PERC Petroleum Research Center

Reactive Transport Models with Geomechanics to Mitigate Risks of CO2 Utilization and Storage

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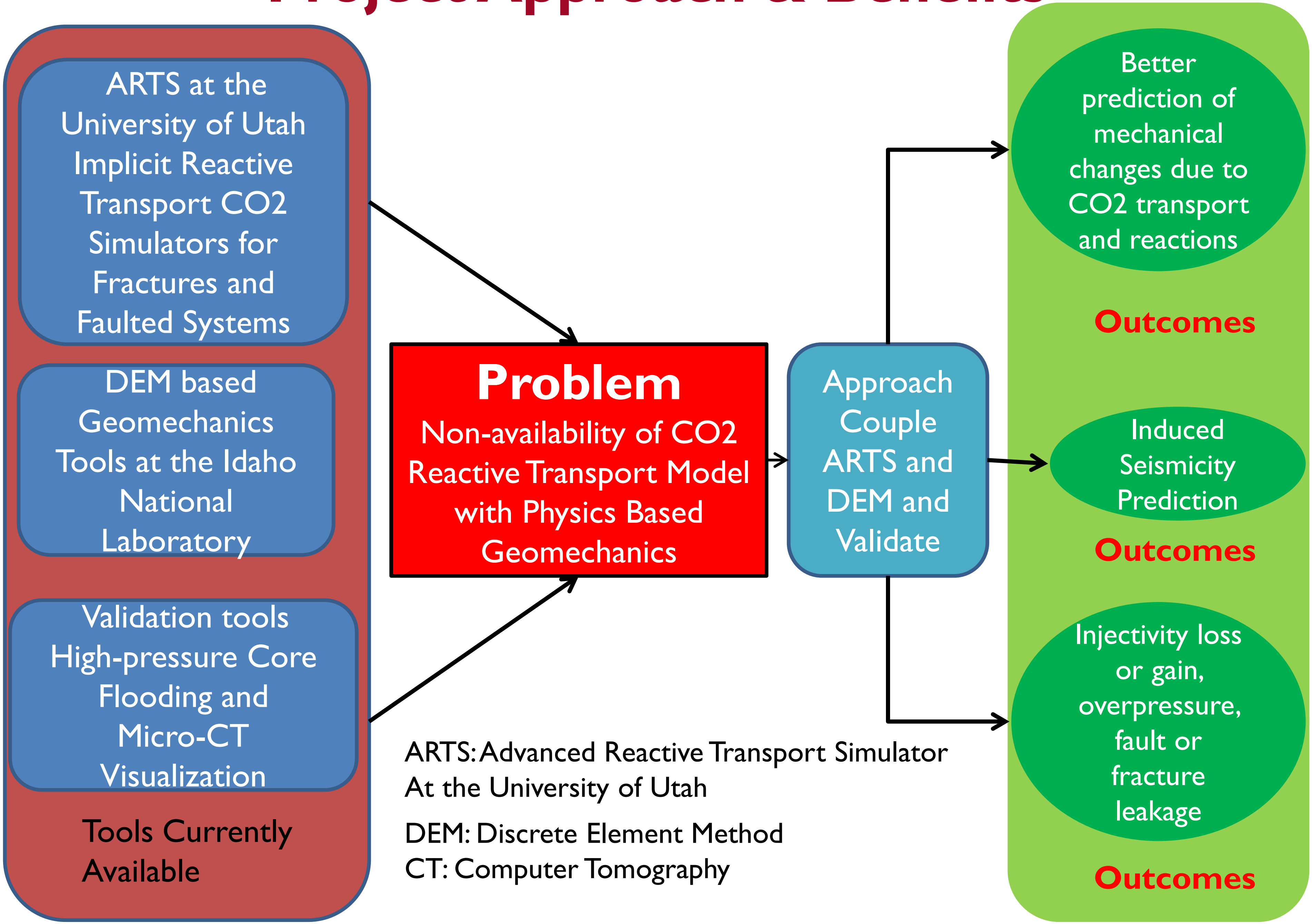
INL Idaho National Laboratory

Carbon Dioxide Sequestration

- Large scale injection of CO_2
- Mechanisms: trapping, dissolution, carbonation
- Is safe storage of large amounts of CO_2 feasible?
- Risks
  - Overpressure
  - Leaks
  - Mechanical integrity of the seals
  - Induced seismicity
- Extensive work and publications on each and every aspect

Integrated, physics-based, geochemical and geomechanical model capable of predicting fracturing and slipping of natural fractures

Project Approach & Benefits



ARTS at the University of Utah Implicit Reactive Transport CO2 Simulators for Fractures and Faulted Systems

DEM based Geomechanics Tools at the Idaho National Laboratory

Validation tools High-pressure Core Flooding and Micro-CT Visualization

Tools Currently Available

Problem

Non-availability of CO2 Reactive Transport Model with Physics Based Geomechanics

Approach Couple ARTS and DEM and Validate

Better prediction of mechanical changes due to CO2 transport and reactions

Outcomes

Induced Seismicity Prediction

Outcomes

Injectivity loss or gain, overpressure, fault or fracture leakage

Outcomes

ARTS: Advanced Reactive Transport Simulator At the University of Utah

DEM: Discrete Element Method

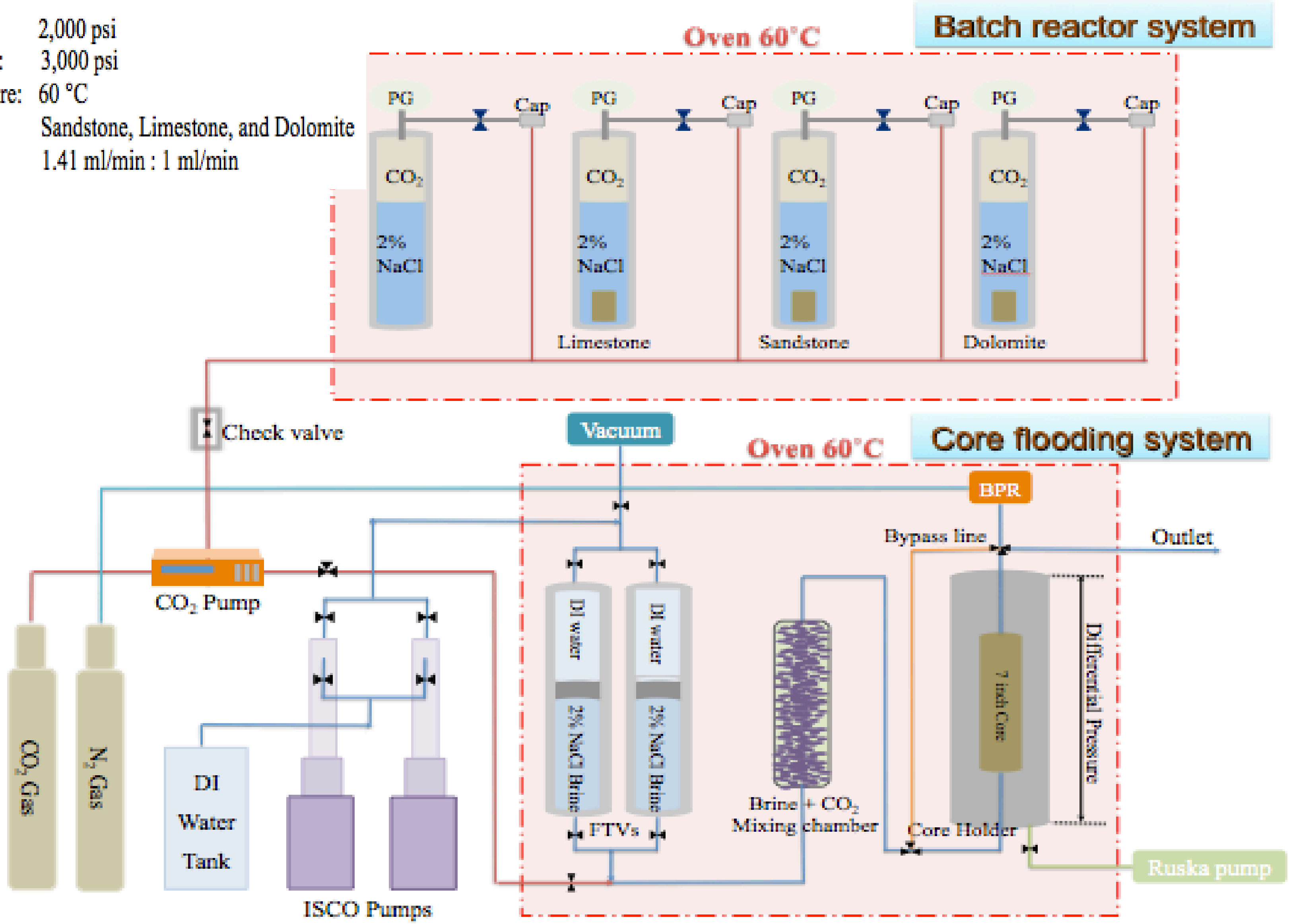
CT: Computer Tomography

Project Scope

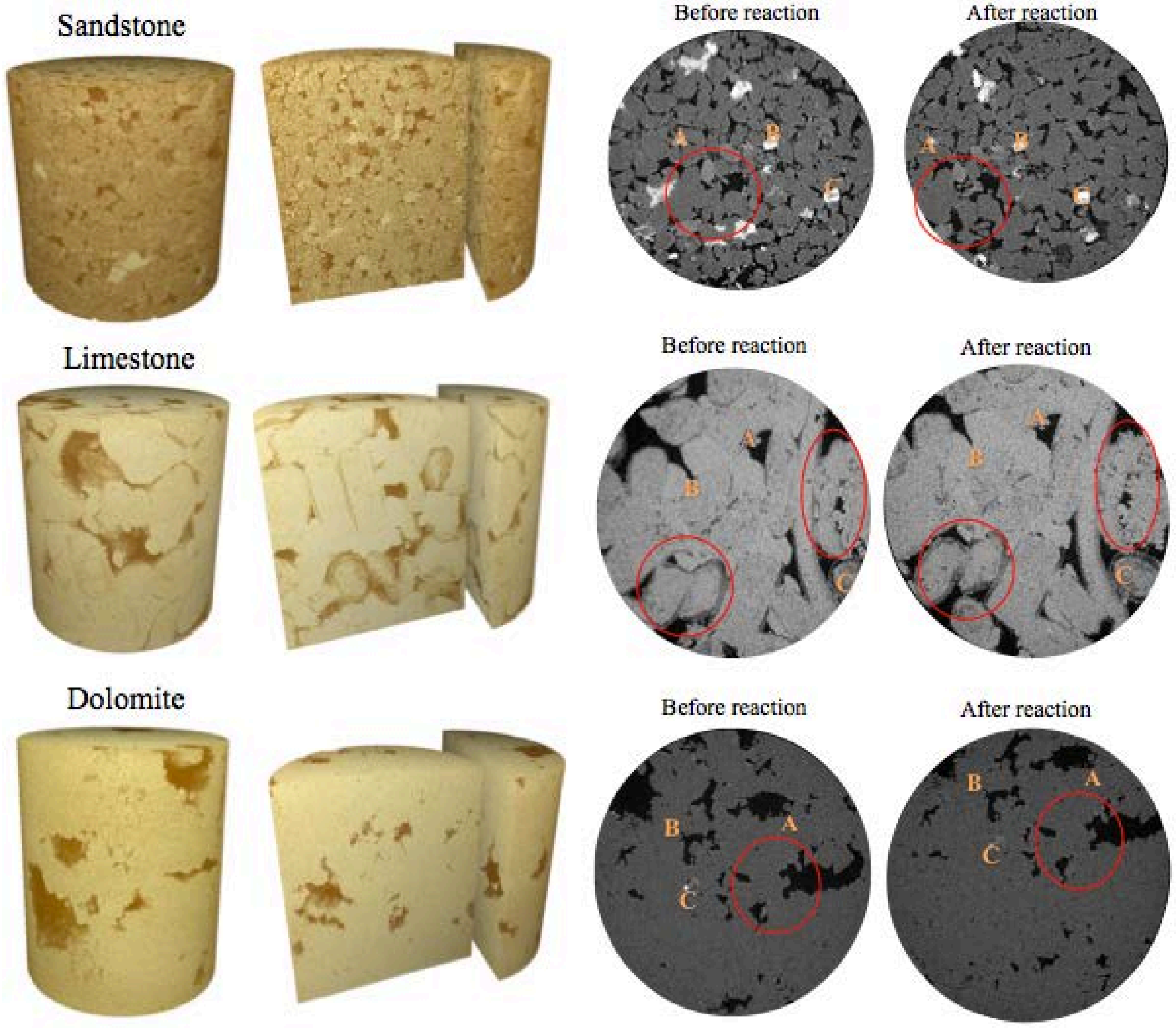
- Experimental study for model validations
  - Corefloods
    - Three possible mineralogies, sa
    - Characterization using XRD, ICP-MS
  - High-resolution micro computed tomography
- Modeling
  - Multiphase reactive transport simulator – ARTS
  - Discrete-element model (DEM) for geomechanics from INL
  - Different coupling schemes: fully coupled vs. sequential coupling

