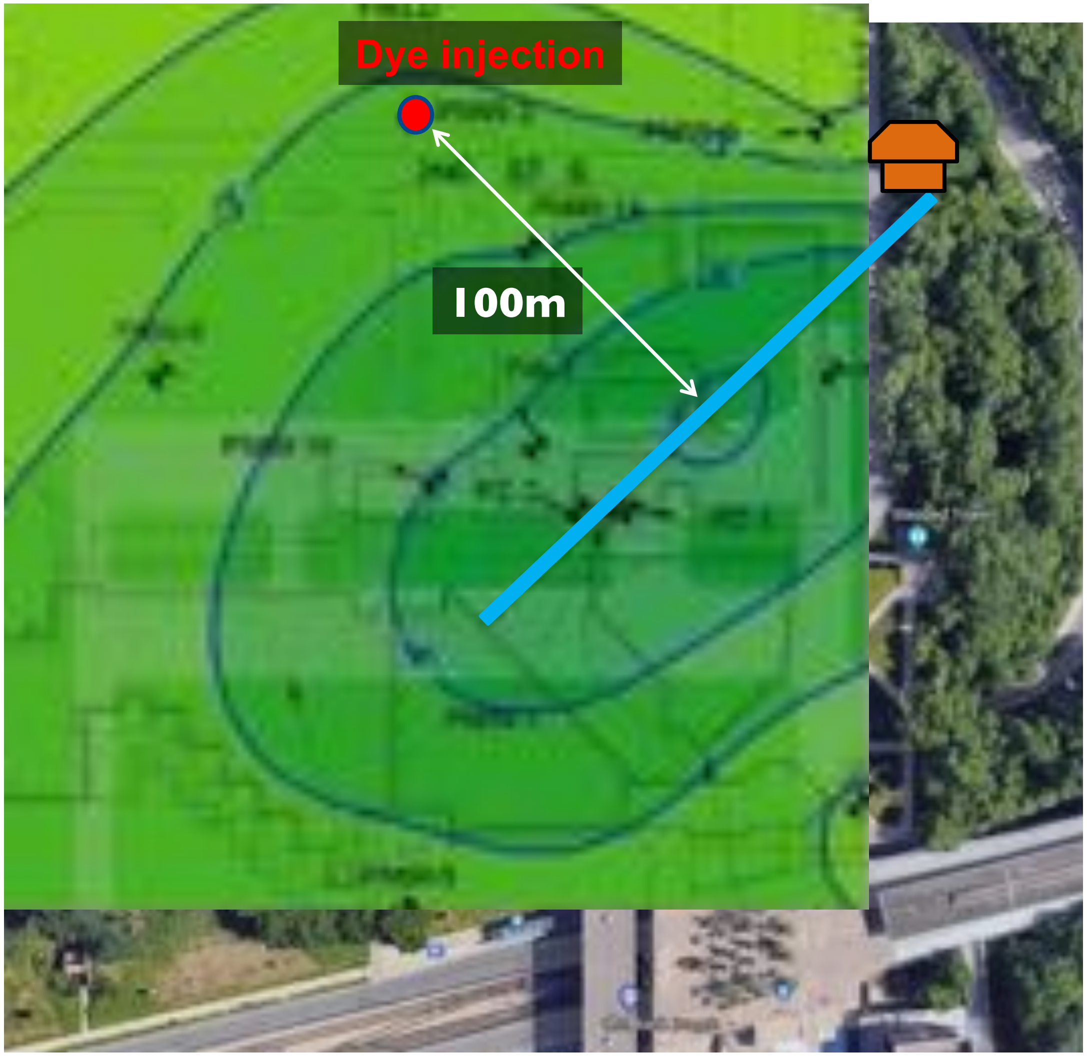


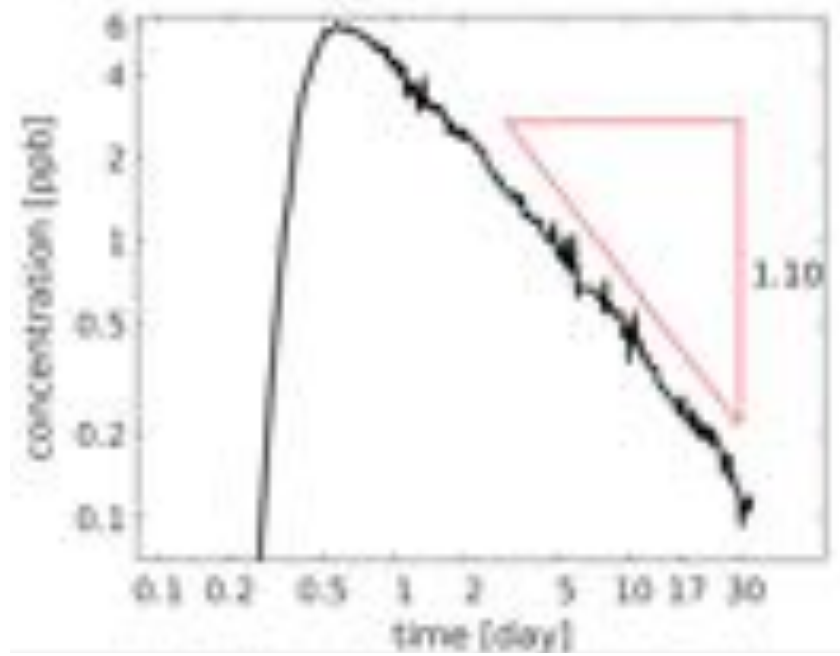
Tracer injection (fluorescein)

