

**Project ESD14089:**  
**Numerical and Laboratory Investigations for  
Maximization of Production from Tight/Shale Oil  
Reservoirs: From Fundamental Studies to  
Technology Development and Evaluation**

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Sharon Borglin, Marco Voltolini, Alejandro Queiruga  
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U.S. Department of Energy  
National Energy Technology Laboratory  
Mastering the Subsurface Through Technology, Innovation and Collaboration:  
Carbon Storage and Oil and Natural Gas Technologies Review Meeting  
August 1-3, 2017



# Presentation Outline

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- Programmatic slides
  - Goals, Benefits
  - Project Overview
- Technical Status
  - Task List and Updates
  - Code Development
  - Reservoir Simulation Studies
  - Laboratory Studies
  - Molecular Simulation Studies
- Accomplishments to Date
- Appendix

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# Benefit to the Program

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**Goal:** Address critical gaps of knowledge of the characterization, basic subsurface science, and stimulation strategies for shale oil resources to enable efficient resource recovery from fewer, and less environmentally impactful wells

**Benefits:**

- Increases in production (from a very low base, 5%)
- Identify and evaluate development improvement strategies
- Increases in reserve estimates
- Enhanced energy security

# Project Overview: Goals and Objectives

**By using** multi-scale laboratory investigations (nano- to core-scale) and **numerical simulations (from molecular to field-scale) to:**

- Identify and quantify the mechanisms involved in hydrocarbon production from such tight systems,
- Describe the thermodynamic state and overall behavior of fluids in the nanometer-scale pores of these tight media,
- Propose new methods for low-viscosity liquids production from tight/shale reservoirs
- Investigate a wide range of such strategies, and identify the promising ones to quantitatively evaluate their expected performance

## **Success criteria**

- Develop methods to compare a number of possible light tight oil production methods
- Identify and compare a number of possible light tight oil production methods

# Gantt Chart

Budget Period	#1				#2			
	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8
Task 1: Project Management and Planning	M1							M1
Task 2: Continuation of evaluation of enhanced liquids recovery		M2				M3		
Task 3: 3D Analysis and Modeling of the Transport and Long-Term Fate of Proppants				M4				
Task 4: Multi-scale laboratory studies of system interactions			M5		M6			
Task 5: Molecular simulation analysis of system interactions				M7				

- Production simulation tasks and code development on or ahead of schedule
- Laboratory and molecular simulation tasks set up and underway

**Budget: \$214.5K in FY2015, \$214.5K in FY2016  
\$240K in FY2017, Proposed \$240K in FY2018.**

# Task Description – Task 1

## **TASK 1: Project Management and Planning**

- Management strategy in place, technical team in place
  - PI: G. Moridis, Co-PI: M.T. Reagan
  - Lab studies: T. Kneafsey, S. Borglin
  - Visualization studies: J. Ajo-Franklin, **M. Voltolini**
  - MFD studies: G. Waychunas
  - Simulation and code development: G. Moridis, **A. Queiruga**, M. Reagan

Status: **COMPLETED & ONGOING**

# Task Description – Task 2

## **TASK 2: Continued Evaluation of Enhanced Recovery**

**FY15-16:** Tasks 2, 3, 4, 7, 8

Define the feasibility parameters, the specific objectives and metrics of the screening study. Then, evaluate recovery strategies accounting for all known system interactions

Status: **COMPLETED**

**Success:** predicted increase by >50% in production/recovery over a 3-5 year period (or economic viability of well)

**Phase II:** ongoing simulation tasks continue as Task 2



# Task Description – Task 2

## **TASK 2: Continued Evaluation of Enhanced Recovery**

**Continue to evaluate recovery strategies accounting for all known system interactions.**

**Previous FY15-16 work examined displacement processes:**

- Traditional continuous gas flooding (i.e. natural gas) using parallel horizontal wells
- Water-alternating-gas (WAG) flooding (poor)
- Added CO<sub>2</sub> properties modules → CO<sub>2</sub> injection

# Task Description – Task 2

## **TASK 2: Continued Evaluation of Enhanced Recovery**

**Continue to evaluate recovery strategies accounting for all known system interactions.**

**Current FY17-18 work examines additional processes**

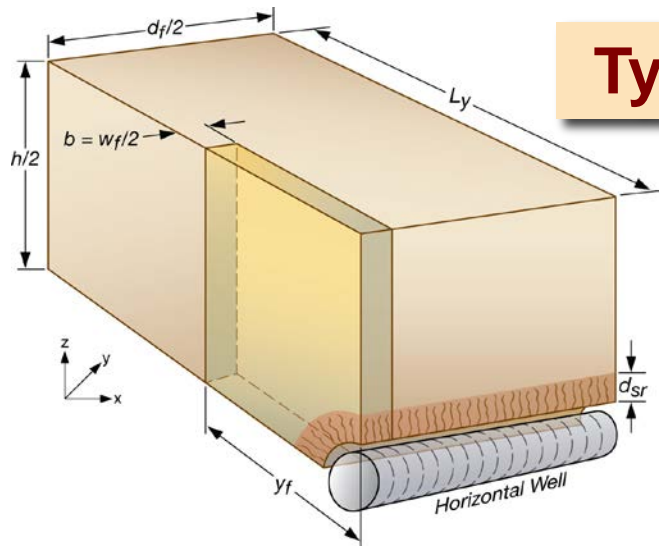
- Updated **thermophysical properties** and PVT relationships using previous laboratory results
- **Examination of additional injection fluids** (CO<sub>2</sub> vs. N<sub>2</sub> vs. CH<sub>4</sub>) for viscosity reduction via gas dissolution
- Further examination of the effect of **secondary and native** fractures
- Further simulation of **heavier, more complex oil phases** (C<sub>14+</sub>, API 36-39)
- **Thermal processes**, viscosity reduction caused by heating
- **Extensive code updates, upgrades, and enhancements**

# Task Description – Task 2

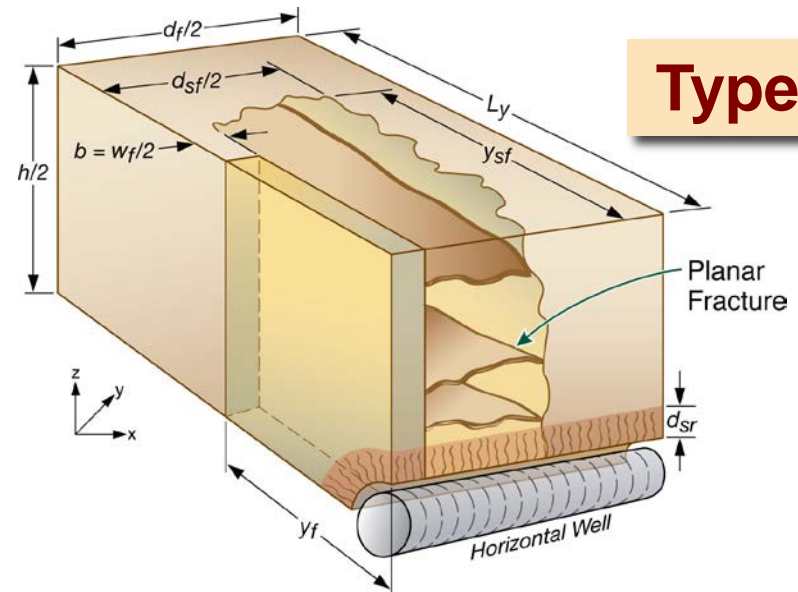
## TOUGH+MultiComponentPhase (T+MCP) Code

- Conventional and tight/shale oil (heavy) simulations, CO<sub>2</sub> enhanced oil recovery, CH<sub>4</sub>- and CO<sub>2</sub>-hydrate formation
- **Fully compositional simulator**
- Oil, H<sub>2</sub>O
- Salt(s)
- Up to 11 gas components (C<sub>1-3</sub>, CO<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>, etc.)
- **Fully non-isothermal**
- **Enhanced oil physical properties relationships (viscosity)**
- Maximum 15 equations/element, 100,000s of elements in 3D
- Massively parallel capabilities (features merged with pTOUGH+)