Experiments on Reactions

Core Pressure: 2,000 psi
Confining Pressure: 3,000 psi
Reaction temperature: 60 °C
Cores (7"): Sandstone, Limestone, and Dolomite
CO_2 : Brine: 1.41 ml/min : 1 ml/min



Micro-CT Imaging



Batch Results – ICP MS

All concentrations in mg/Kg

	Na	Mg	Si	Cl	K	Ca
LoD	2	0.004	400	2	7	13
Blank	878	0.21	<400	1211	<7	<13
Sandstone	901	45.9	<400	1251	34	154
Limestone	878	9.8	<400	1229	8	571
Dolomite	861	182.5	<400	1233	10	302

Limestone and dolomite show dissolution

Experimental Conclusions

- Significant visible dissolution with increased porosities in limestone and dolomite
- Lesser dissolution in sandstone – still visible in micro-CT
- ICP-MS results confirm the dissolution findings
- XRD values before and after do not show significant changes

Multiscale Reactive Transport Modeling and High-Performance Computing

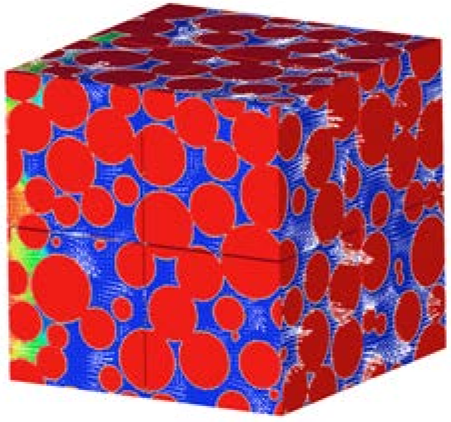
✓ Pore-scale reactive transport models developed at INL

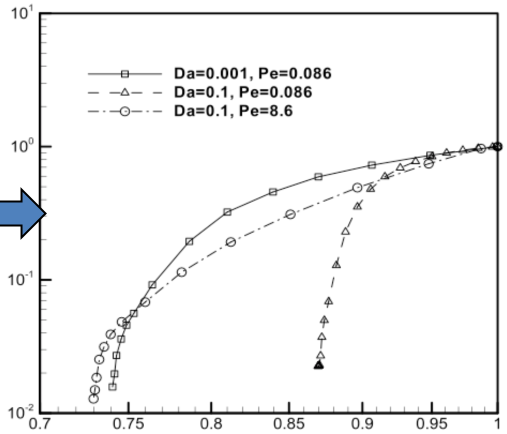
  – *Level set; Phase field; Smoothed particle hydrodynamics*

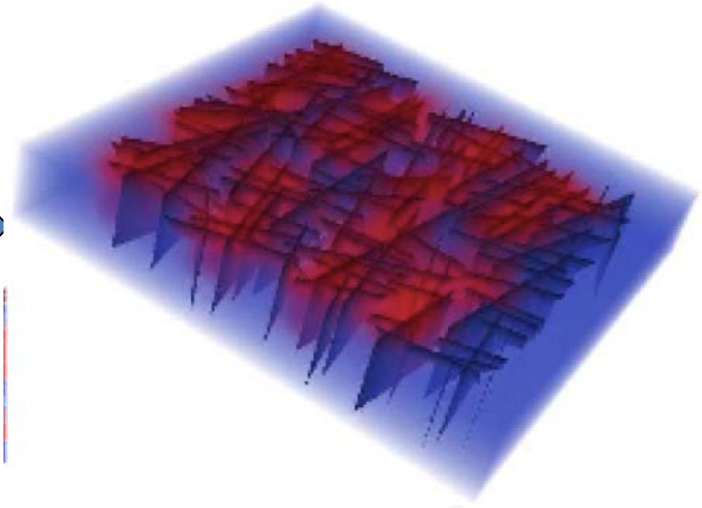
✓ Advanced reactive transport simulator (ARTS)

  ▪ *Fully coupled, fully implicit approach*

  ▪ *Massively parallel; Adaptive mesh refinement (AMR)*





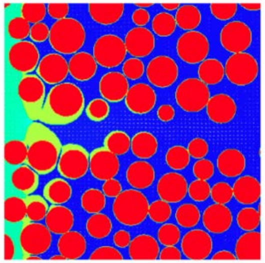


Pore-scale Reactive Transport Modeling

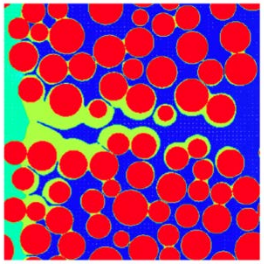
- ✓ Permeability-porosity evolution due to mineral precipitation/dissolution under different transport and reaction regimes

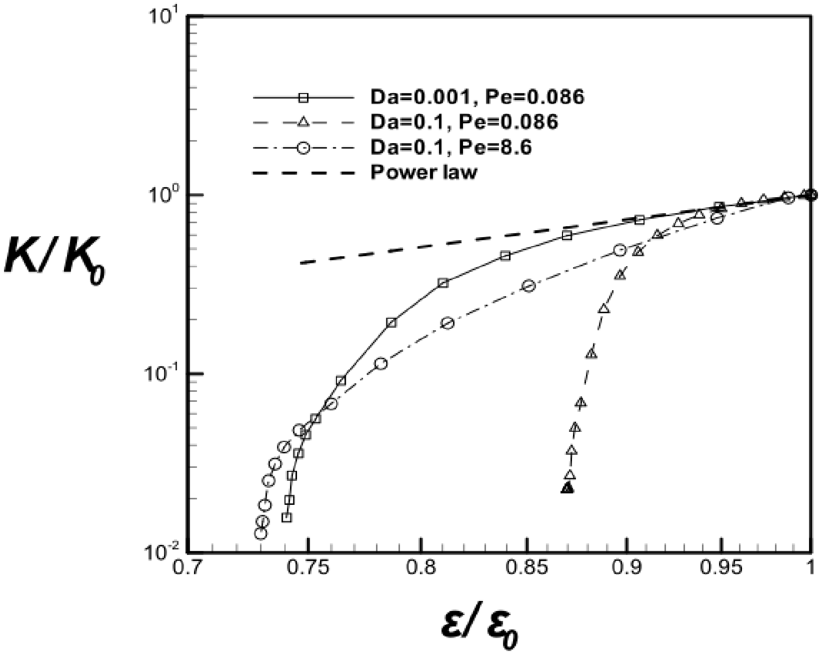
Diffusion dominated transport & slow reaction
Pe=0.086, Da=0.001

Diffusion dominated transport & fast reaction
Pe=0.086, Da=0.1

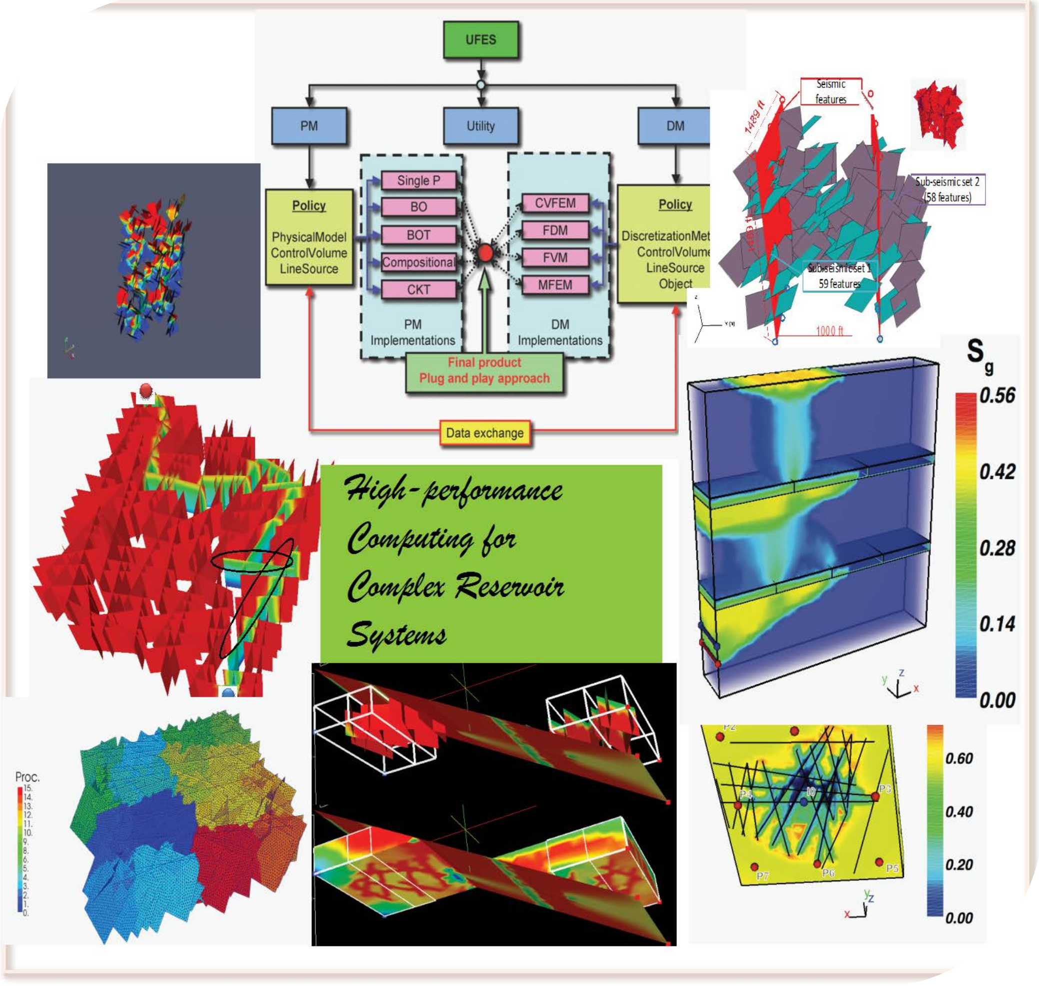


Advection dominated transort & fast reaction
Pe=8.6, Da=0.1





A Geochemical Simulator For Complex Geometries (DFN)