Water sampling

Dye tracing in collaboration with Scott Alexander, Calvin Alexander.
Collaboration with Bay West.

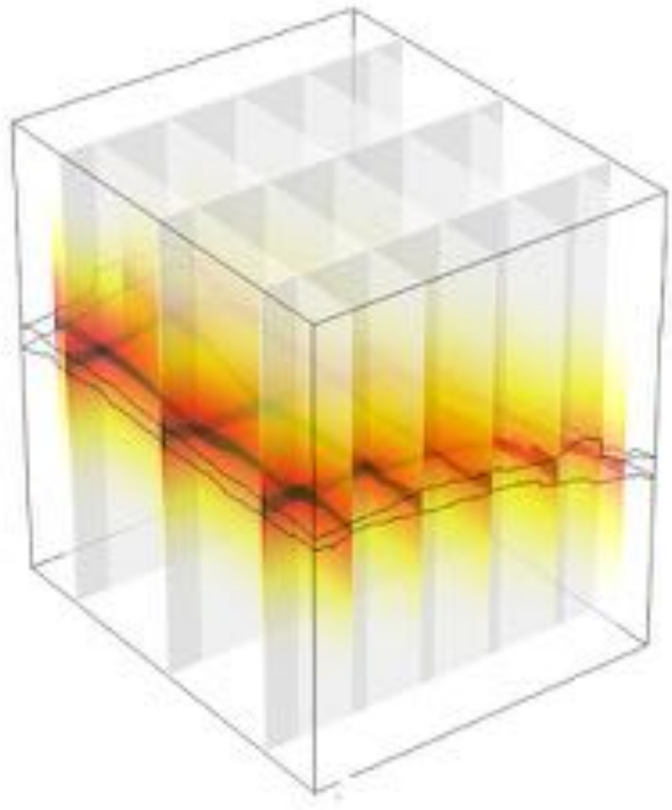
Strong power-law tracer tailing with slope ~1 is observed