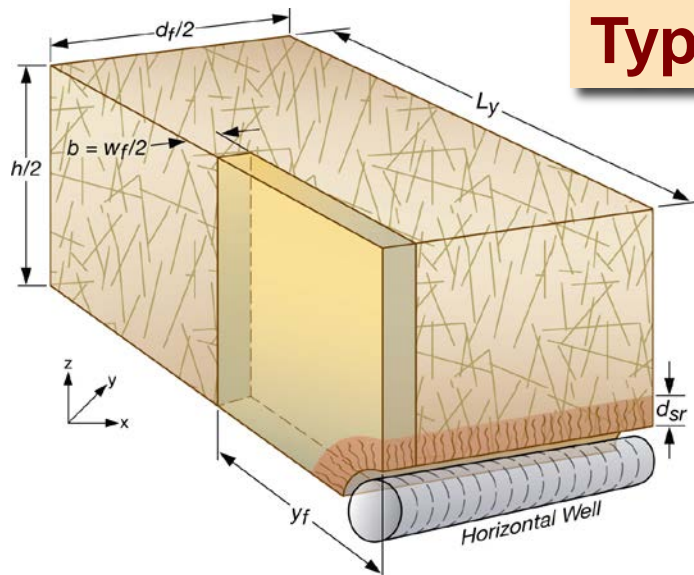
# Types of fractured systems



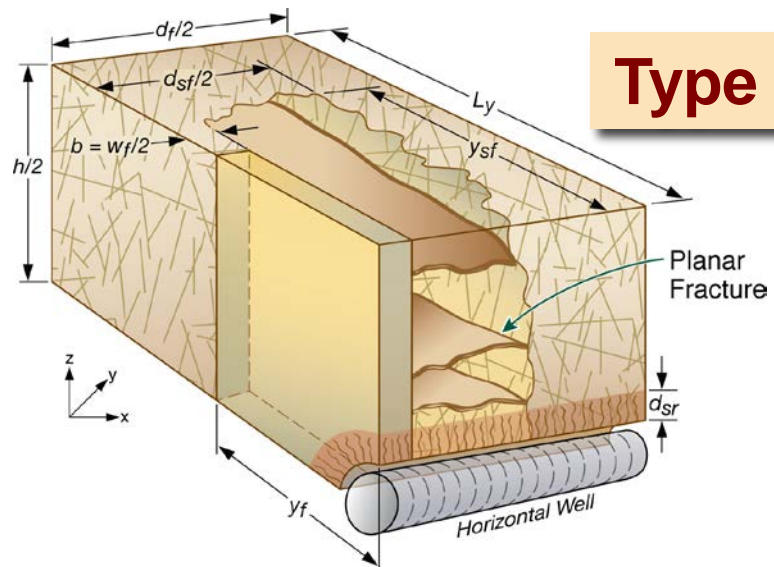
**Type I**



**Type II**



**Type III**



**Type IV**

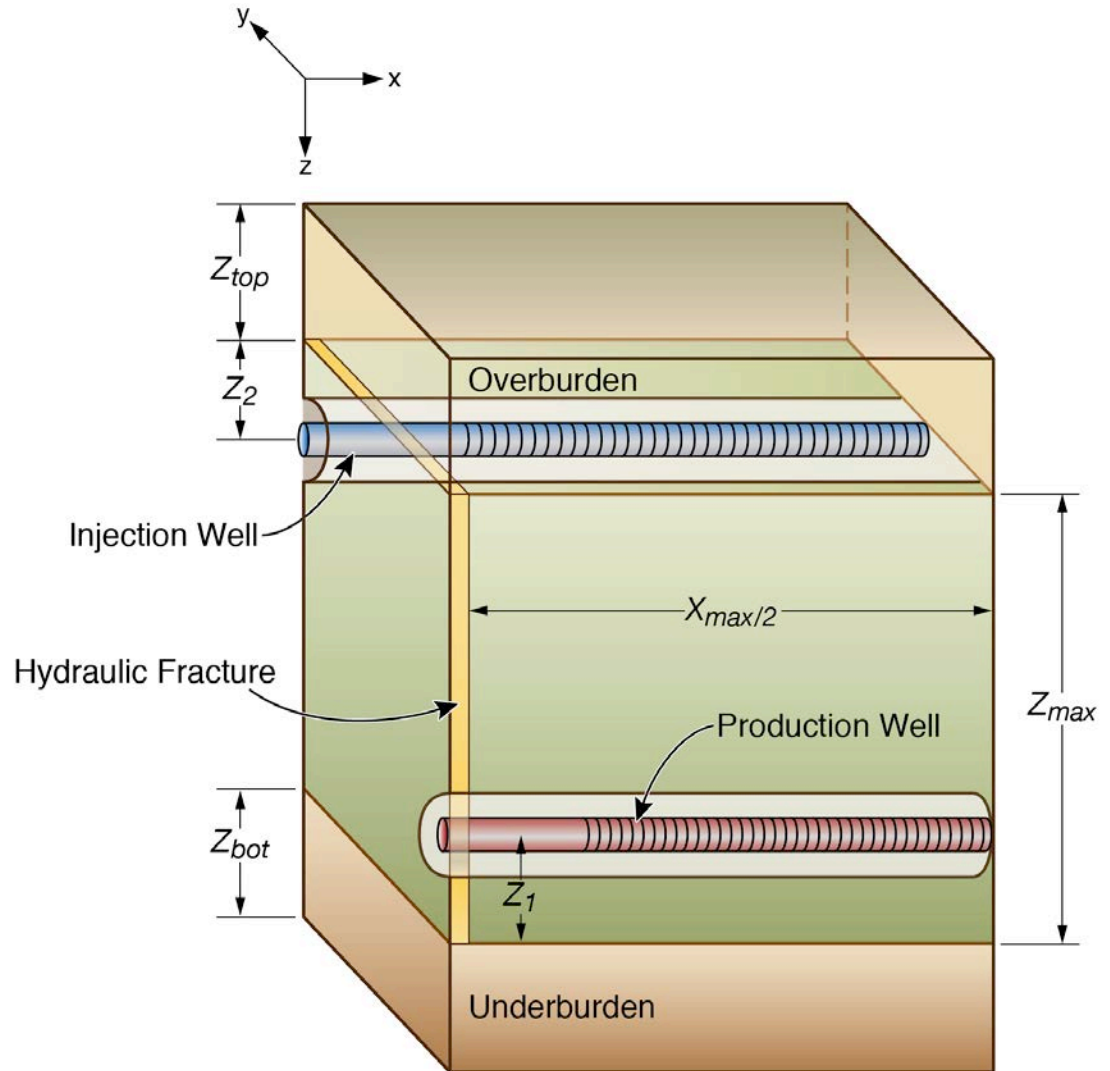
# SHALE OIL PRODUCTION: Domain stencil

## REFERENCE CASE

$$X_{\max}/2 = 15 \text{ m (49 ft)}$$