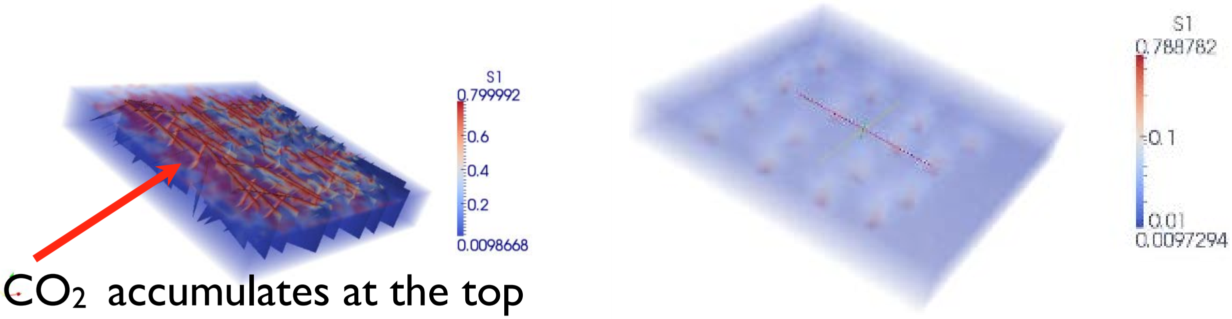


- A fully implicit non-isothermal geochemistry compositional simulator
- Unstructured mesh
- Different discretization and fracture representation methods
- Verification and validation
- Applications and parallelization performance evaluation

Coupled DFN-Porous Matrix Results

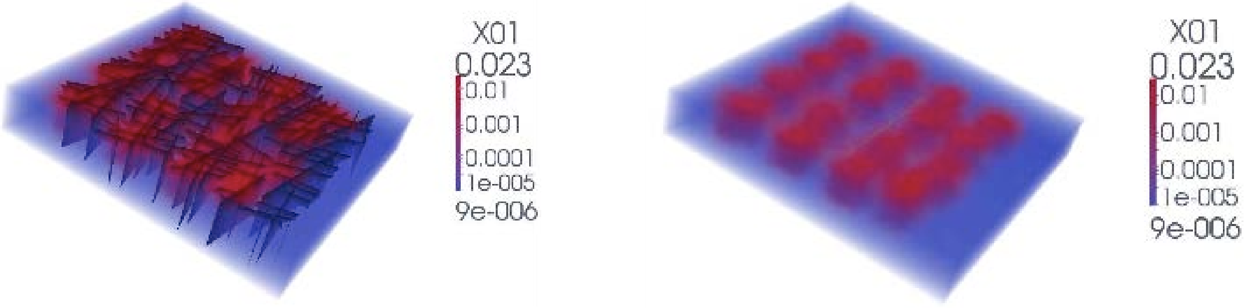
–The fracture/fault effect: fracture network case

Free and dissolved CO_2 distribution at 100 days with or without fracture network



Almost all free CO_2 accumulates at the top due to channeling through fractures.

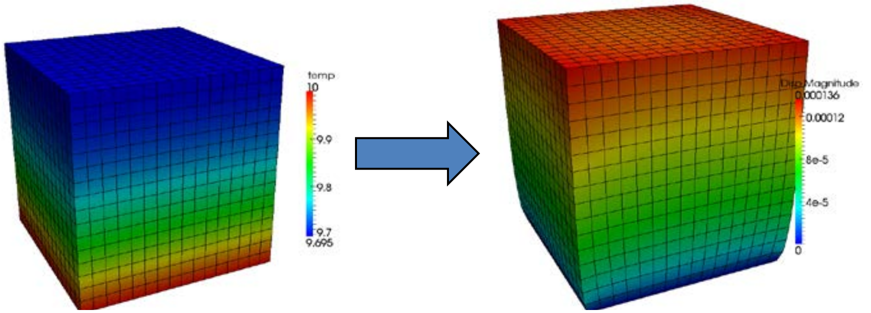
Free CO_2 distribution with or without fracture network



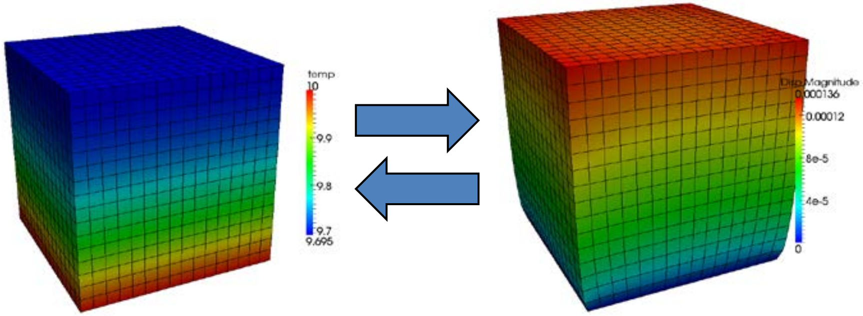
Dissolved CO_2 distribution with or without fracture network

Numerical Modeling of Coupled Processes

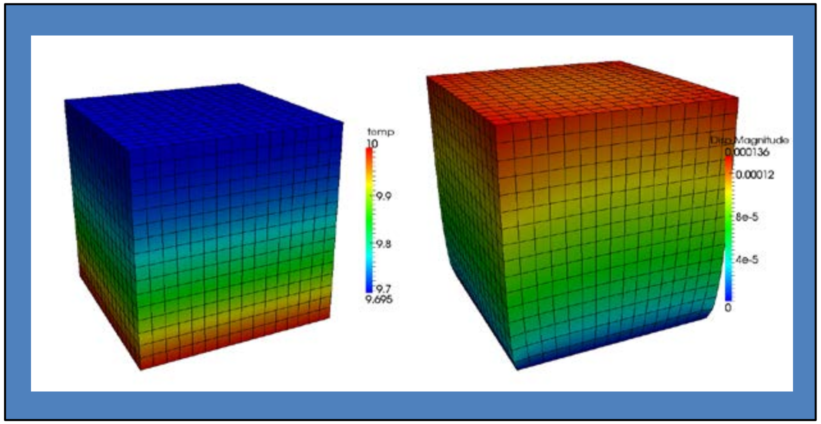
- Loose Coupling / Operator Split
    1. Solve PDE1
    2. Pass Data
    3. Solve PDE2
    4. Move To Next Timestep



- Sequential Coupling w/Iteration
    1. Solve PDE1
    2. Pass Data
    3. Solve PDE2
    4. Pass Data
    5. Return to 1 Until Convergence
    6. Move To Next Timestep



- Fully Coupled
    1. Solve PDE1 and PDE2 simultaneously in _one_ system
    2. Move To Next Timestep



Jacobian-free Newton Krylov (JFNK) Solution For Nonlinear Coupled THMC Processes

- Newton's method is used to solve the nonlinear system

$$\mathbf{F}(\mathbf{u}) = 0,\ \ or\ \mathbf{F}(\mathbf{u}^{n+1}) < tol$$

- The resulting linear system and nonlinear iteration are

$$\mathbf{J}\delta\mathbf{u}^{n+1} = -\mathbf{F}(\mathbf{u}^{n}) = 0,\ \ \mathbf{u}^{n+1} = \mathbf{u}^{n} + \delta\mathbf{u}^{n+1}$$

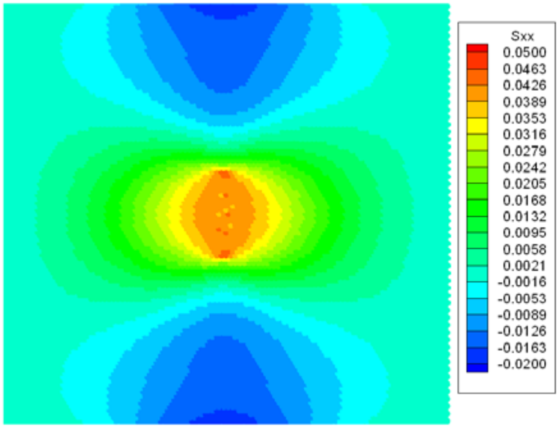
- Using a Krylov method (GMRES) to solve the linear system only requires a matrix-vector product (the Jacobian never appears alone)

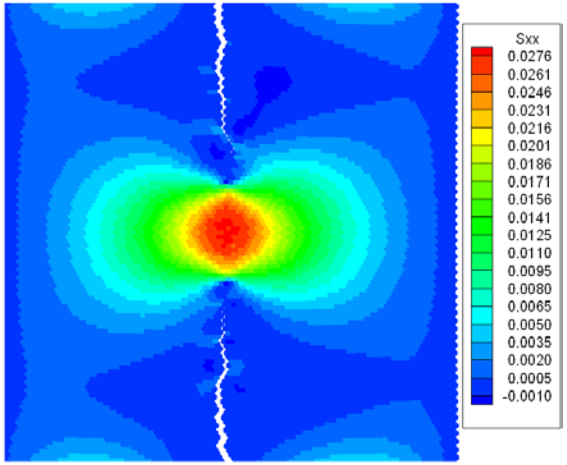
$$\delta\mathbf{u}^{n+1,k} = a_0\mathbf{r}_0 + a_1\mathbf{J}\mathbf{r}_0 + a_2\mathbf{J}^2\mathbf{r}_0 + \ldots + a_k\mathbf{J}^k\ \mathbf{r}_0$$

- This matrix-vector product (for generic **v**) may be approximated by

$$\mathbf{J}\mathbf{v} \approx \frac{\mathbf{F}(\mathbf{u} + \epsilon\mathbf{v}) - \mathbf{F}(\mathbf{u})}{\epsilon}$$

Challenges for Simulating Geomechanical Response Due to Injection



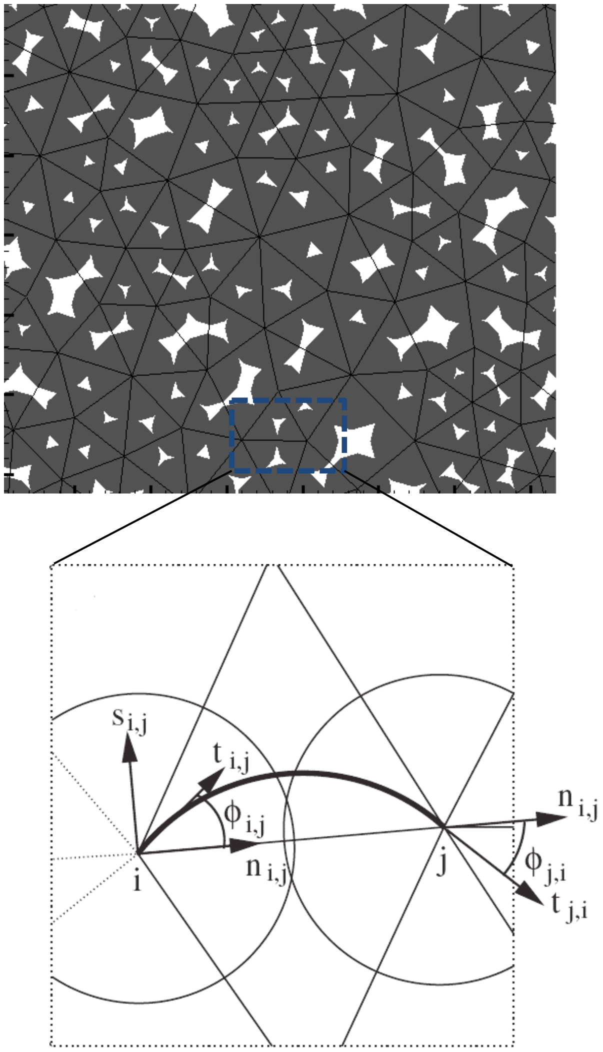


- Fracturing coupled with flow:
  - ✓ Initiation & propagation of new cracks during injection
  - ✓ Interactions between hydraulic fractures and natural existing fractures
  - ✓ Permeability changes of fractures as fluid pressure and temperature change
- Conventional continuum thermoporoelastic models are inadequate:
  - ✓ Empirical laws to trigger failure
  - ✓ Empirical laws for post-failure mechanics: sliding, dilation etc.