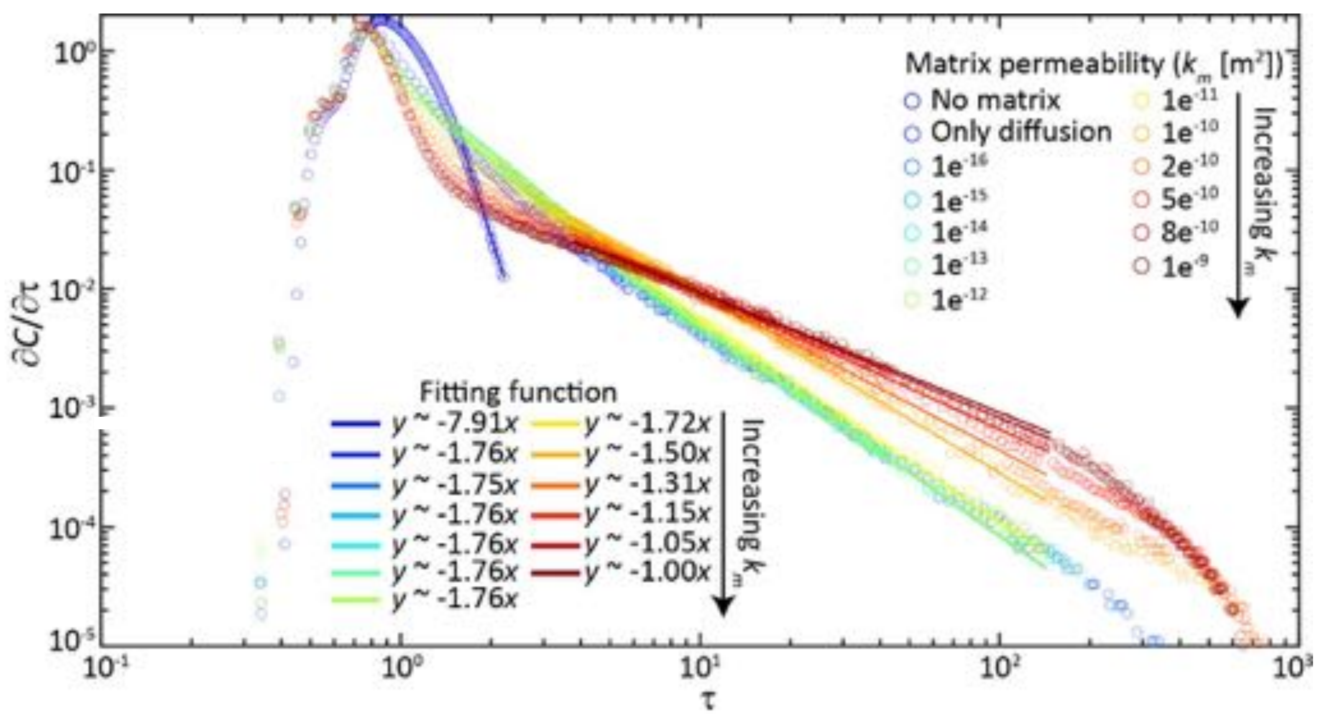




Hypothesis: Interaction between main fracture flow paths and surrounding rock matrix

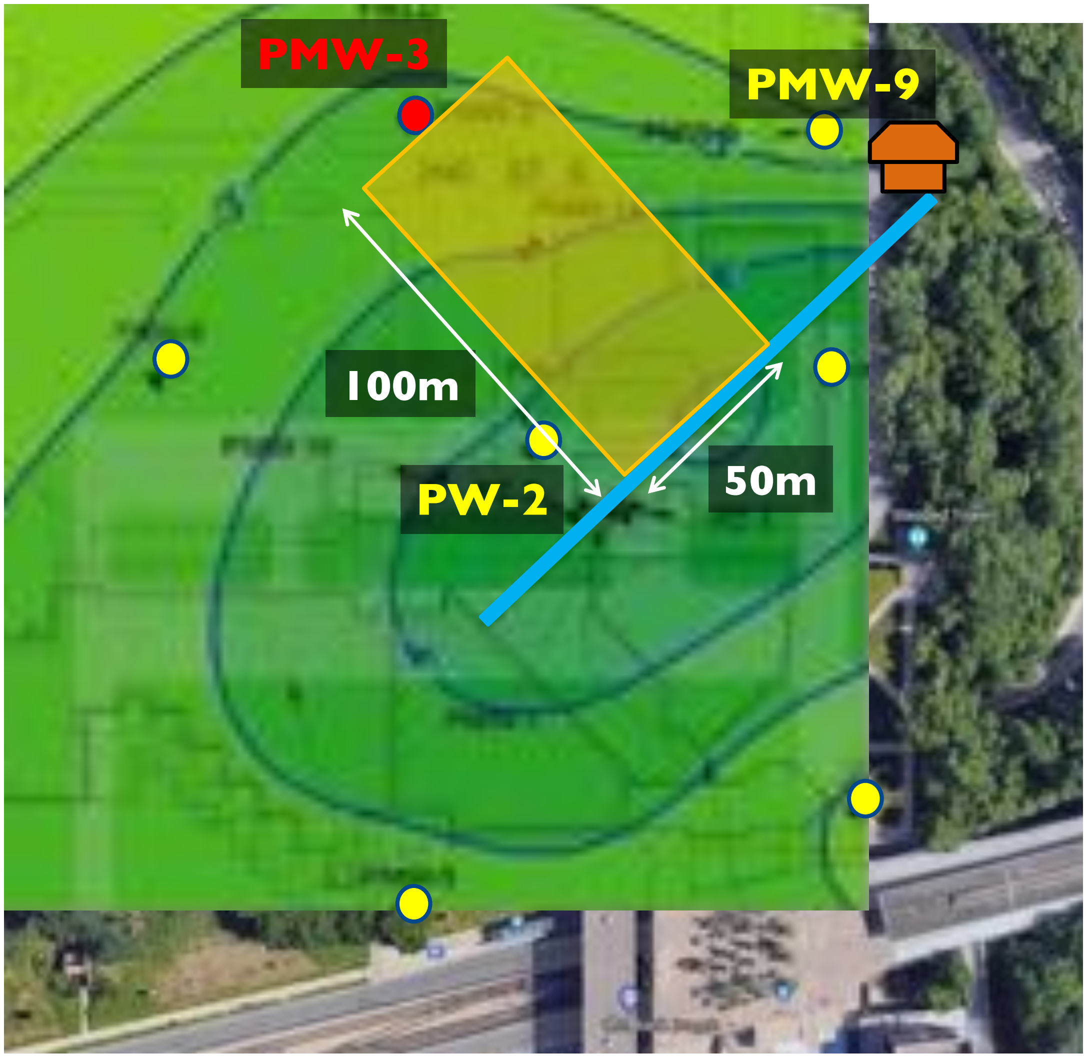
Increase in matrix permeability is shown to cause strong tailing