## Extremely fine discretization

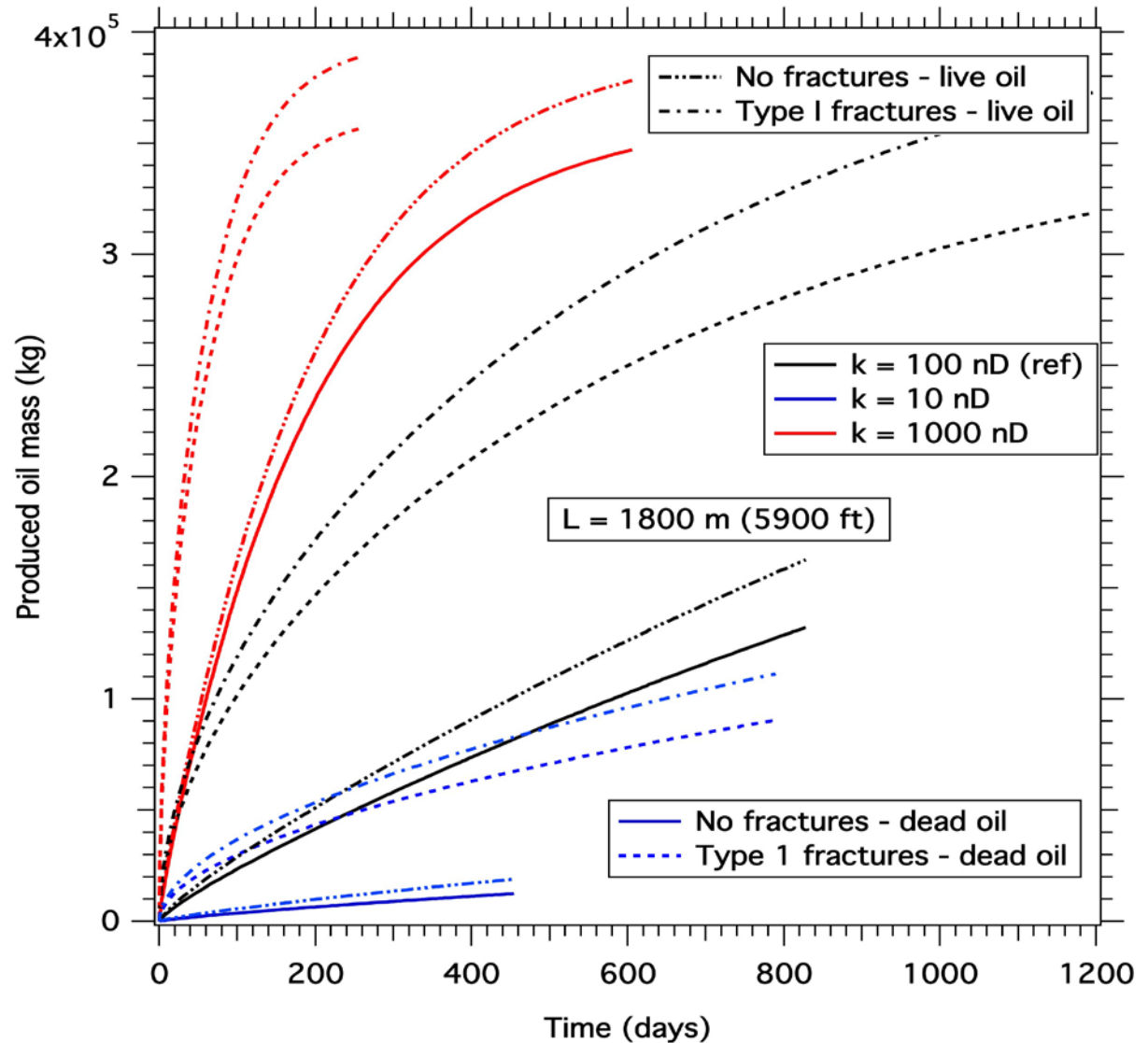
370,000 elements with no- and Type I fractures; 740,000 elements with Types II to IV fractures



# SHALE OIL PRODUCTION: Task 2

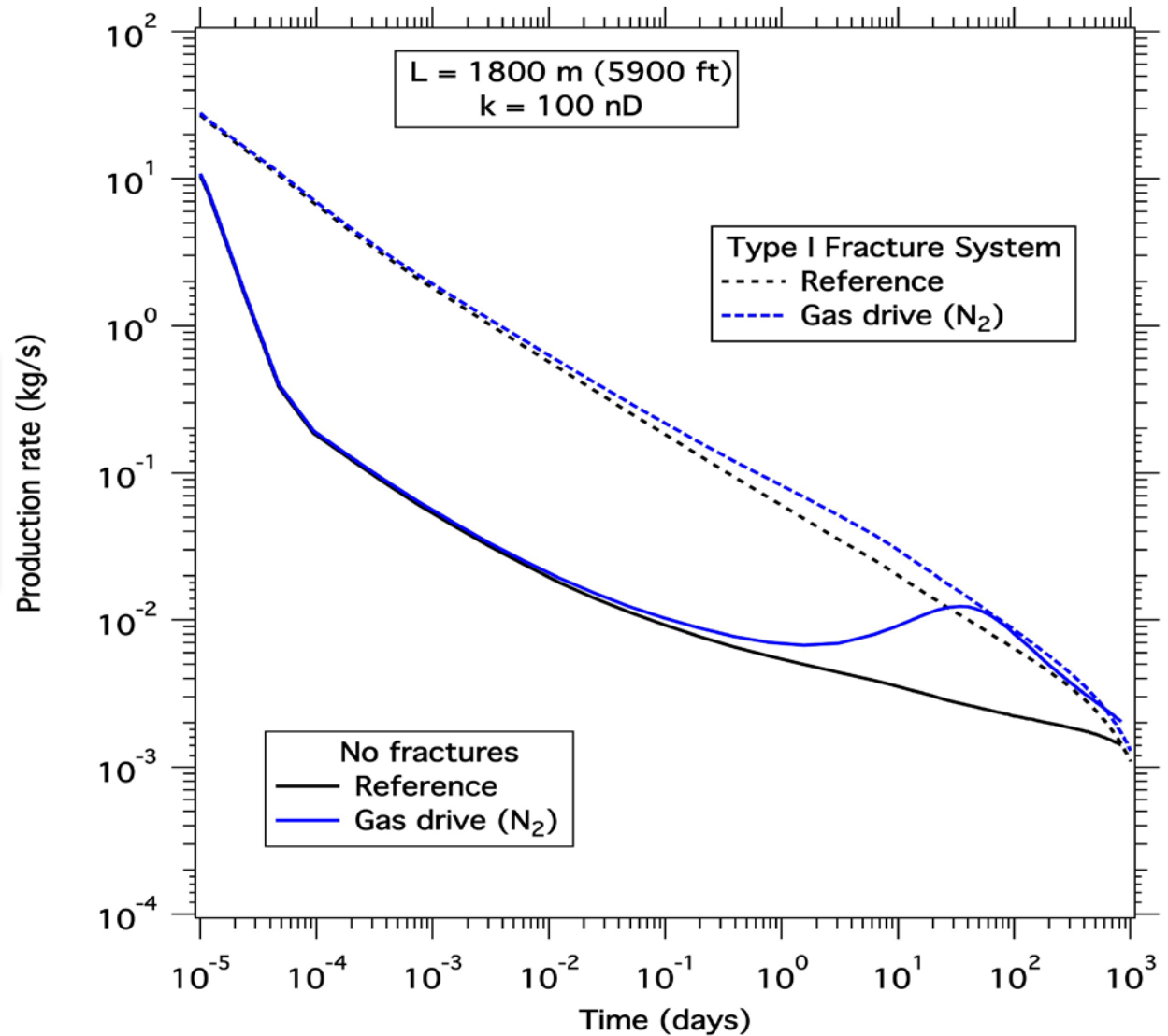
Effect of  
fracturing and  
of matrix  
permeability