- Need more "**physics**" based models for more robust modeling:
  - Fracture propgations,
  - Reactivation of pre-existing fractures and permeability evolutions

Discrete Element Model (DEM) for Fracturing and Geomechanics Under Stimulations

DEM Model Framework



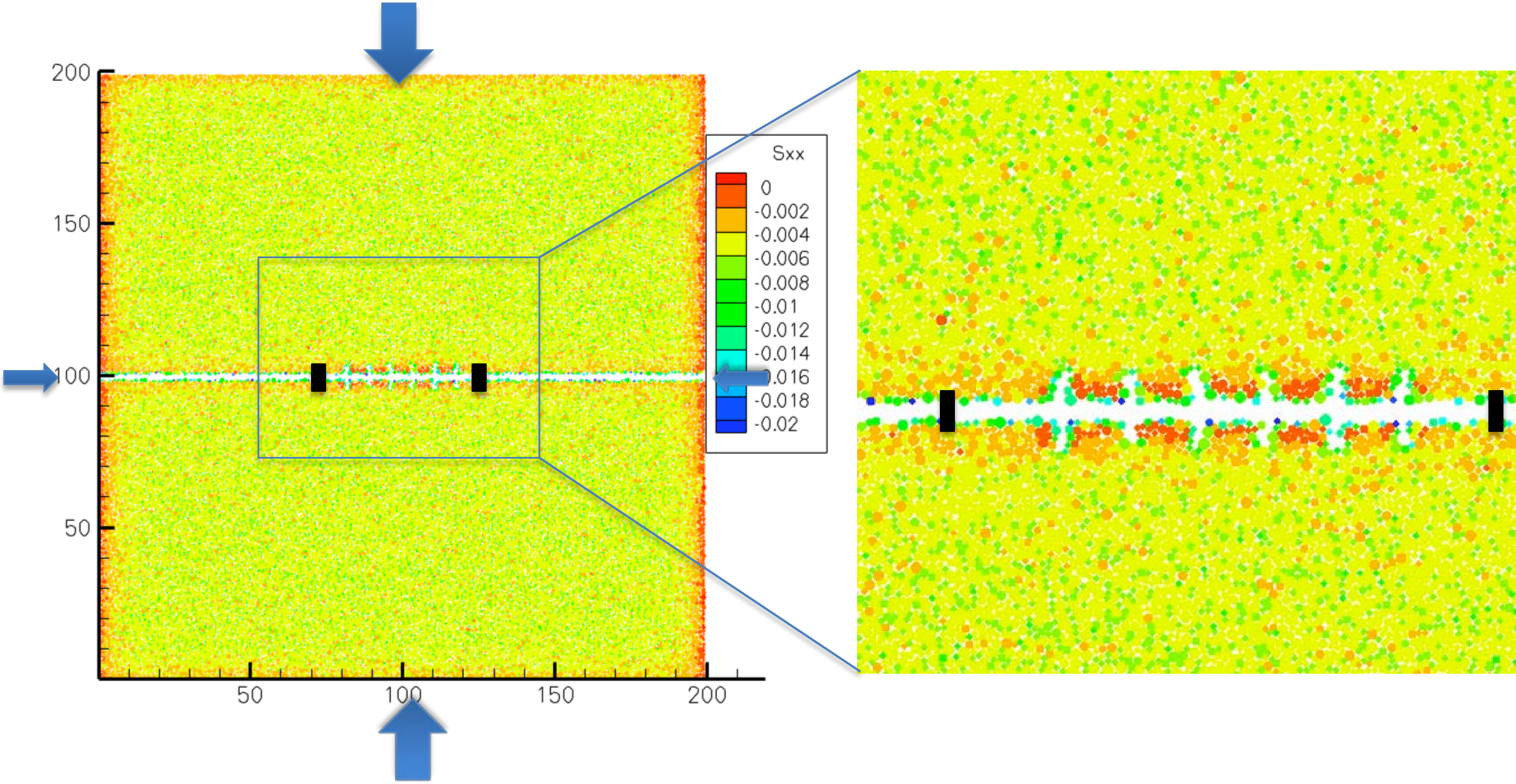
- Represent material, including heterogeneity and anisotropy, by a network of mechanical elements connected by springs or beams, elastic or viscoelastic, etc.)
- Impose boundary conditions (stress, strain)

Force and Moment Balance

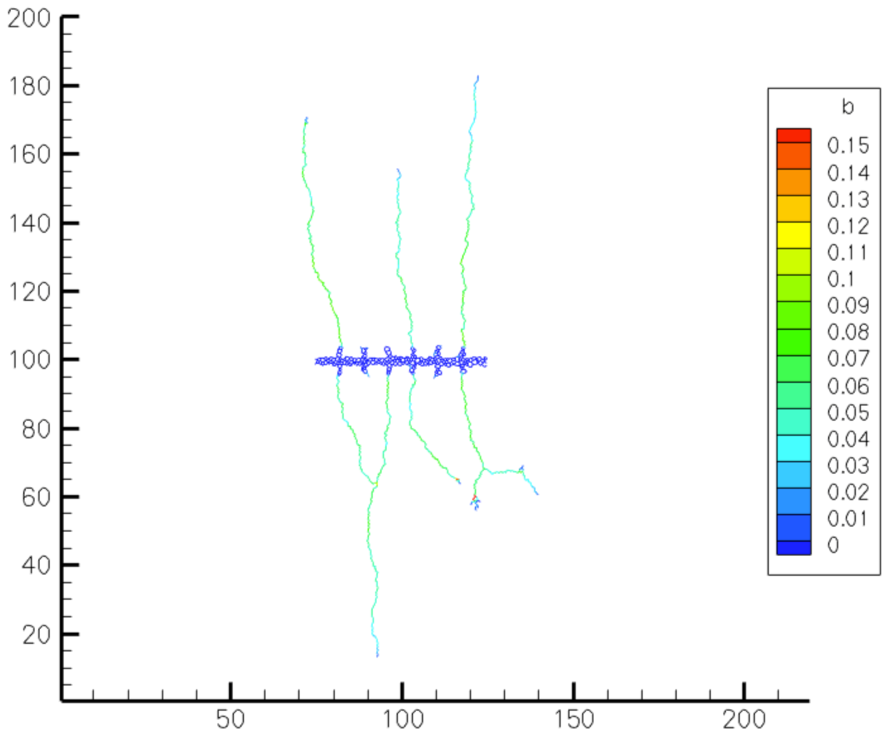
$$\vec{F}_{i,j} = k_n(d_{i,j} - d^0_{i,j}) + k_s \frac{1}{2}(\varphi_{i,j} + \varphi_{j,i})\vec{s}_{i,j}$$

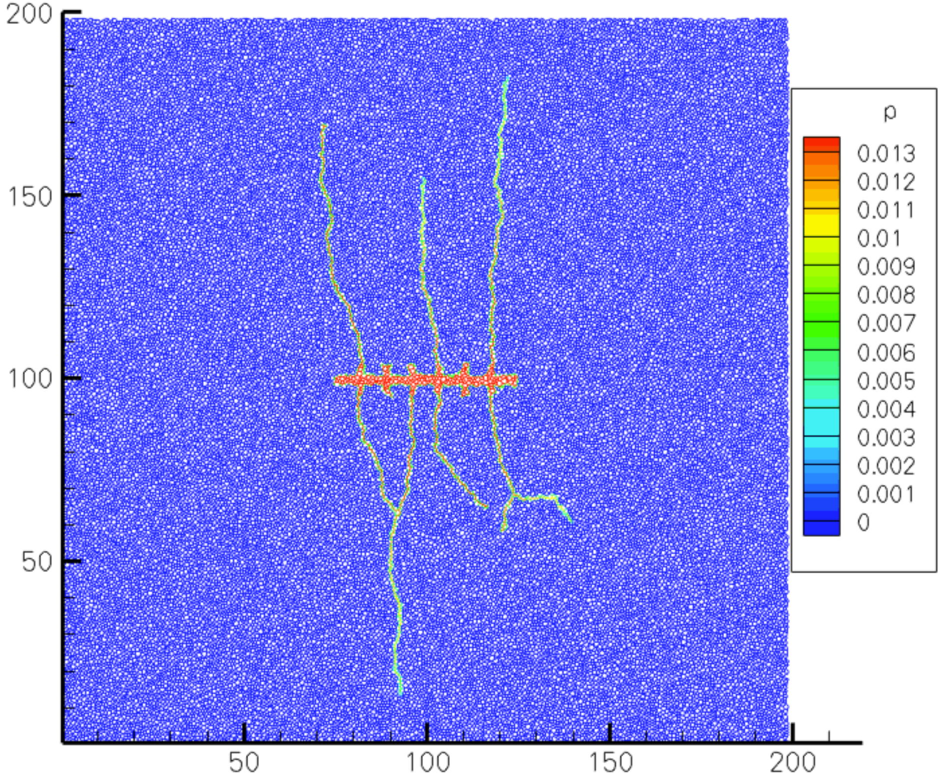
$$\vec{M}_{i,j} = k_s d[\frac{\Phi}{12}(\varphi_{i,j} - \varphi_{j,i}) + \frac{1}{2}(\frac{2}{3}\varphi_{i,j} + \frac{1}{3}\varphi_{j,i})]$$

Simulations of multistage hydraulic fracturing



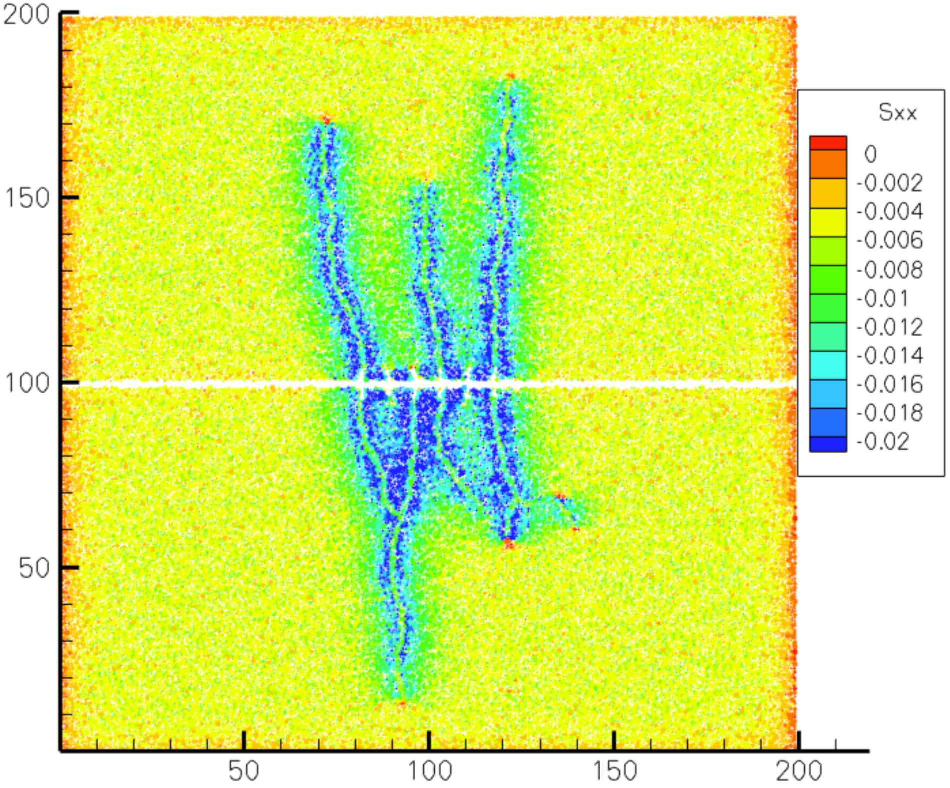
Mutlistage hydraulic fracturing at high injection rate