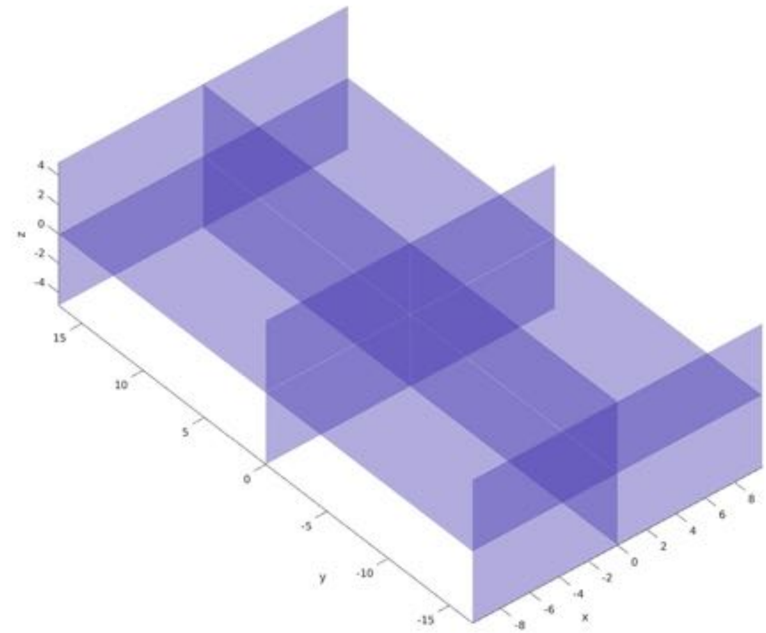


L. Wang, S. Yoon, L. Zheng, T. Wang, X. Chen, and P. K. Kang, under review.

Flow and transport modeling of the fractured aquifer



Domain size: 100m x 50m x 12m



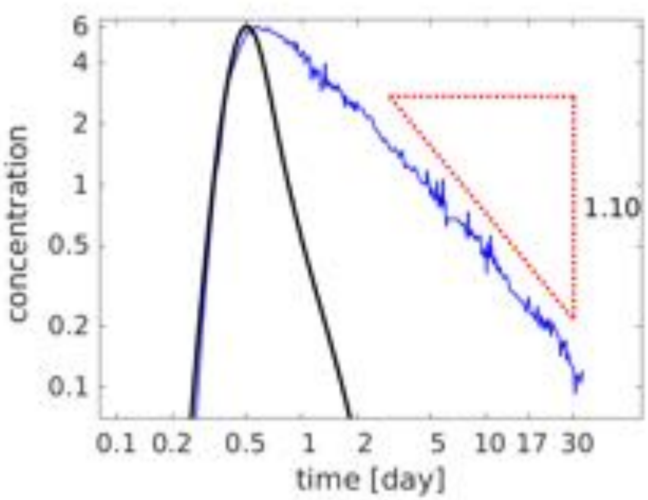
DFNWORKS DISCRETE FRACTURE NETWORK

PFLOTRAN

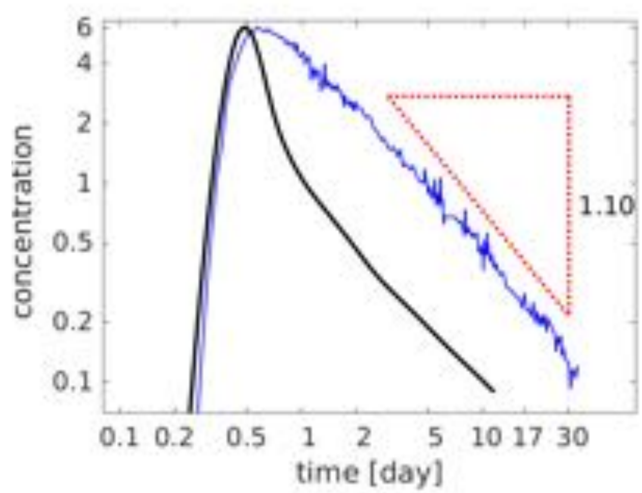
A Massively Parallel Reactive Flow and Transport Model for describing Subsurface Processes

Sensitivity Analysis Results (Matrix Permeability & dispersivity)

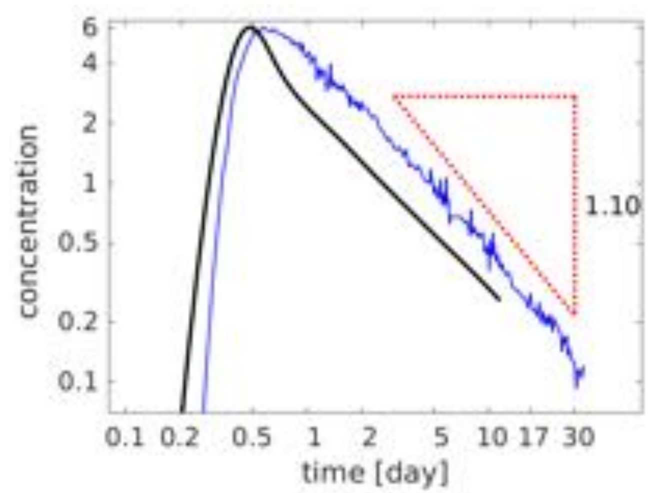
Low matrix permeability (10^{-14})
Longitudinal dispersivity $\alpha_L = 0.1$