Effect of  
dissolved  
gas



# SHALE OIL PRODUCTION: Task 2

**Displacement  
process: N<sub>2</sub>  
drive**

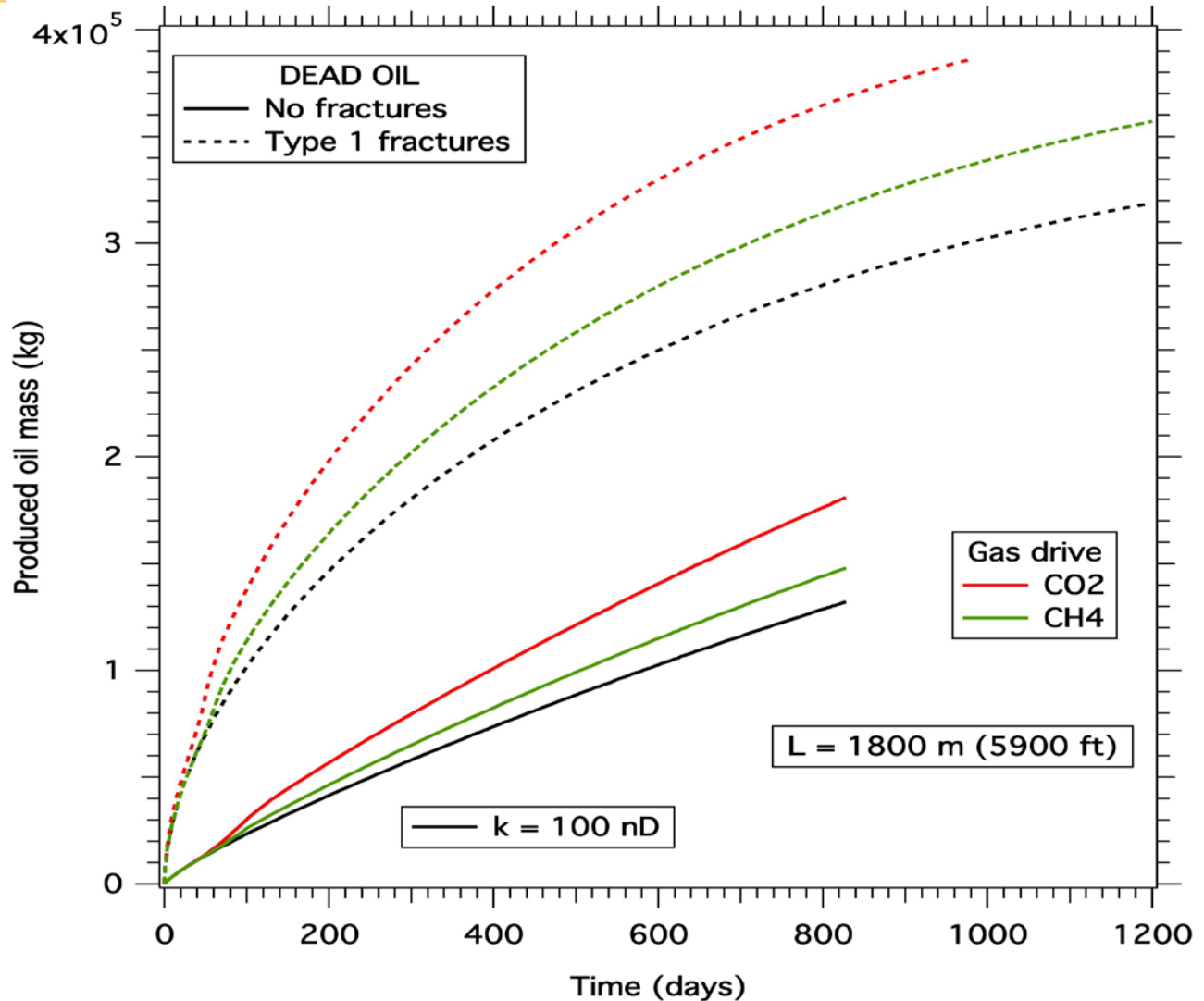


# SHALE OIL PRODUCTION: Task 2

**CO<sub>2</sub> vs. CH<sub>4</sub>**

**Displacement  
process: gas  
drive**

**CO<sub>2</sub>  
superiority?**





# SHALE OIL PRODUCTION: Task 2

## HOWEVER:

- Anecdotal evidence that **CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub> mixture more effective** in shale oil recovery
- (Super) Light (C8-C14) vs. heavier oil (C14+)?
- Repeating simulations with an oil with an API gravity of 36-39 (CH<sub>4</sub> vs. CO<sub>2</sub>) in Q3/Q4
- Currently, the effect of the CH<sub>4</sub>/C<sub>2</sub>H<sub>6</sub> is unknown; **laboratory studies may clarify**

# Future Work – Task 2

**Work in Budget Period #2 will complete the work described in the SOW.**

- Completion and analysis of simulations examining the relative effects of **primary, secondary, and natural fractures** ← **LARGE GRIDS**
- Completion of simulations of production enhancement methods for fractured systems, with a focus on:
  - 1) Displacement processes,
  - 2) Gas drives/flooding,
  - 3) Viscosity reduction, and
  - 4) Combined/interacting processes
- Increased complexity/gravity of the oil phase
- Relative effectiveness of CH<sub>4</sub>, CO<sub>2</sub>, and other injected species
- Completion of documentation of all techniques shown to be inefficient or impractical

# Task Description – Task 3

## **TASK 3: 3D Analysis and Modeling of the Transport and Long-Term Fate of Proppants**

- Develop (from first principles) a 2D/3D numerical model of fluid flow and proppant transport
- Analyze the effect of stresses on the embedment of the proppants into the matrix
- Incorporate elements of the numerical models into **TOUGH+ (MCP, RGB)**
- Perform simulations capturing the *PVT* behavior of fluids in shales during hydraulic fracturing operations
- Determine the transport and fate of injected proppants and resulting geomechanical behavior

Status: **AHEAD OF SCHEDULE**

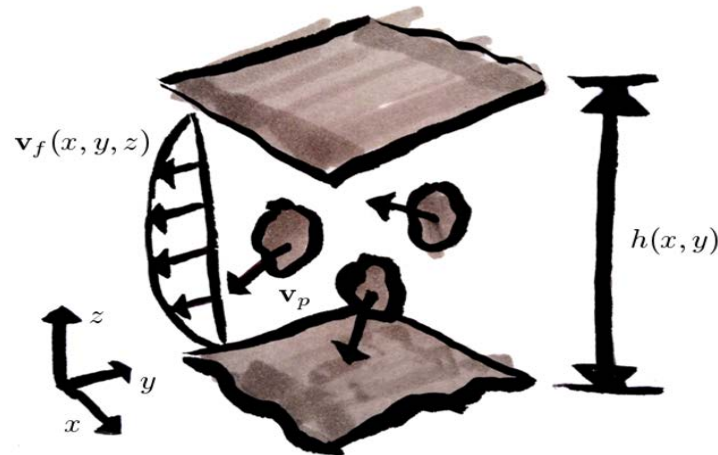
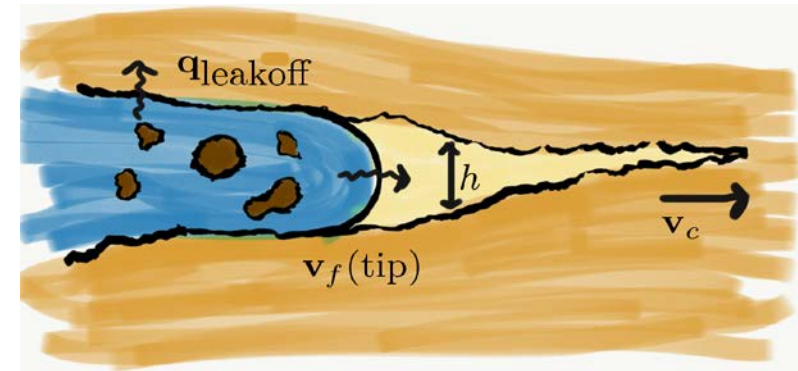
# Fracture Transport Model – Task 3

## Designing a new Numerical Model:

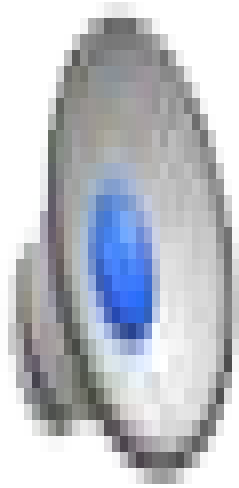
- Solve transport along fracture network during hydraulic fracturing process
- Capture fluid lag behind fracture tip
- Mass conservation approach to proppants
- 2D Finite Element Method

Simplify down to a 2D plane assuming:

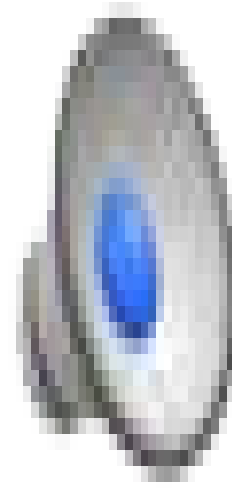
- Fully developed thin-film flow
- Stokes drag
- Uniformly distributed proppants
- Fracture height given from a coupled mechanics code (STONE)



# Preliminary Simulations – Task 3



Proppant-laden fluid injection into a vertically oriented 10m fracture, color indicating pressure. Fluid interface is the 0-contour (thick line)



Proppant-laden fluid injection into a horizontally oriented 10m fracture, color indicating proppant density. Fluid interface is the thick line.

# Upcoming Work – Task 3

## Work for BP #2:

1. Include **mechanics and fracture propagation** into level-set FEM model
2. Couple 2D fracture model to the 3D transport+mechanics codes
3. Embed fractures in 3D space and handle **branching and intersections**
4. Incorporate elements of the numerical models into **TOUGH+(MCP)**
5. Perform coupled simulations and assess the transport and fate of injected proppants and resulting geomechanical behavior