Fracture path

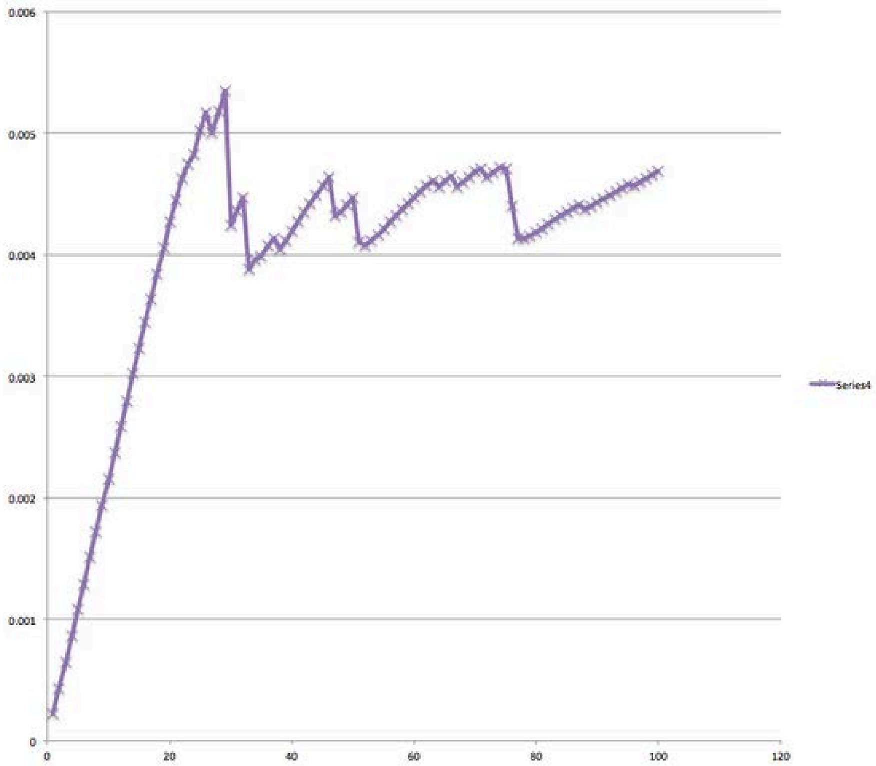

Fluid pressure

Mutlistage hydraulic fracturing at high injection rate

Stress fields

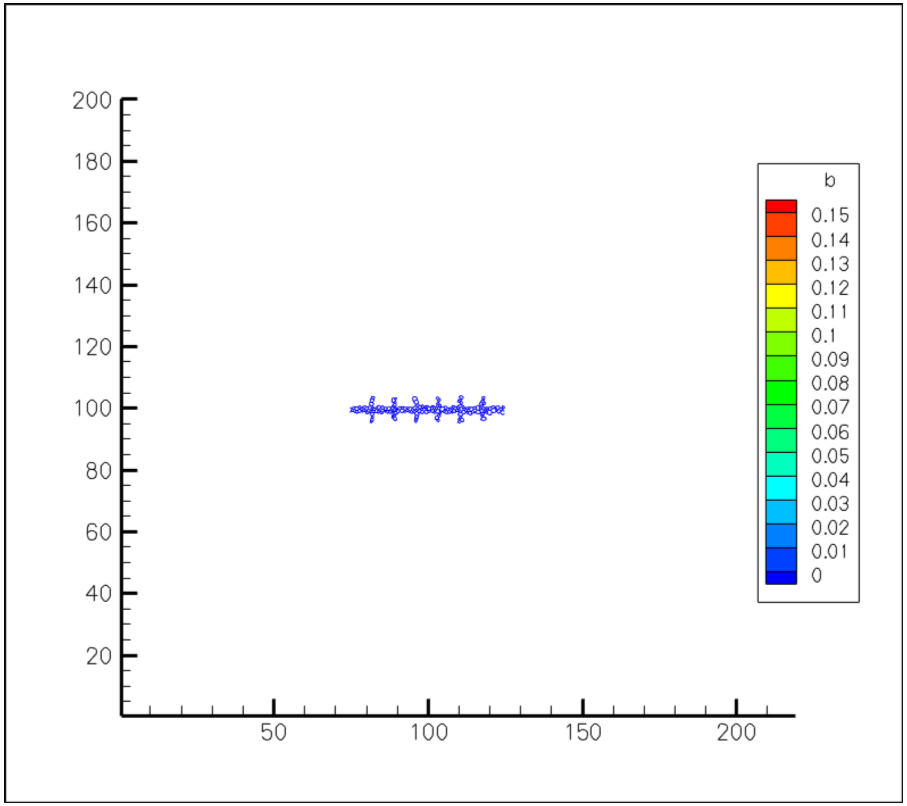


Wellbore pressure

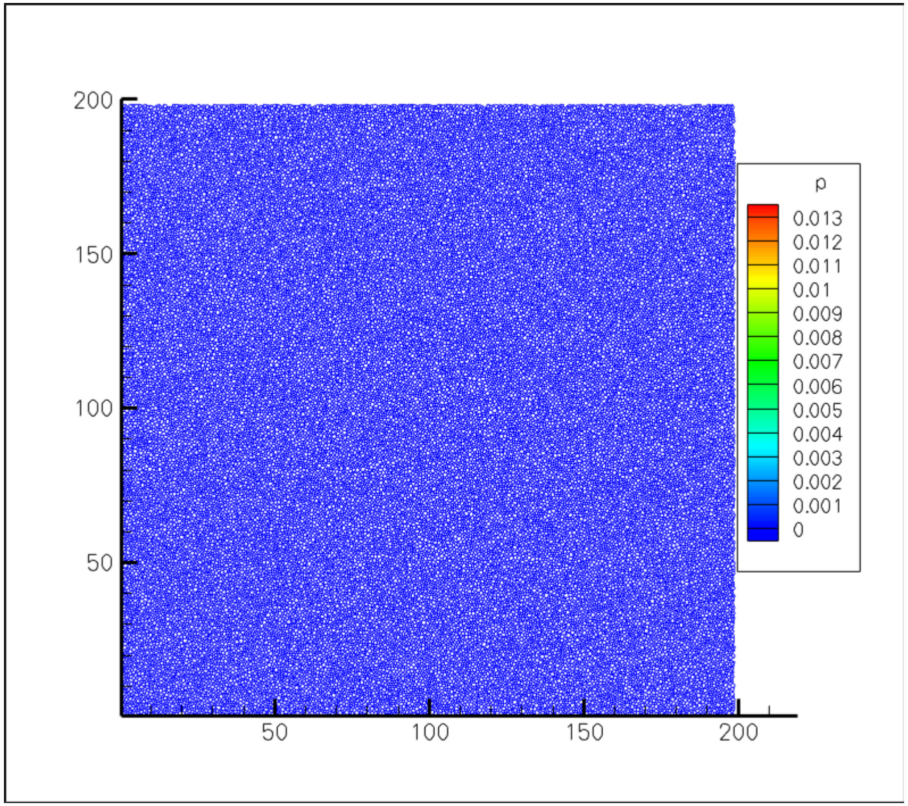


Mutlistage hydraulic fracturing at high injection rate

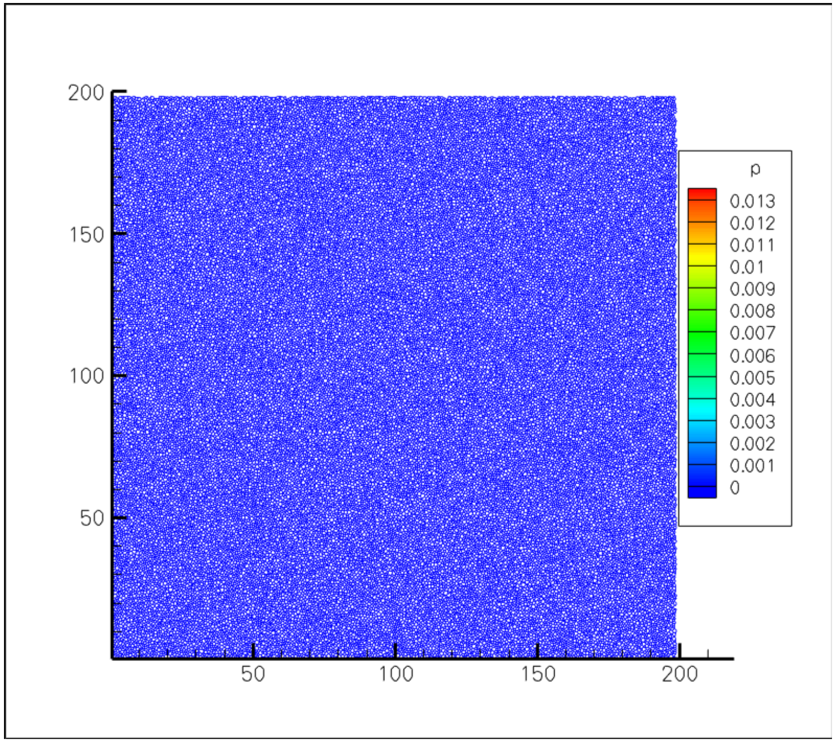
Fracture path

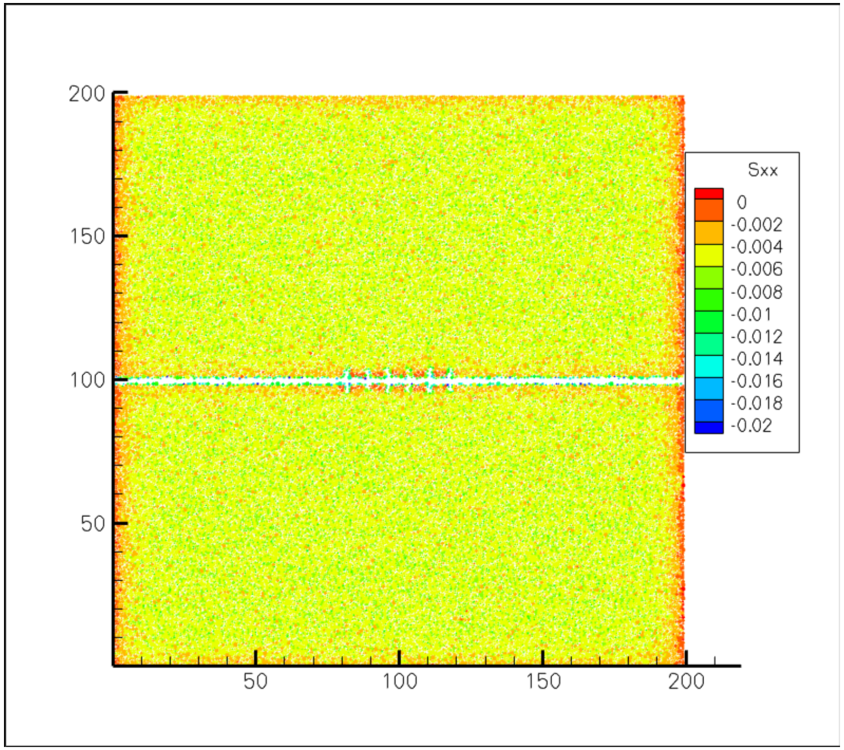


Fluid pressure



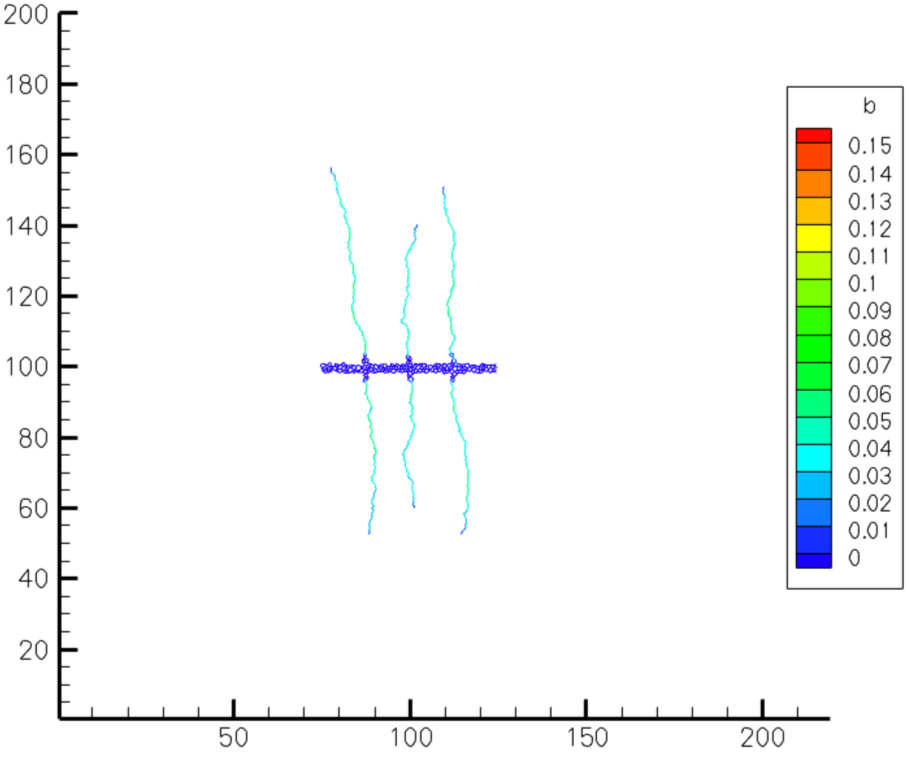
Mutlistage hydraulic fracturing at high injection rate