High matrix permeability (10^{-11})
Longitudinal dispersivity $\alpha_L = 0.1$

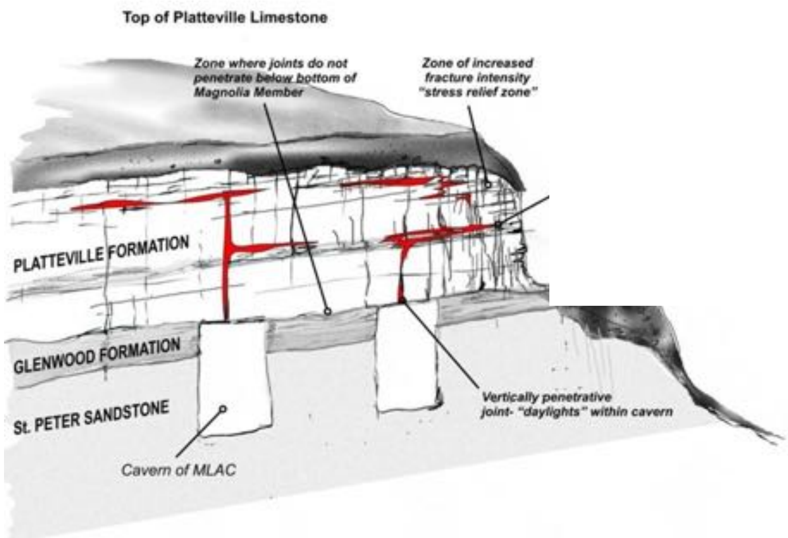


High matrix permeability (10^{-11})
Longitudinal dispersivity $\alpha_L = 1$

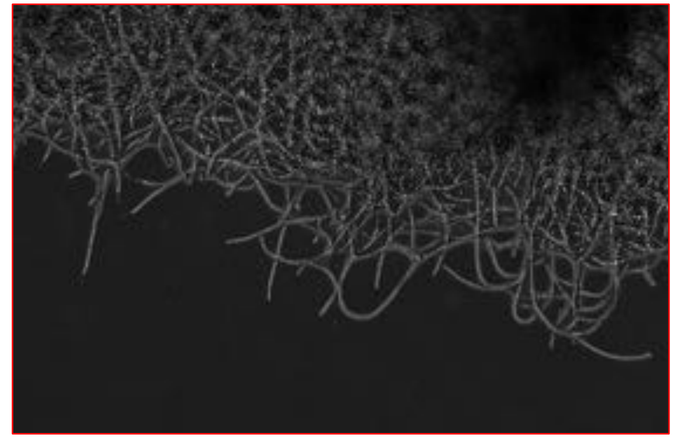


Detailed site characterization is ongoing in collaboration with MGS.

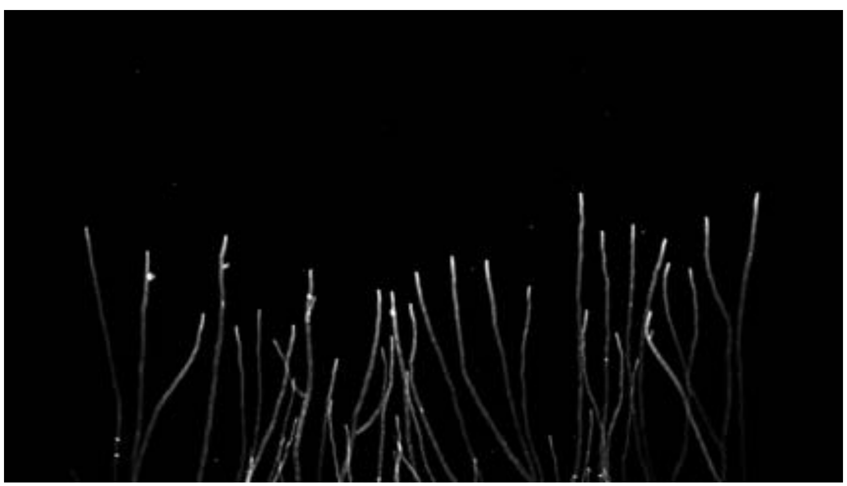
Fungi-enhanced remediation of contaminated fractured aquifer sites