# Task Description – Task 4

## **TASK 4: Multi-scale laboratory studies of system interactions**

### **Subtask 4.1: Sub-Microscopic-Scale Visualization Studies**

#### **Objectives**

- To understand the role of proppants in the evolution of a fracture

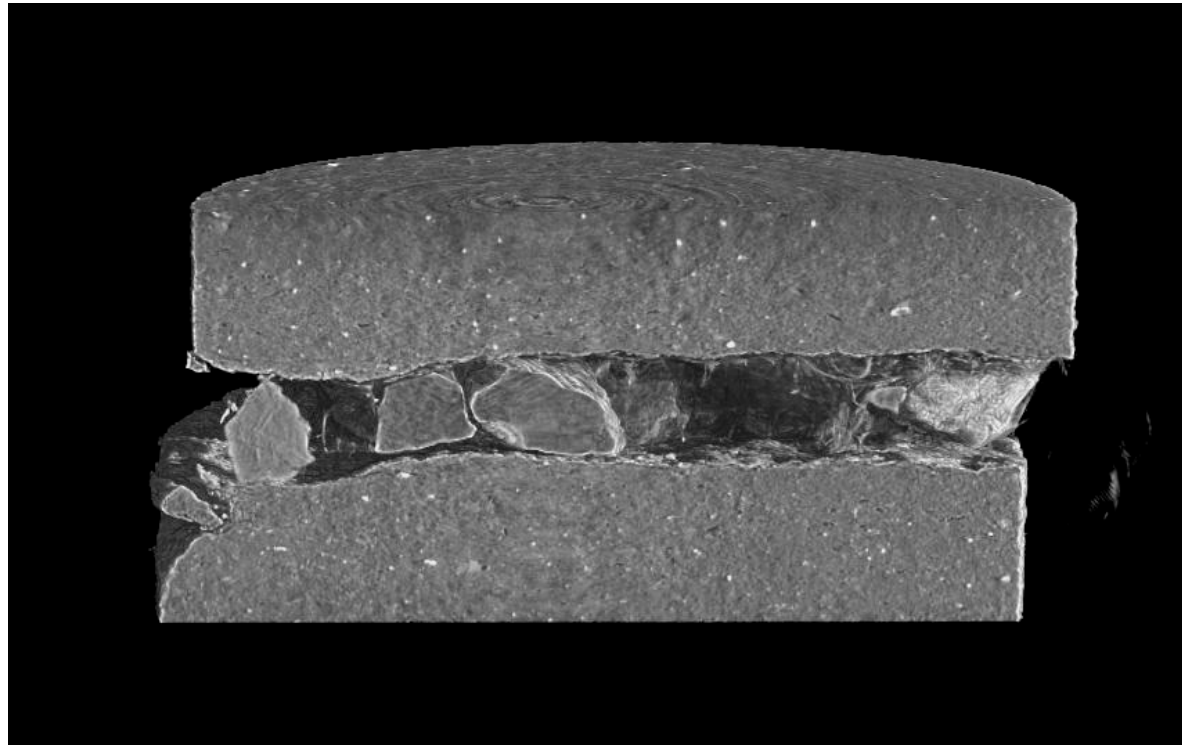
#### **Proppant in a fracture can control the evolution of a fracture, e.g.:**

- **Embedment:** in a plastic rock, the proppant can embed on the surface of the fracture and being inefficient at keeping it open
- **Breakage of the rock:** in a brittle/fragile rock proppant can induce breaking, with fines generation (clogging issues) and decrease of the aperture of the fracture
- **Breakage of proppant:** a strong/rigid rock can induce breakage of the proppant grains, again with fines generation (clogging issues) and decrease of the aperture of the fracture.

**Status: IN PROGRESS**

# Preliminary Test – Task 4

**Preliminary Result:** a combination of both proppant and rock breakage during unconfined compression (progressive increase in axial load) in a relatively brittle Mancos Shale sample:

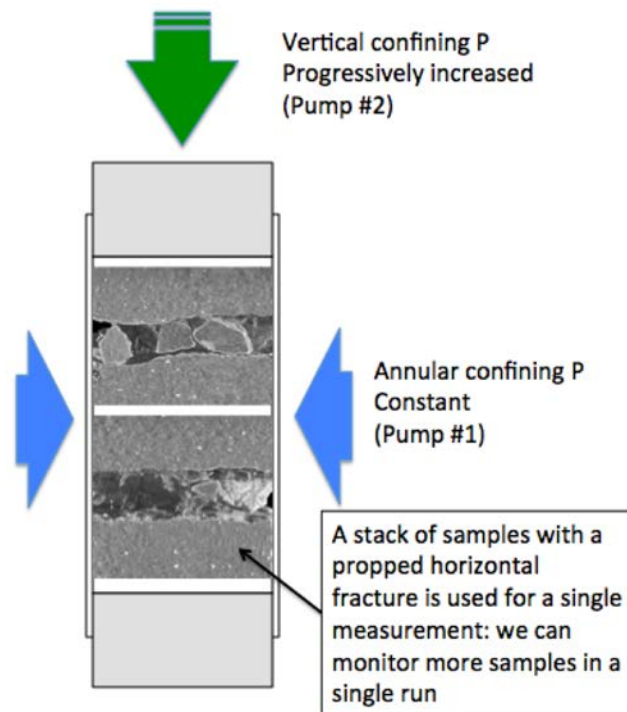
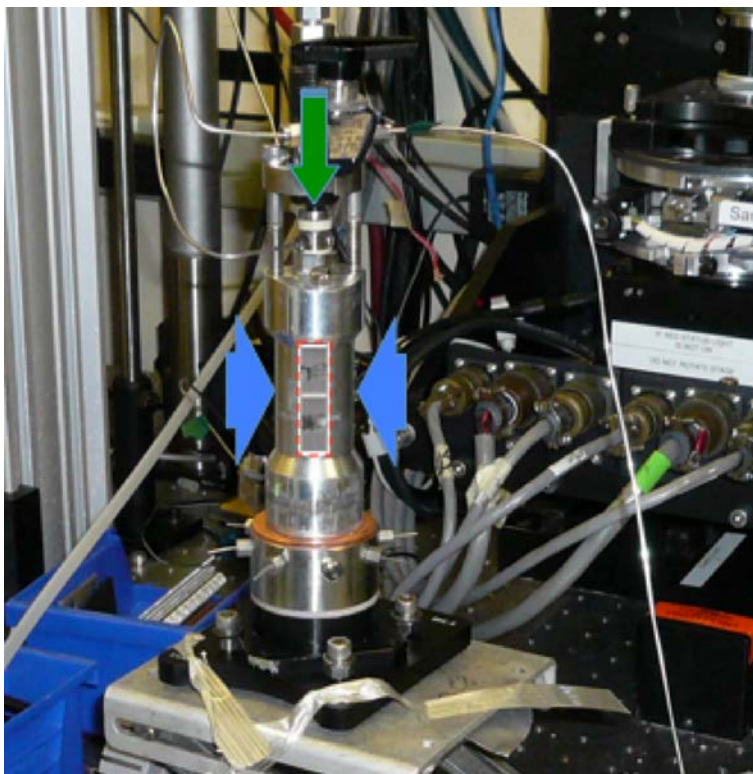


How this changes with rock composition and texture?



# ALS *In Situ* Experiment – Task 4

Plan for the experiment on **July 28<sup>th</sup>-29<sup>th</sup>** at the Advanced Light Source.



- A mini-triaxial cell will be used, thus allowing setting a confining pressure
- Axial pressure is independently set and increased in steps.

# Expected Outcomes – Task 4

- We will learn **about the evolution of the fracture** (volume changes, aperture evolution, flow properties evolution, characterization of microfractures, deformation, etc.)
- Use the 4D datasets to **model** flow properties of the fractures during closure
- **Local strain quantification**
- We can **generalize the observed behaviors** to find e.g. how much clay is needed to have more plastic embedment instead of more brittle breakage, or the load needed to induce close the fractures in different scenarios.

# Task Description – Task 4

## **TASK 4:** Multi-scale laboratory studies of system interactions

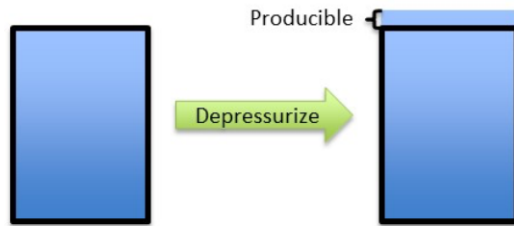
### **Subtask 4.2: Laboratory-Scale Studies**

#### **Objectives**

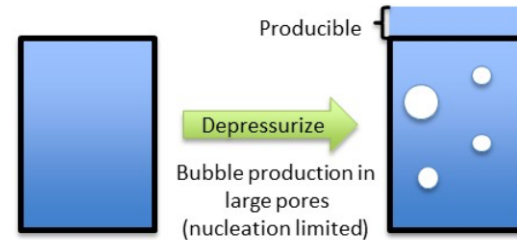
- **Investigate and quantify differences** in possible light tight oil (LTO) EOR techniques suggested by numerical investigation
- Provide **feedback** to simulations
- **Directly observe** proppant transport in variable aperture fractures