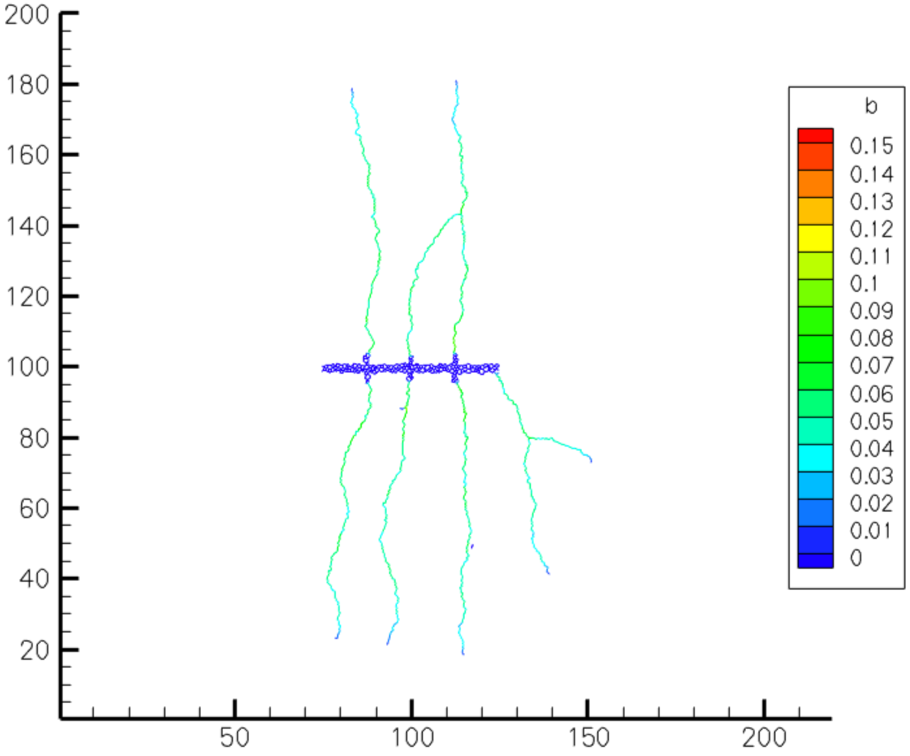


Effects of injection rates

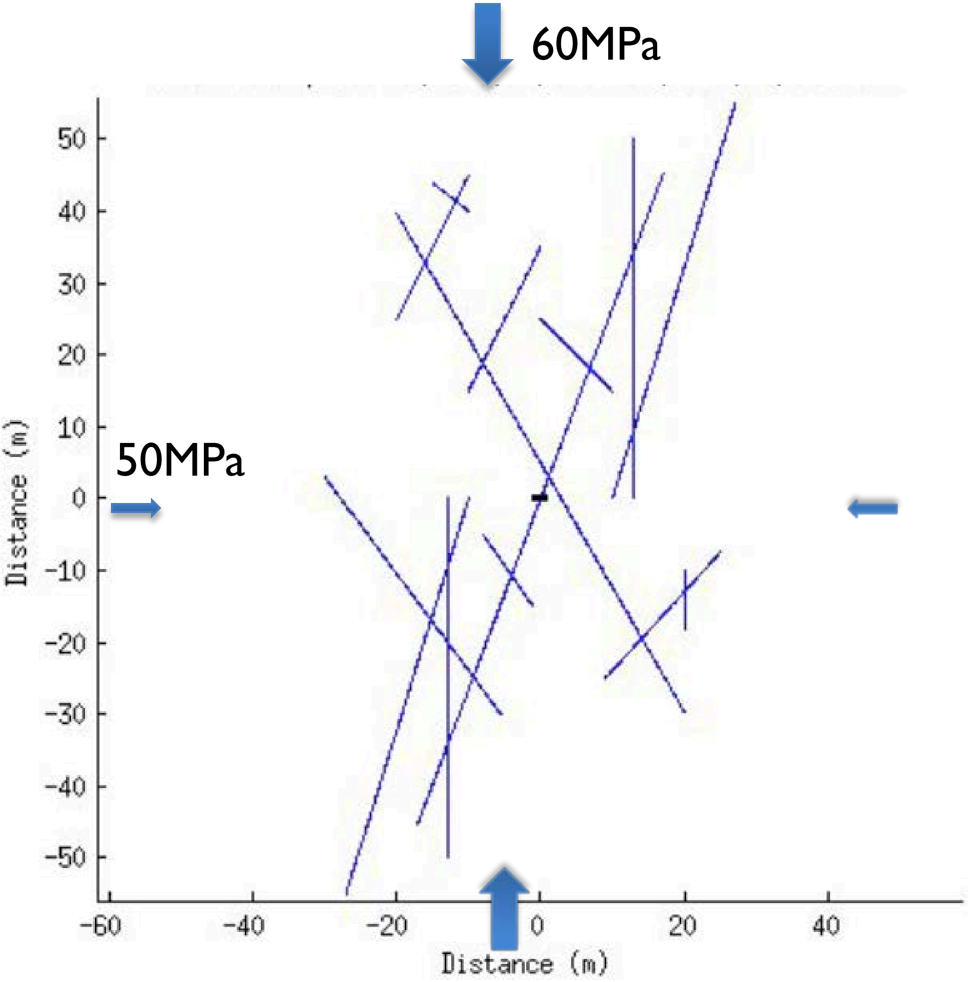
Q



2Q

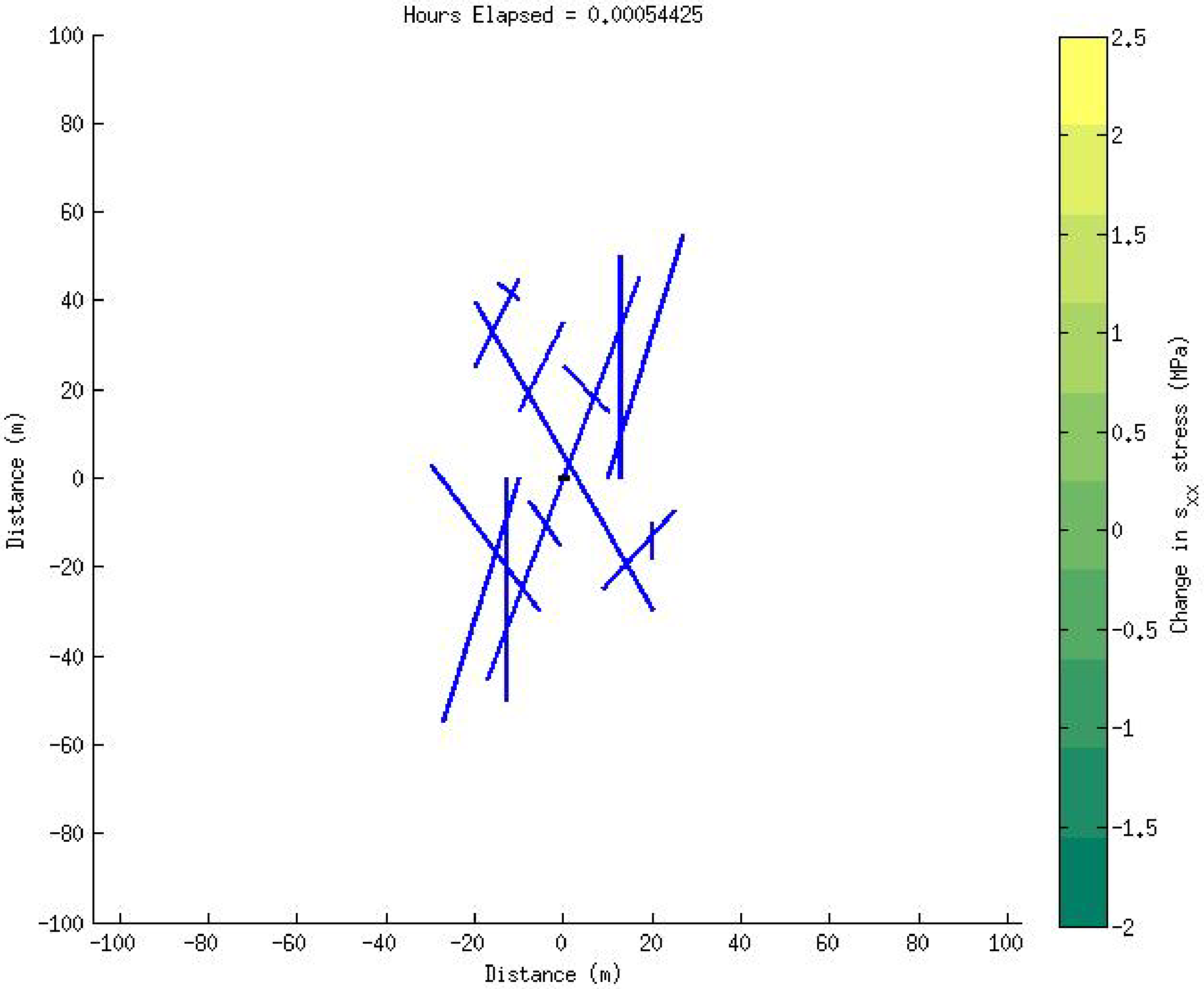


Reactivation of natural fractures

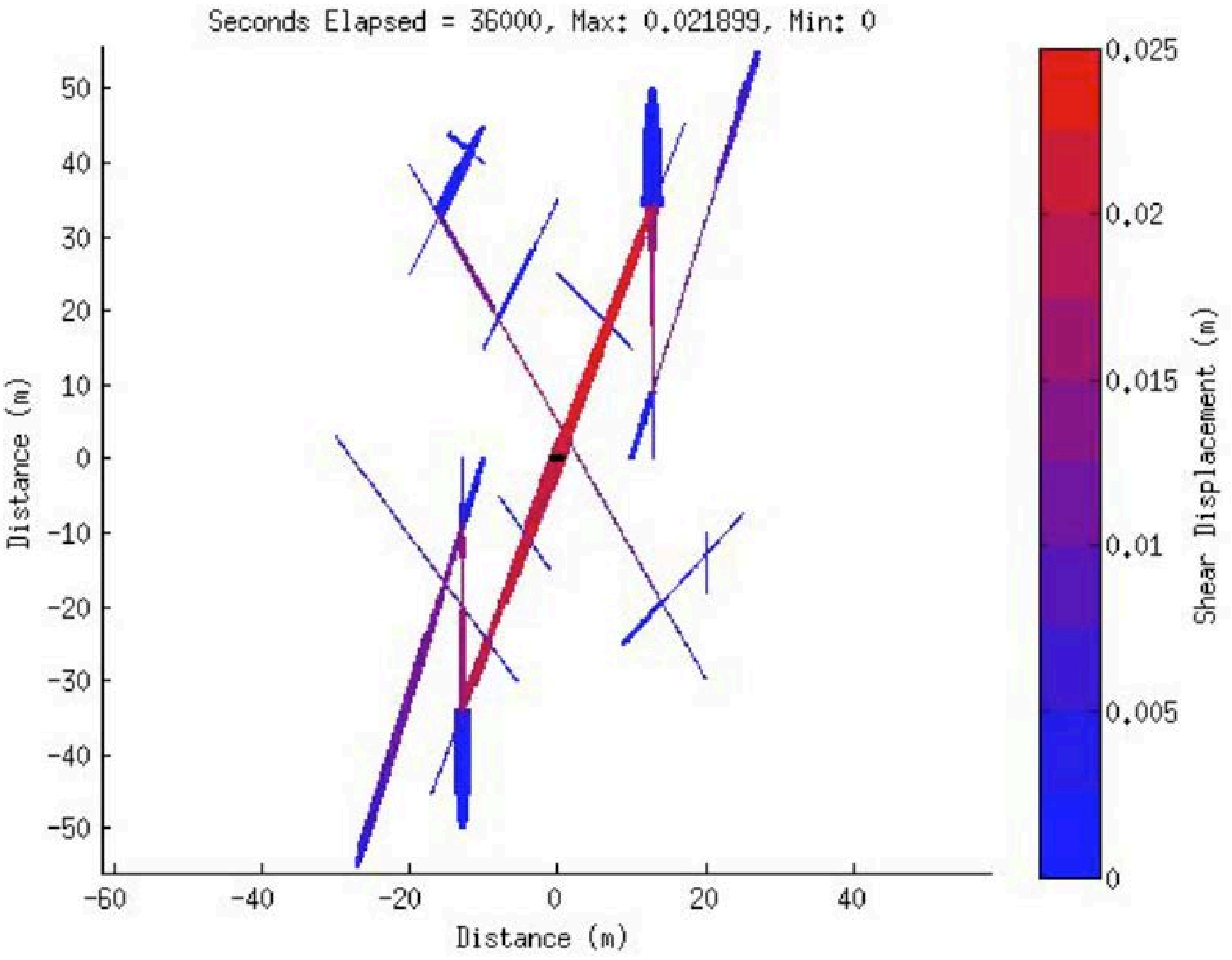


1. Injection rate: 2.5Kg/s
2. Initial fluid pressure: 20MPa
3. Max. injection pressure: 55MPa
4. No leakage from fracture to matrix is considered
5. Only opening and slip of existing cracks are considered

Reactivation of natural fractures



Reactivation of Natural Fractures: slipping vs. openning



Accomplishments to date

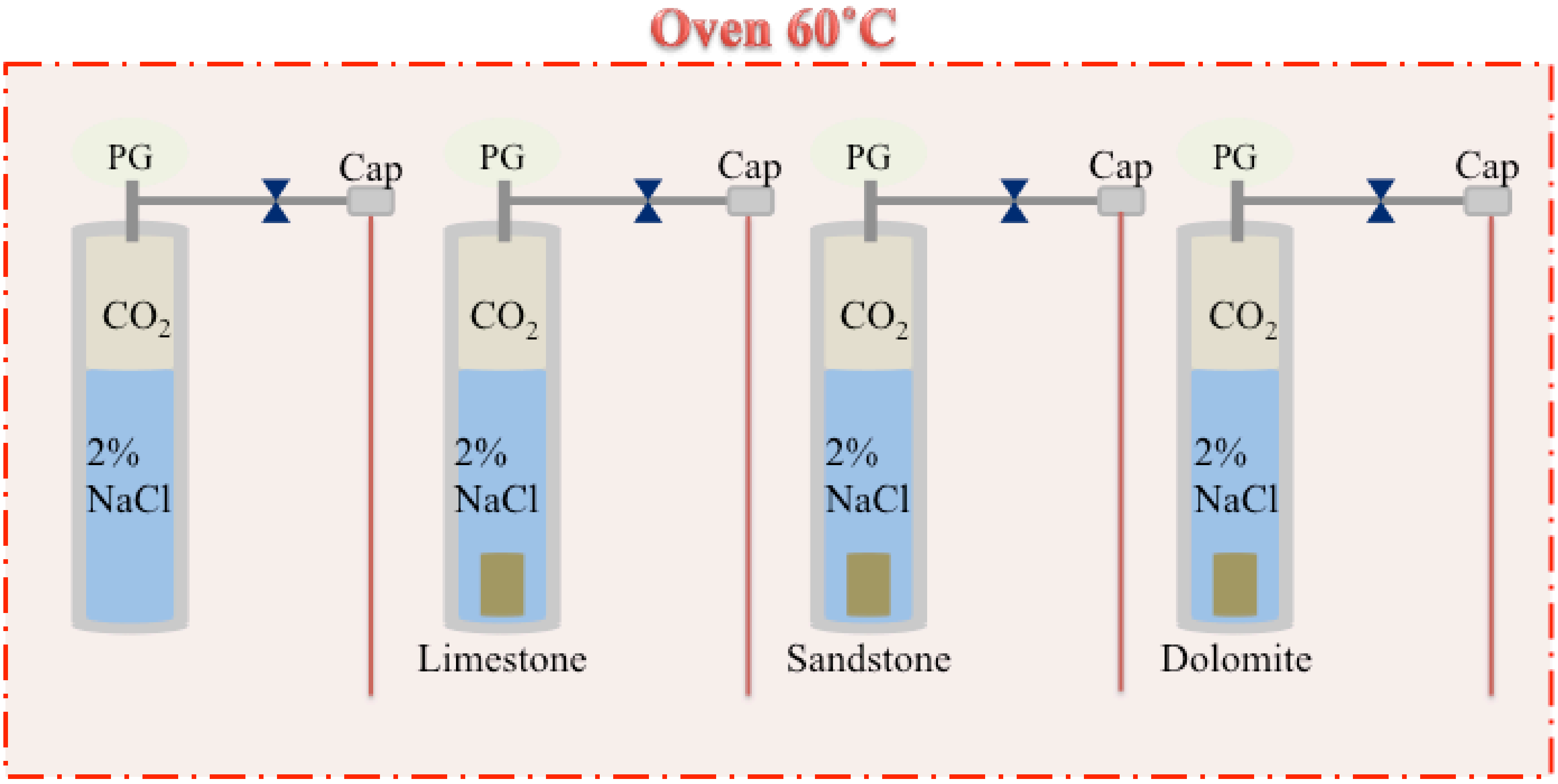
- Developed apparatus for batch and core flooding experiments under elevated temperature and pressure
- Conducted batch experiments for reaction kinetics