Fungi isolated from the site

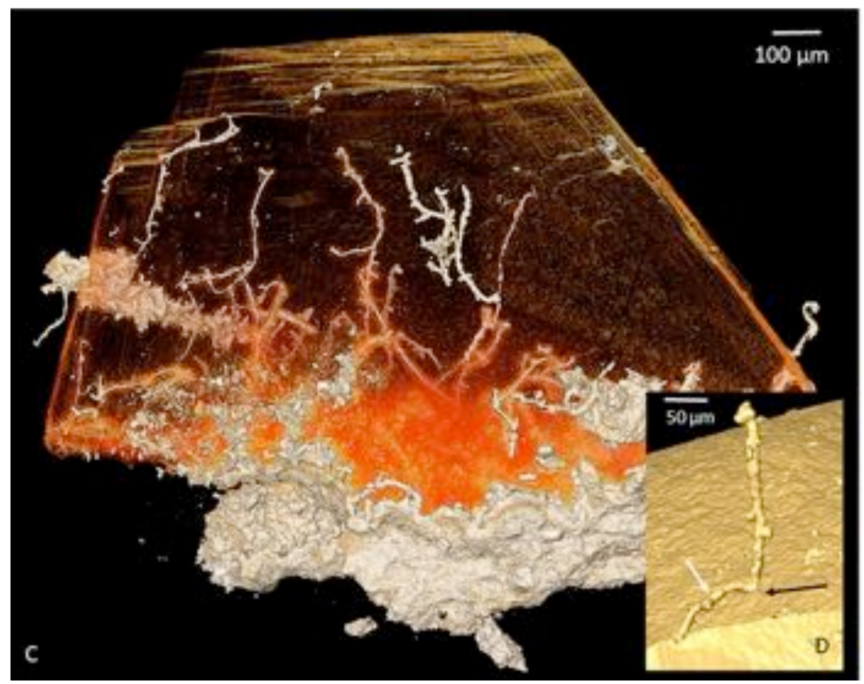


Fungal appressorium is shown to produce pressure up to 200 bar



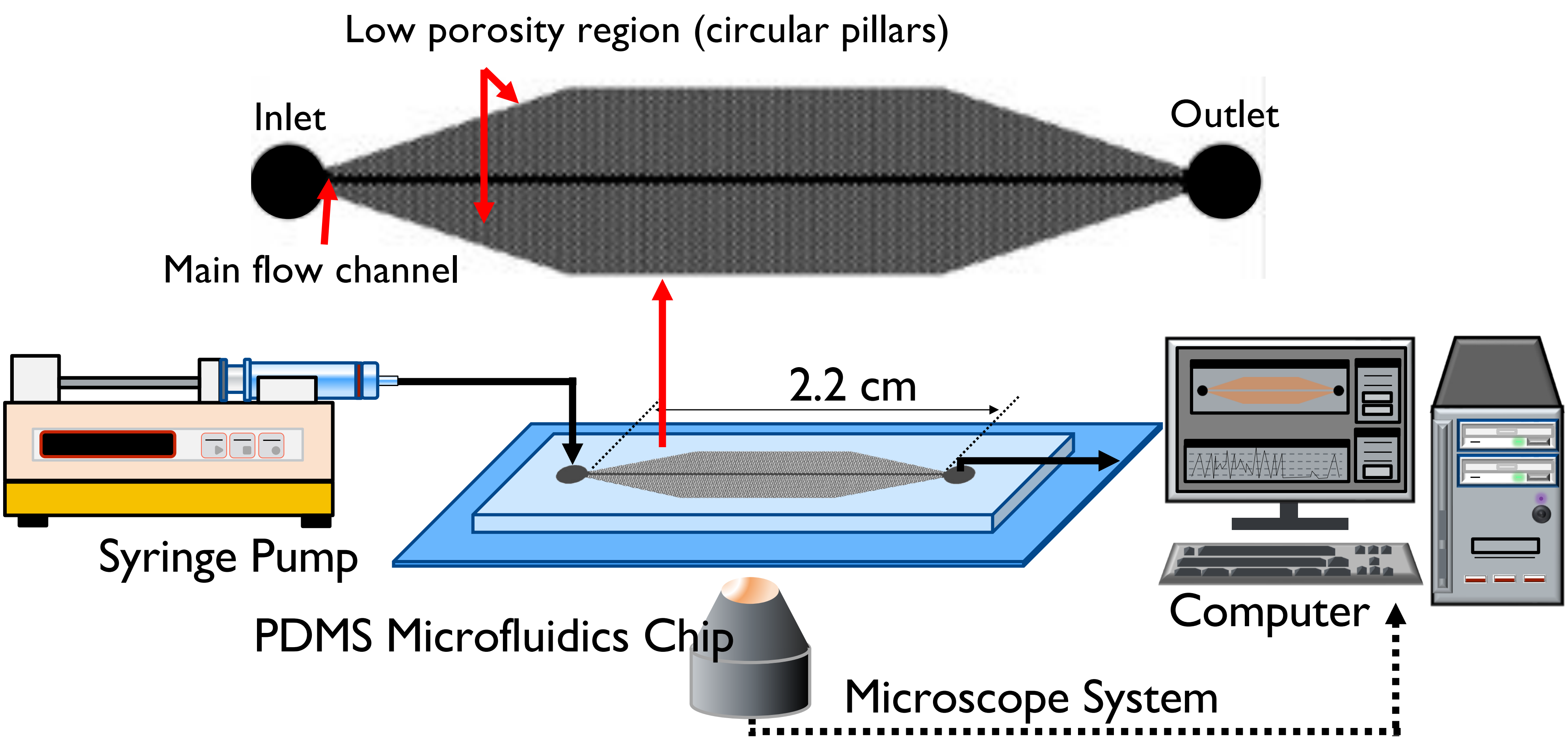
Hoffland, et al (2004). Frontiers in Ecology and the Environment