Status: **IN PROGRESS**

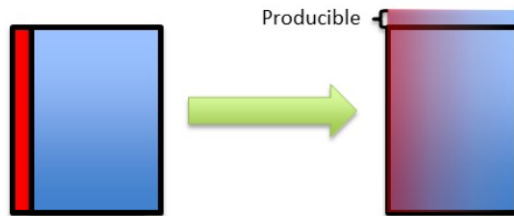
# Task Description – Task 4



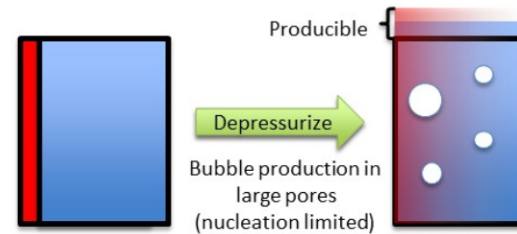
Depressurization



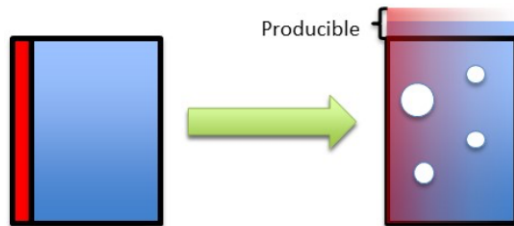
Depressurization with gas



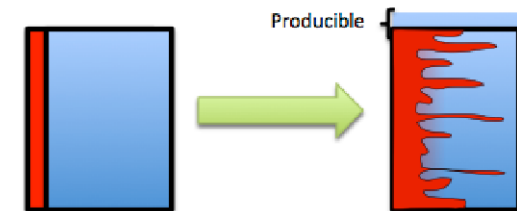
Fluid dissolution into oil



Dissolution with depressurization



Surfactant



Imbibition/Osmotic

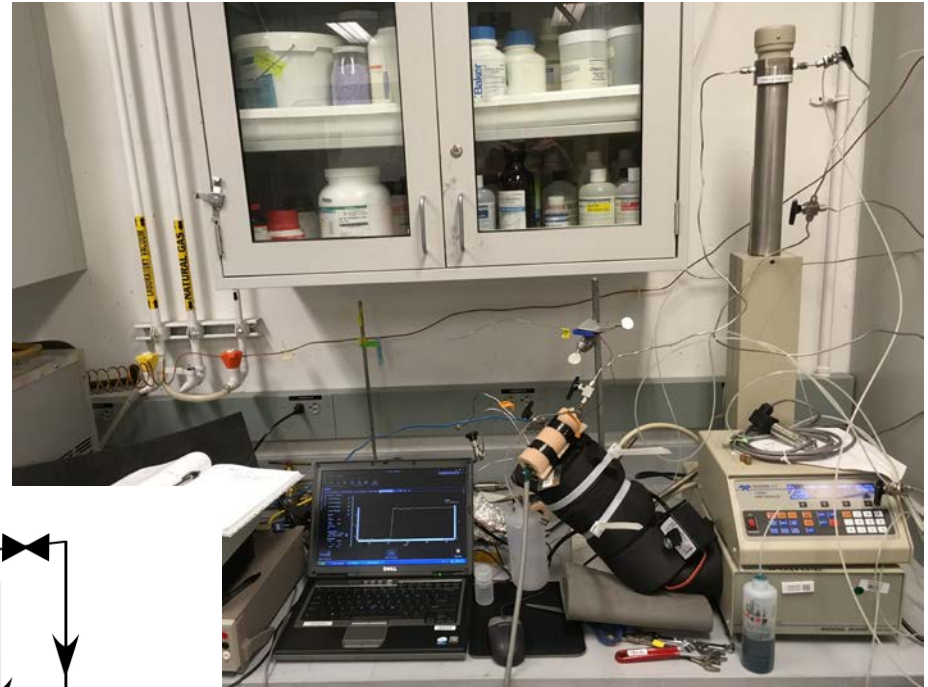
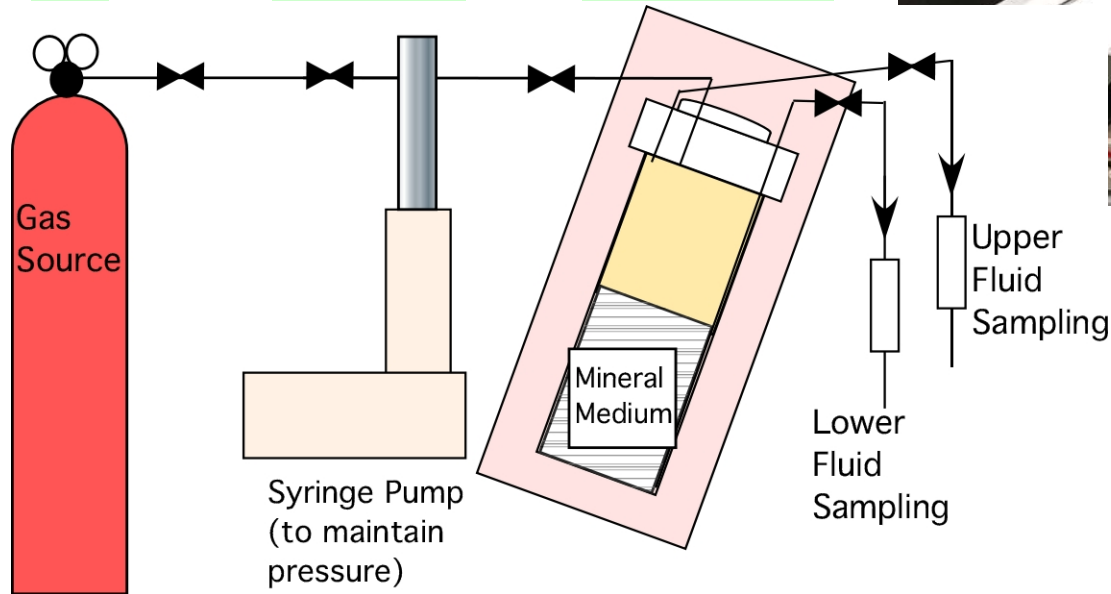
Combinations

# Improved System for Process Eval.– Task 4

Gas or fluid of choice

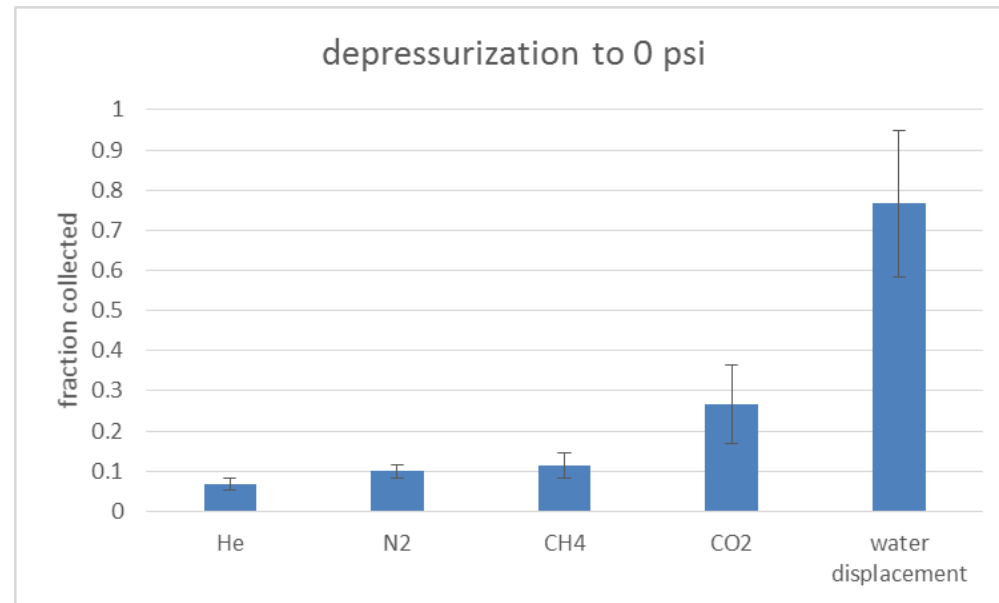
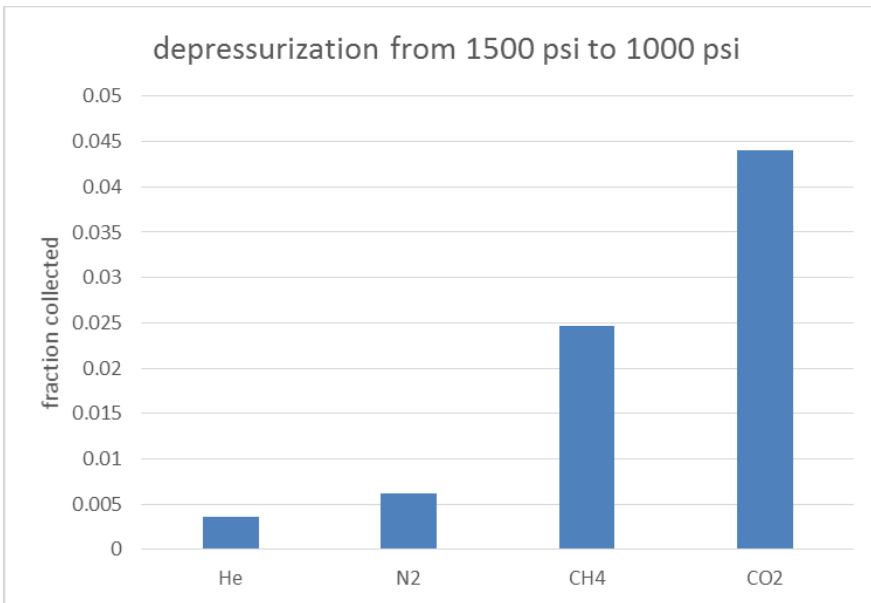
High-pressure syringe pump for pressure control