- Applied pore-scale models for porosity-permeability constitutive relationships for relevant rocks.
- Implemented the porosity-permeability relationships into the continuum reactive transport simulator
- Coupled 2D DEM model with flow simulator under two extremes:
  - Hydraulic fracturing
  - Reactivation of pre-existing fractures

Summary

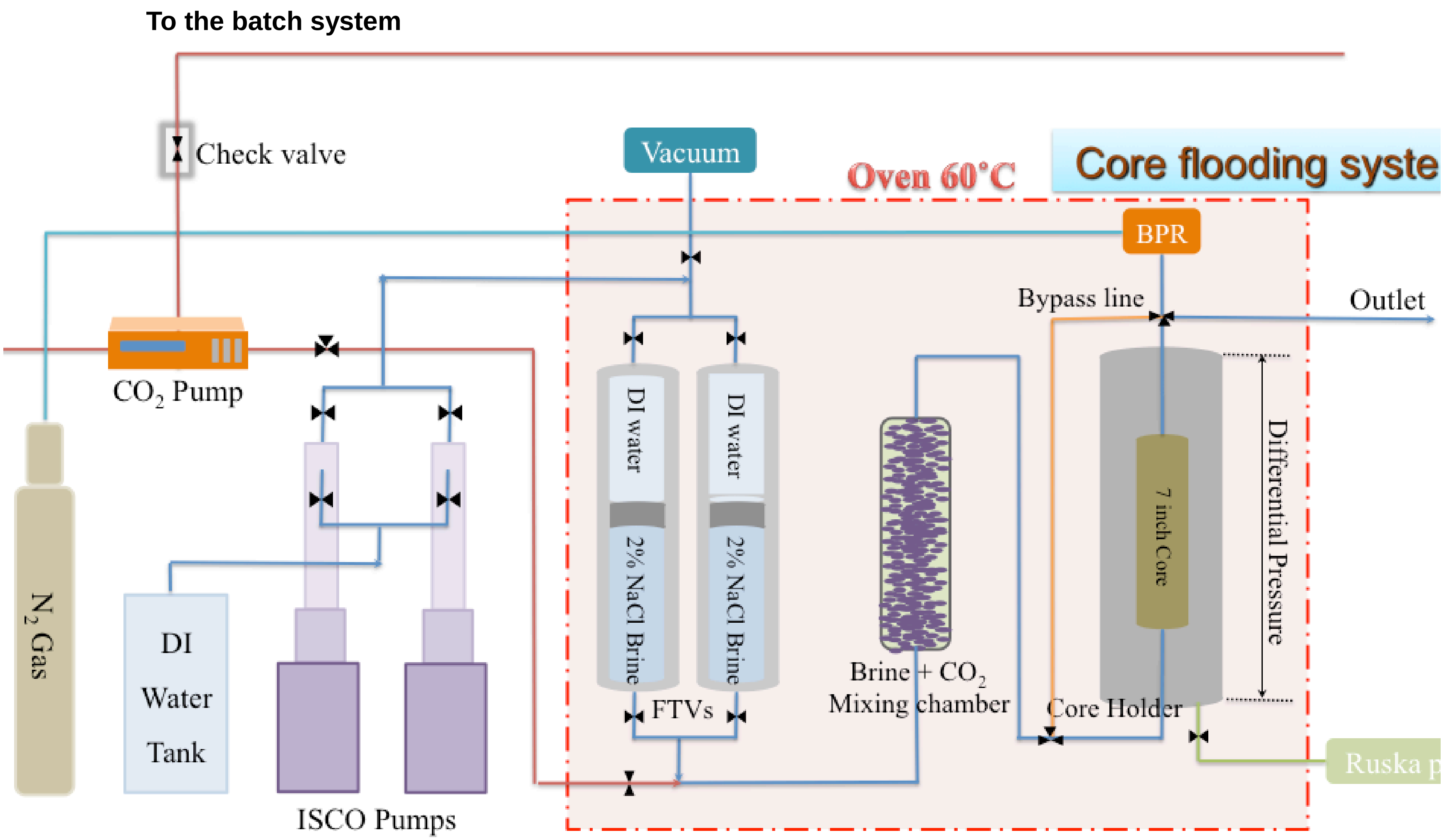
- Key findings:
  - Mineral dissolution and precipitation strongly affects permeability of fractured reservoir
  - Fracturing and geomechanics response are important to wellbore injectivity
- Future plan
  - Core flooding experiments, chemical analysis and core imaging
  - Validate pore-scale and continuum reactive transport models with experiments
  - Coupling 3D DEM with flow simulator