Hyphae penetration into zeolite

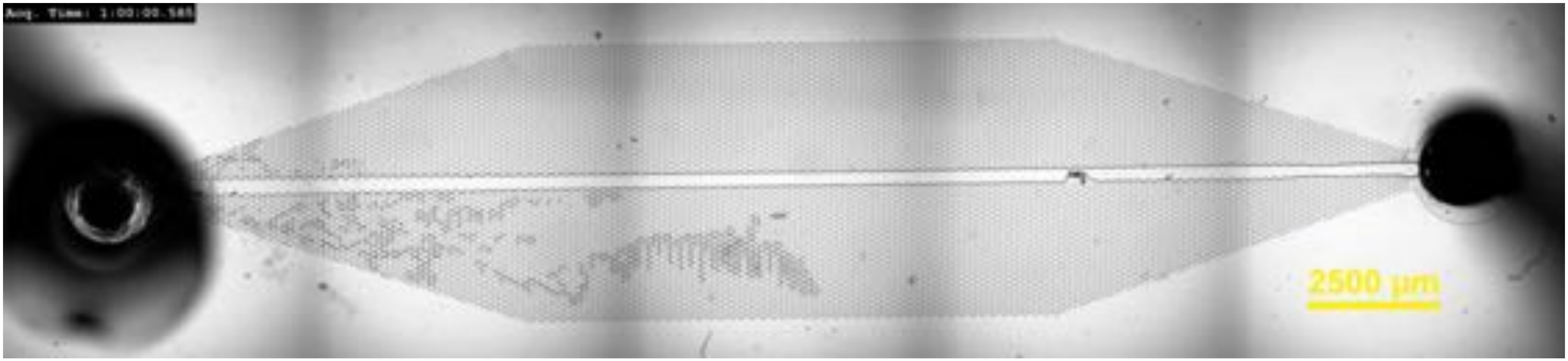


Ivarsson et al (2020). BioEssaysz

Method: Microfluidics system



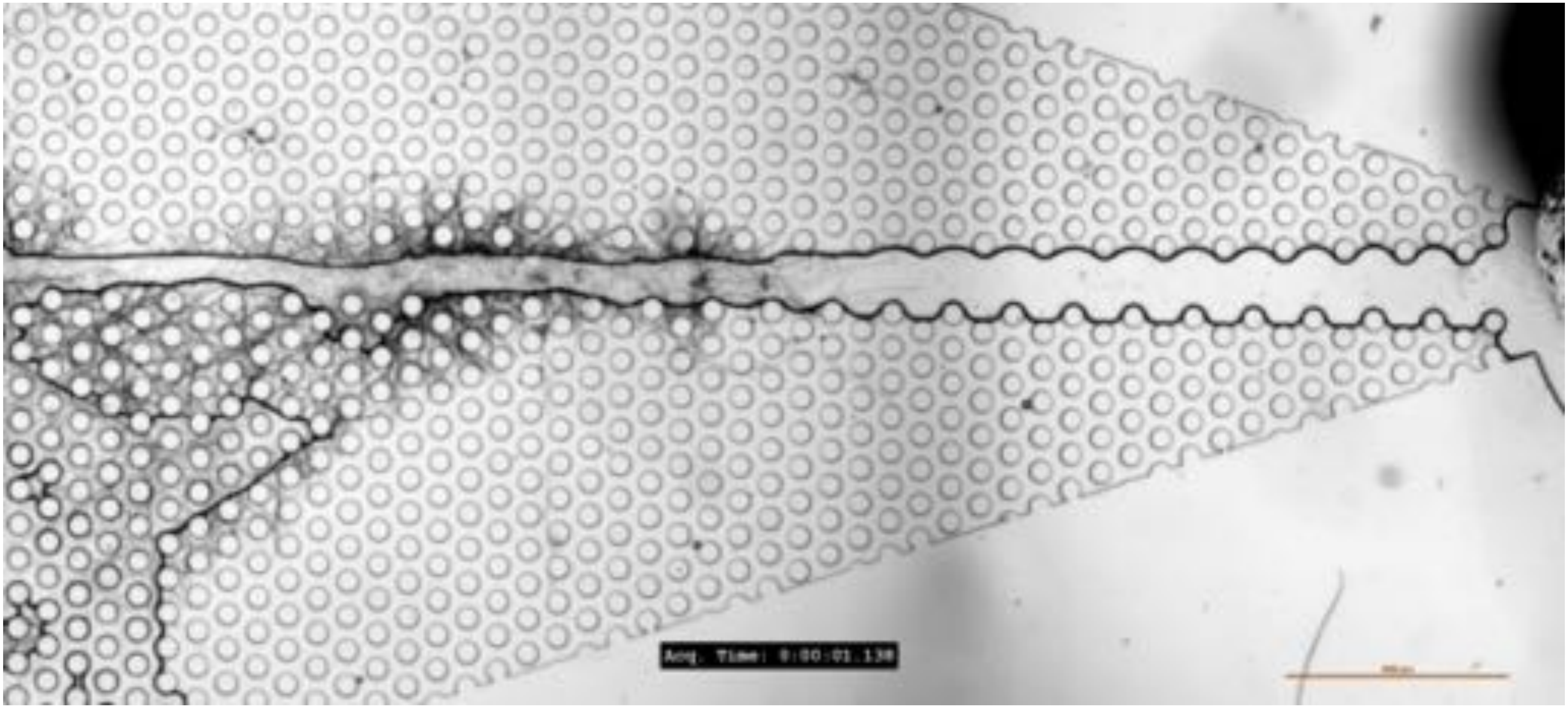
Result: continuous flow over 65 hours



Close-up:

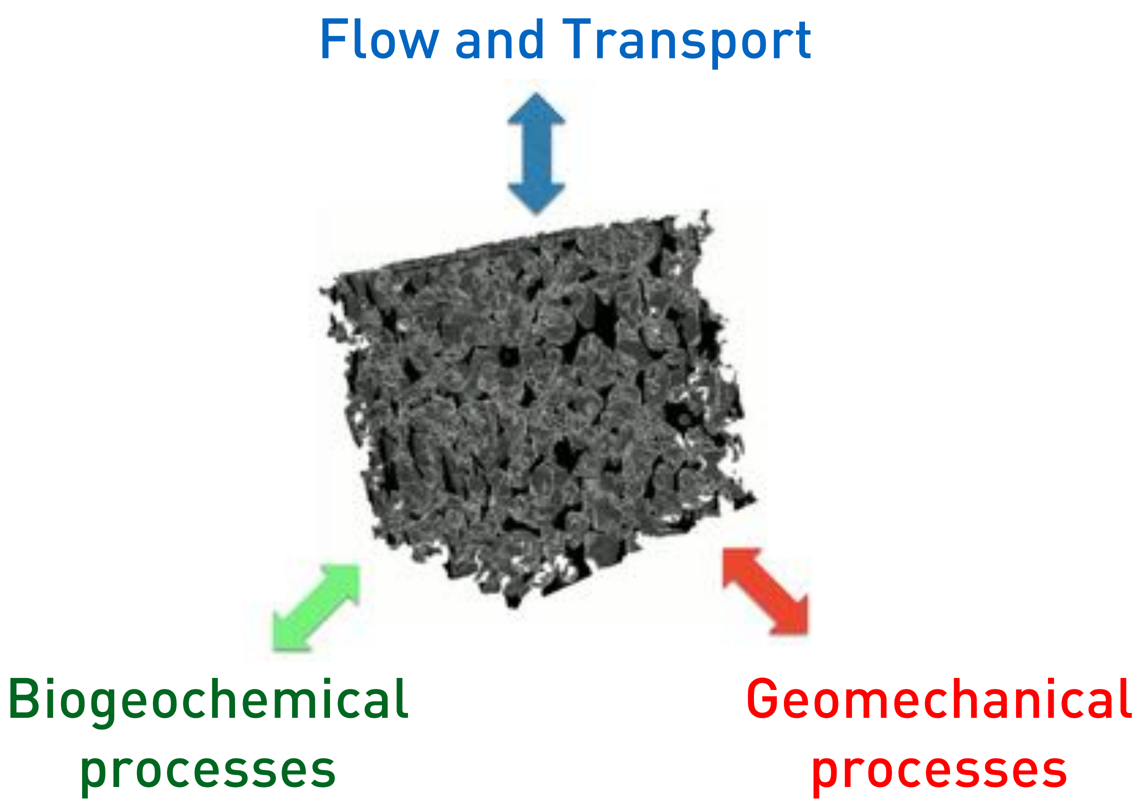
Pore clogging and pressure build-up
→ Pore invasion

Result: When flow is slow



Key Messages

- 3D & Inertia effects can fundamentally change transport, mixing, and reaction dynamics in fractured porous media.
- Machine learning and high-performance computing are opening up new possibilities for predicting transport processes.
- Strong need for better understanding coupled processes involving biogeochemical processes and field-based demonstration.



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3M Non-Tenured Faculty Award

ACS PRF Doctoral New Investigator Award

University of Minnesota College of Science & Engineering

MnDRIVE Environment

Questions?

Contact: pkkang@umn.edu