Porous ceramic disks in layers inside commercial pressure vessel



# Summary – Task 4

scCO<sub>2</sub> > CH<sub>4</sub> > N<sub>2</sub> > He, but water was best.  
CO<sub>2</sub> mass injected >> other gases



# Highlights – Task 4

- Built 2 high-pressure process evaluation test rigs
- Performed 62 tests to evaluate gas dissolution, depressurization, and imbibition
- $\text{scCO}_2 > \text{CH}_4 > \text{N}_2 > \text{He}$ , but water was best
- $\text{CO}_2$  mass injected  $\gg$  other gases

## Next:

- Osmotic displacement (imbibition driven by water activity differences)
- Anisotropic/heterogeneous wetting media
- Sensible technique combinations (avoid permeability jails)
- **Proppant transport** in fractures and corners (**Task 3**)

# Task Description – Task 5

## **TASK 5: Molecular Simulation Analysis of Pore-Scale Interactions**

### **FY15-16 Accomplishments**

- Constructed basic pore simulation system
- Conducted simulations involving flow of water, water plus alkanes, water plus carboxylic acids, and water plus multiple species

### **Results:**

- Characterized differences in the nature of the surface interactions with each species separately
- Characterized surface interactions when species are mixed
- In particular, carboxylic acids appear to help bind alkanes to the pore edge surfaces
- We expect similar effects with substituted alkanes, such as carboxylic, amino, hydroxyl and other functional groups that have some hydrophilic character.



# Task Description – Task 5

## FY17 Objectives (BP #1)

- **Generate larger model clay pore** with appropriate terminations and surface protonations
- Recalibrate earlier simulations to larger scale frame

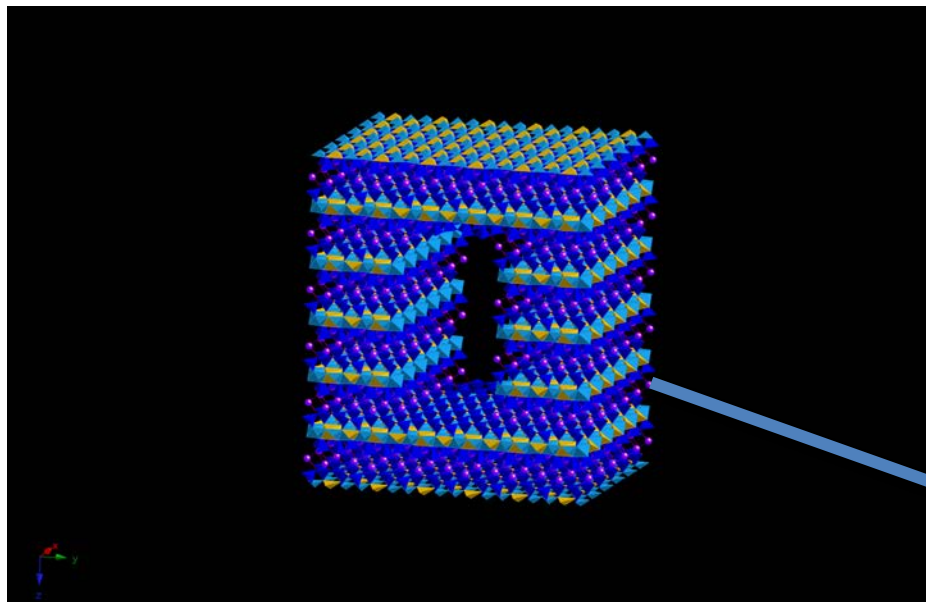
## FY18 Objectives (BP #2)

- Flow simulations for small clay pore model, then extension to **60,000 molecule frame**
- **Comparison of results with imaging** via electron microscopy (as available) on the 2-5 nm scale
- **Compare earlier results** with larger pore model
- Examine behavior of less soluble alkanes with carboxylic acids
- Examine molecular behavior with high organic content fluid

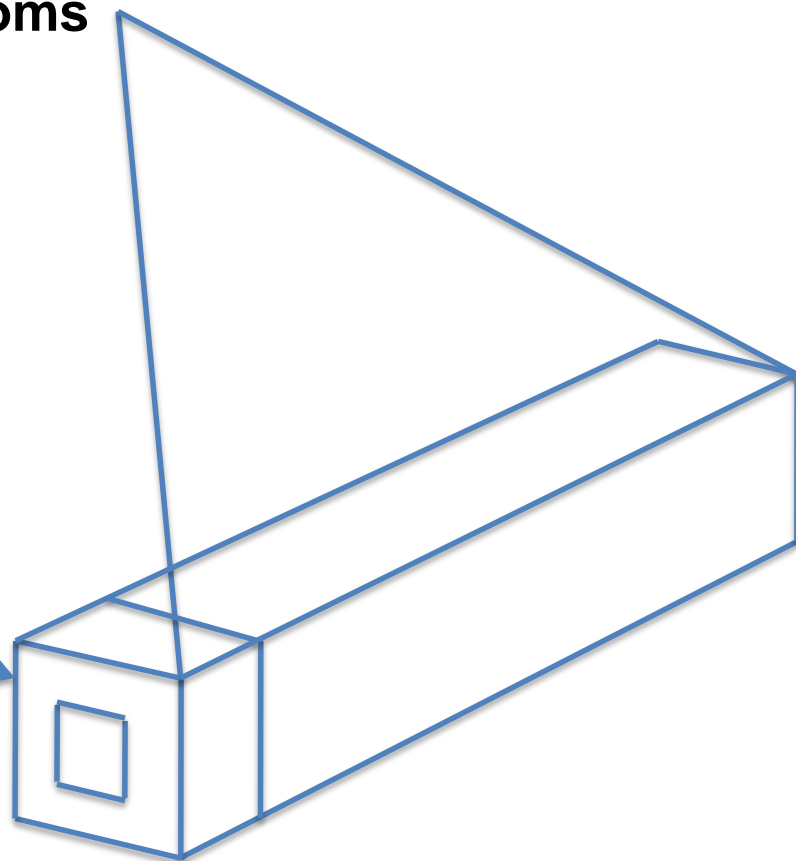
Status: **IN PROGRESS**

# Molecular Simulations – Task 5

**New pore model 6x number of atoms**



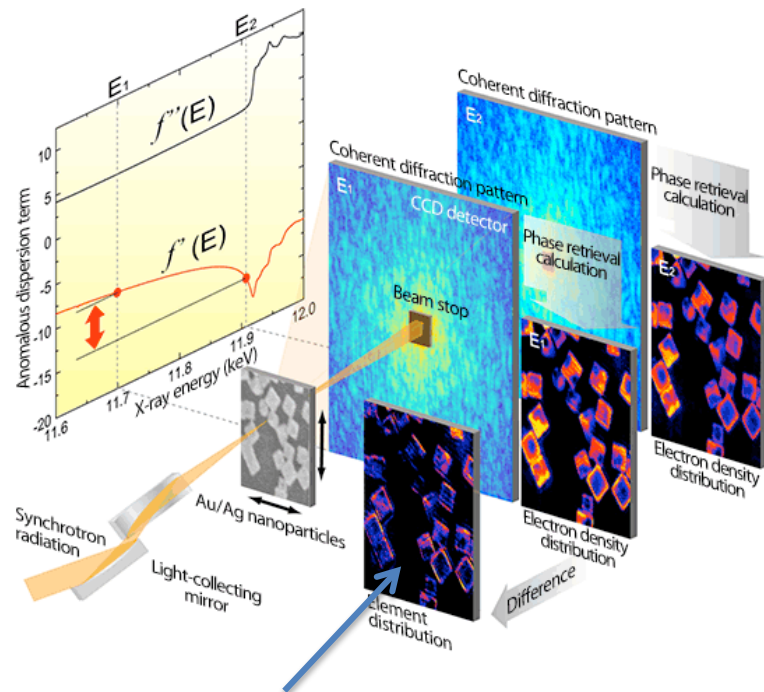
**6x6x6 clay cell model with 3 x 3 x 2 nm pore used in past simulations with reactive fluids ca. 10,000 atoms (uses periodic boundary conditions); protonation determined by contemporary analyses of surface charge behavior (e.g. Bickmore)**