- Backup slides

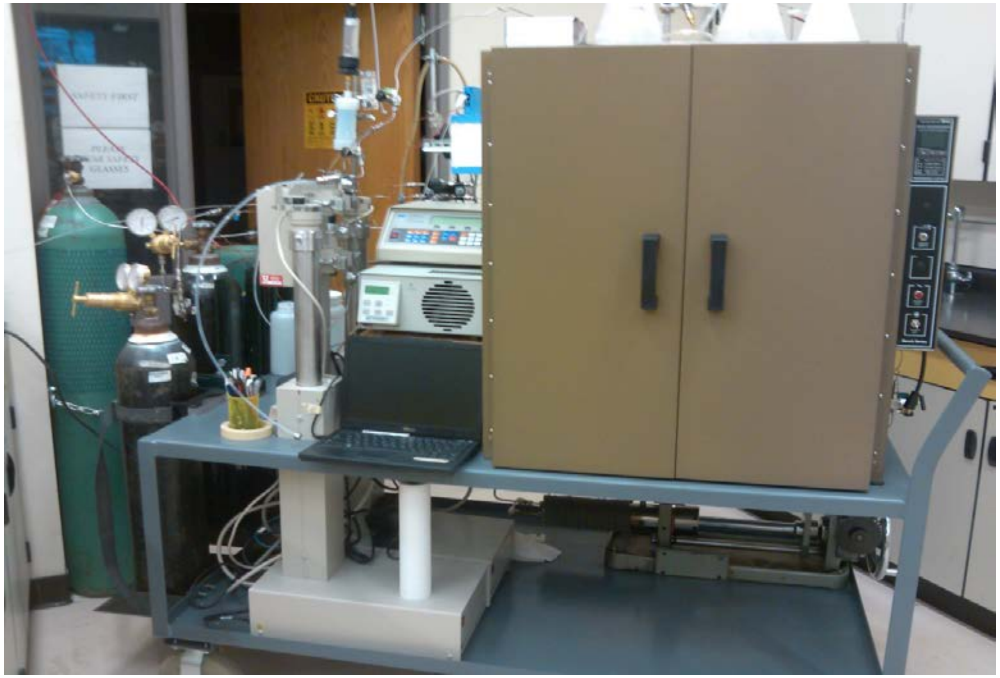
Batch Experimental System



Coreflooding System

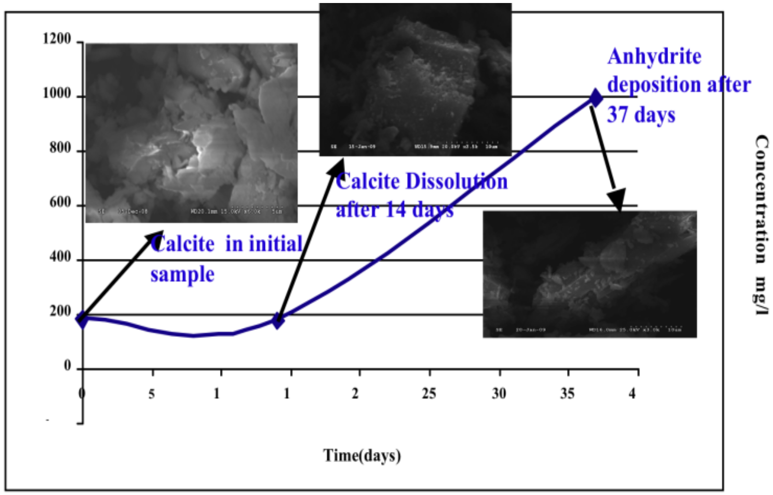


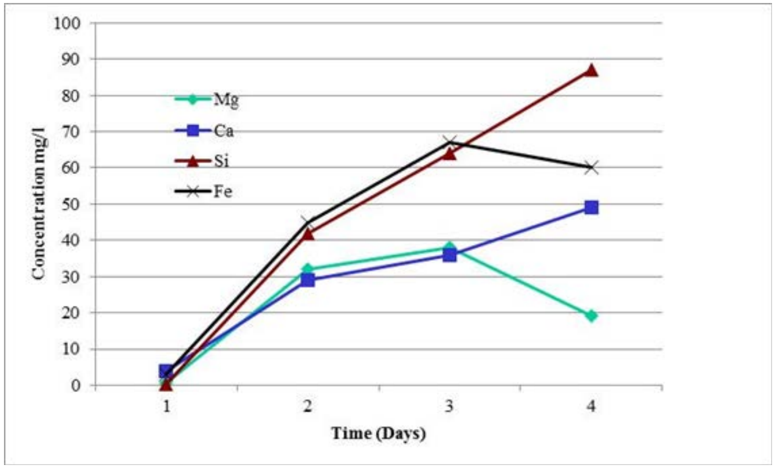
Experimental System



Additional Results

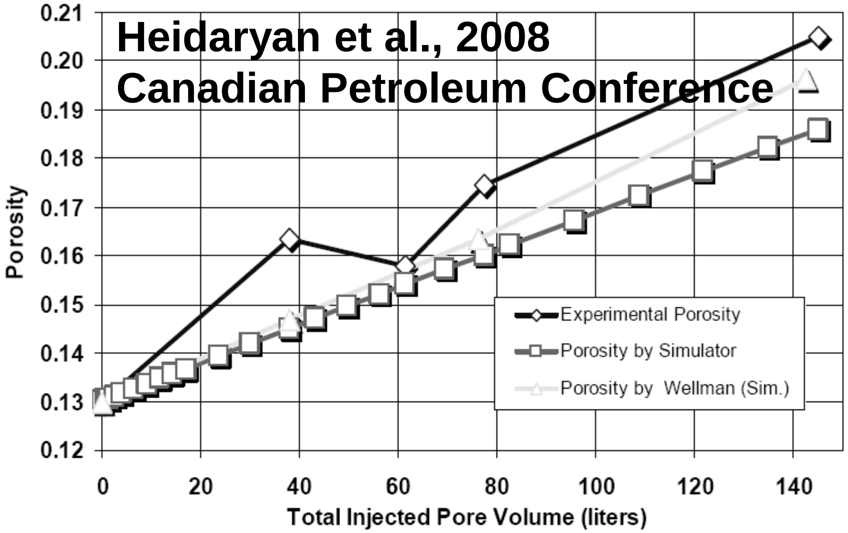
- Dissolution with limestone
- Dissolution and reprecipitation with peridotite
- Effect of gas chemistry
  - Presence of SO_2 in CO_2 causes continuous dissolution of carbonate. anhydrite formation detected
- Implications on injectivity and pressurization



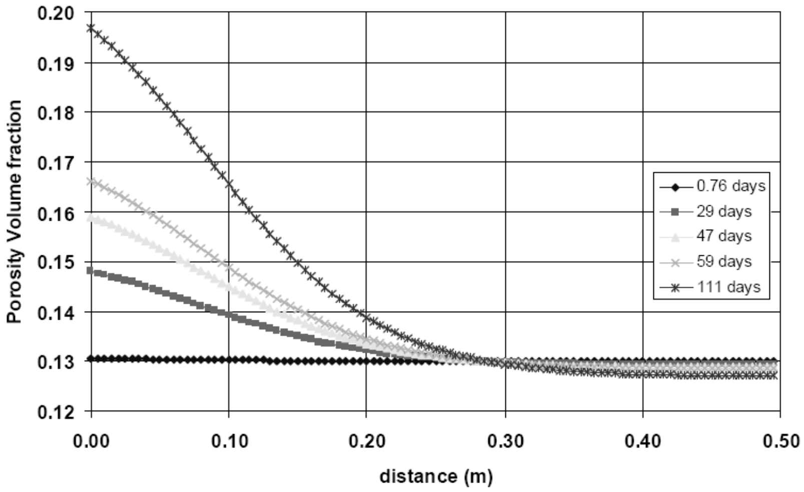


Review of Core Floods

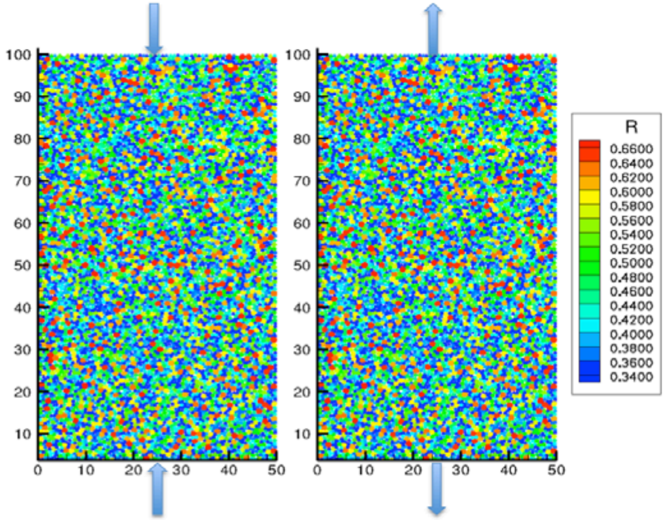
- Generally increased porosity in calcitic/dolomitic systems near injection points
- Carbonation and decreased porosity at the end of the sample over time



Heidaryan et al., 2008
Canadian Petroleum Conference

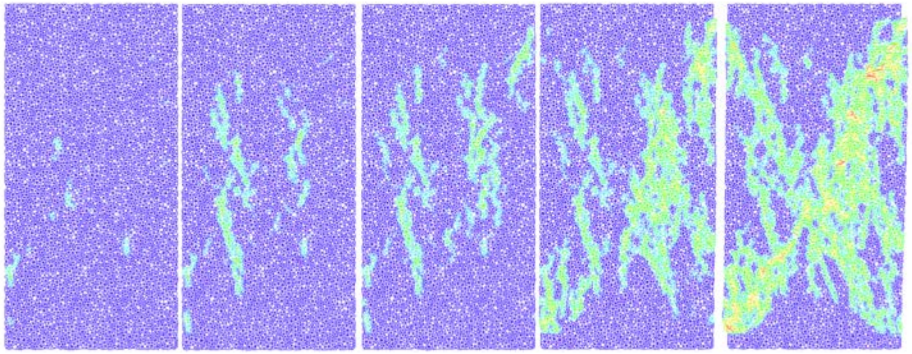


DEM Parameter Calibration Using Uniaxial Compression and Tension Tests

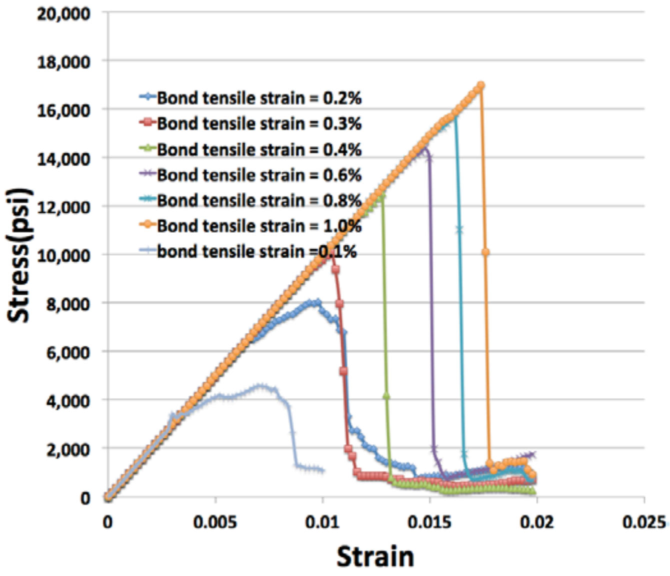


Relationships developed between DEM bond parameters and bulk mechanical properties:

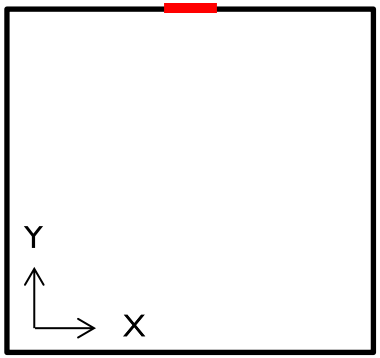
- Young's modulus (E)
- Poisson's ratio (v)
- Tensile strength (S_t)
- Compressive strength (S_c)



Simulated nucleation, propagation and growth of microfractures and the final macroscopic failure of rock sample



Model Validation: DEM vs. FEM



Model Parameters

Unconfined boundaries

T_{heater} = 1000 °F

E = 1.0 x 10^6 psi

V = 0.23

α = 2.36 x 10^{-5} °F^{-1}

D = 0.55 ft^2/day

t = 40 hours

Satisfactory match between DEM and FEM in linear elastic regime