**Proposed next model with 3 x 18 x 2 nm pore ca. 60,000 atoms**

# Future Work – Task 5

Goal: Comparing actual pores with simulations

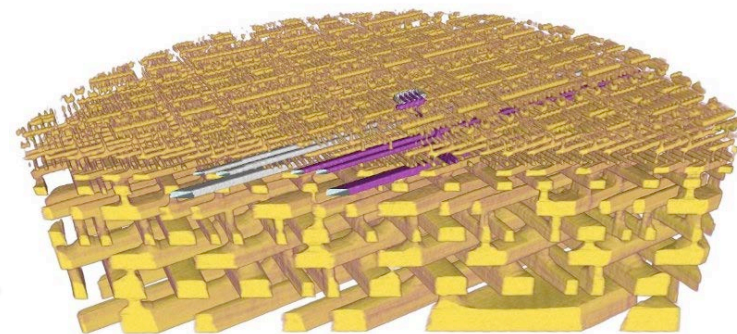


Early work at Molecular Foundry featured Au-Ag nanoparticles; initial studies on clay materials have been attempted

Ptychography tomography used to image 3D structure of Silicon chip at the individual transistor level (14 nm resolution)

## X-ray Ptychography

- requires **coherent** synchrotron source
- can measure *in situ*
- resolution potentially on nm scale with complete chemical (element) sensitivity
- could distinguish among different types of carbon (e.g. -CH, -COOH, -CS)



Holler et al Nature 2017



# Accomplishments to Date

- Development and testing of **T+MCMP**: shale oil/gas all-purpose simulator
- **Evaluation of production enhancement** via:
  - Gas injection (multiple species)
  - Viscosity reduction
  - Thermal enhancement
  - Fracture extent/type
- Development of new **proppant transport** model and code
- **Construction** of 2 high-pressure process evaluation test rigs
  - Performed **62 tests** to evaluate gas dissolution, depressurization, and imbibition
- Prepared for **ALS visualization of cracks and proppants** under **confining pressure**
- **First MD/MFD simulations** of molecular/pore-scale surface phenomena

# Synergy Opportunities

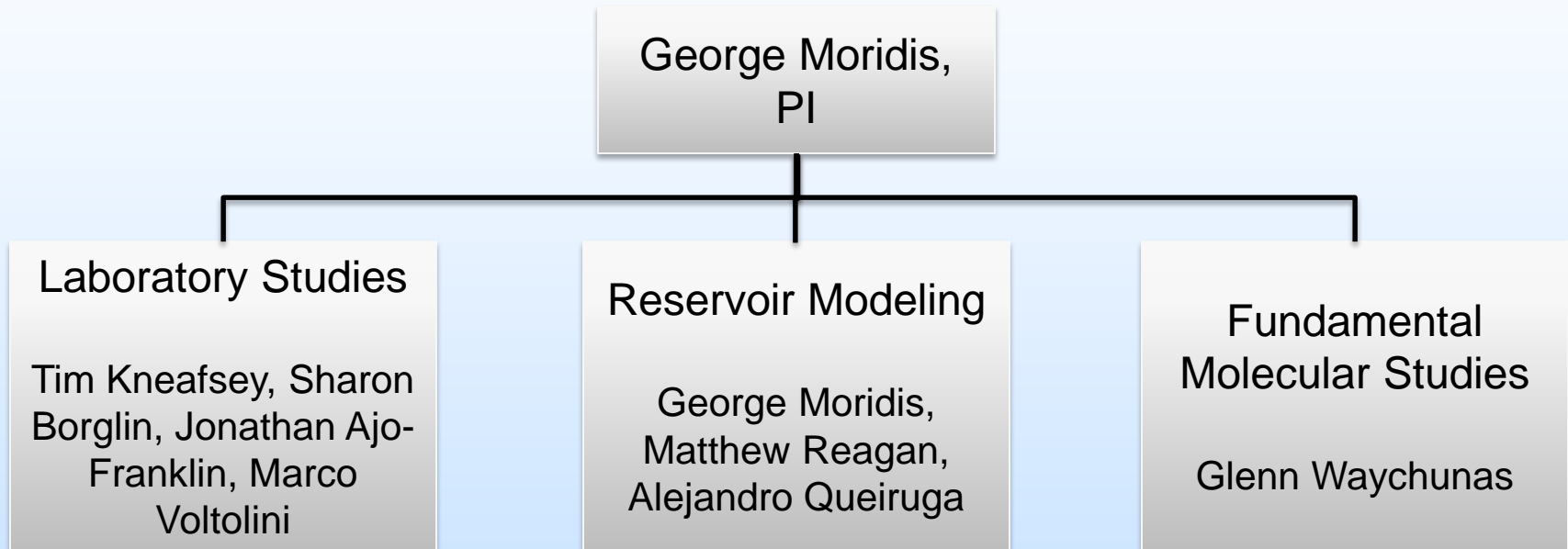
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- Phase II objectives include collaboration goals with other NETL-funded work
- Clear synergies are apparent in approaches, measurements, and analysis of data among similar project themes
- **Comparisons of results** obtained using the various approaches builds confidence in the results and the program

# Appendix

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# Organization Chart



# Technical Status: Phase I Milestones

MILESTONES		
TASK Title/Description	Planned Completion Date (after project inception)	Verification Method
<b>Task 2: Definition of metrics and methodology for screening production strategies</b>	3 months (Budget Period #1)	Topical Report
<b>Task 3: Evaluation of enhanced liquids recovery using displacement processes</b>	7 months (Budget Period #1)	Topical Report
<b>Task 4: Evaluation of enhanced liquids recovery by means of viscosity reduction</b>	9 months (Budget Period #1)	Topical Report
<b>Task 5: Multi-scale laboratory studies of system interactions</b>	17 months (Budget Period #2)	Topical Report
<b>Task 6: Molecular simulation analysis of system interactions</b>	13 months (Budget Period #2)	Topical Report
<b>Task 7: Evaluation of enhanced liquids recovery by means of increased reservoir stimulation, well design and well operation scheduling</b>	18 months (Budget Period #2)	Topical Report
<b>Task 8: Evaluation of combination methods and of new strategies</b>	18 months (Budget Period #2)	Topical Report



# Tasks & Milestones

MILESTONES		
Title/Description	Planned Completion Date (after project inception)	Verification Method
<b>M1:</b> Task 1: Project Management and Planning	1 month and 24 months (Budget Periods #1 & 2)	PMP and regular reports
<b>M2:</b> Documentation of techniques indicated to be inefficient or impractical (Task 2)	6 months (Budget Period #1)	Report documenting inefficient production techniques
<b>M3:</b> Development of a compendium of appropriate production strategies and their respective effectiveness (Task 2)	18 months (Budget Period #2)	Draft of compendium
<b>M4:</b> Deployment of the enhanced TOUGH+ simulator with proppant-modeling capability (Task 3)	12 months (Budget Period #1)	Completion of simulations demonstrating the capabilities of the code, including validation runs.
<b>M5:</b> Completion of tests evaluating the comparative effectiveness of water and scCO <sub>2</sub> injection on LTO recovery (Task 4)	9 months (Budget Period #1)	Completion of experiments, description of comparative effectiveness.
<b>M6:</b> Completion of proppant transport apparatus and initial observations of proppant distribution (Task 4)	15 months (Budget Period #2)	Report documenting the apparatus, and results of initial observations of proppant distribution.
<b>M7:</b> Determination of geometry and character of clay mineral grain surface-fluid molecular attachments and flow for basal and edge planes (Task 5)	12 months (Budget Period #1)	Successful completion of simulations using new molecular models.

