Simulation of the Shale Oil System: from Molecular Fluid Dynamics to Reservoir Scale

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

George Moridis, Matthew Reagan, Glenn Waychunas, Tim Kneafsey, Sharon Borglin, Jonathan Ajo-Franklin, Marco Voltolini
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Mastering the Subsurface Through Technology, Innovation and Collaboration:
Carbon Storage and Oil and Natural Gas Technologies Review Meeting
August 16-18, 2016

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Presentation Outline

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

Benefit to the Program

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 various mechanisms involved in hydrocarbon production from such tight systems,
- Describe the thermodynamic state and overall behavior of the various 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

Technical Status: Phase I Milestones

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

Technical Status: Phase I Milestones

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Task 5: Multi-scale laboratory studies of system interactions	17 months (Budget Period #2)	Topical Report
Task 6: Molecular simulation analysis of system interactions	13 months (Budget Period #2)	Topical Report
Task 7: Evaluation of enhanced liquids recovery by means of increased reservoir stimulation, well design and well operation scheduling	18 months (Budget Period #2)	Topical Report
Task 8: Evaluation of combination methods and of new strategies	18 months (Budget Period #2)	Topical Report

Phase I Complete

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Research Challenges & Approach

Numerous challenges: from fundamental to technology development

Approach

- Fundamental studies to technology development and evaluation (in parallel)
- Gain a deeper understanding of the dominant processes that control production from tight reservoirs
- Develop appropriate and effective production strategies.

Phase 1: 18 months, FY15-16 (completed)
Phase 2: 24 months, FY17-18 (commencing)

Task 2: Metrics and Screening Methodology

Define the feasibility parameters, the specific objectives and metrics of the screening study, and the corresponding methodology for the evaluation of the various strategies to be investigated.

Status: COMPLETED

Successful strategy = increases by >50% in production/recovery over a 3-5 year period (or economic viability of well)

Not possible to use a single metric/approach. Two approaches in defining recovery:

- Based on resource-in-place and function of well spacing
- Based on resource-in-place and function of Reservoir Stimulated Volume (RSV)

Additional issues: Difficulties in describing drainage areas (heterogeneity), stage and cluster spacing

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Task 3: Enhanced Recovery (Displacement)

Evaluation of enhanced recovery using displacement processes

Evaluate "standard" recovery strategies (via simulation) involving displacement processes, accounting for all known system interactions:

- Traditional continuous gas flooding (i.e. natural gas) using parallel horizontal wells (Phase I)
- Water-alternating-gas (WAG) flooding, and
- Huff-and-puff injection/production strategies using lean gas/rich gas in a traditional (single) horizontal well with multiple fractures (Phase II).

Additional numerical evaluations, as warranted by the results:
updated thermophysical properties and PVT relationships

Task 3: Enhanced Recovery (Displacement)

Code Development: TOUGH+MultiComponentMultiPhase (T+MCMP)

- **Builds on NETL-funded TOUGH+ codes (TOUGH+HYDRATE)**
- **Builds on RPSEA-funded codes for modeling shale properties (TOUGH+RealGasBrine)**
- **Conventional and tight/shale oil (heavy) simulations**
- **CO_2 enhanced oil recovery (CH_4, N_2)**
- **Shale-specific physics:** sorption, non-Darcy effects, Knudson diffusion, Forchheimer flow, etc.
- CH_4- and CO_2-hydrate formation (adapted from NETL hydrates studies)
- "Fully compositional" model, fully non-isothermal
- Up to 3 oil components, H_2O, salt, and up to 18 gas components
- Minimum 1, maximum 23 equations/element
- **A platform for all further numerical simulation**

Task 3: Shale Oil Production

PROGRESS: Simulation Studies

REFERENCE CASE: DEPRESSURIZATION

- **TOUGH+MCMP**

- **Eagle Ford shale oil properties**
- **Reservoir depth**: 6560 ft
- **Constant bottomhole pressure (P = 1500 psia)**
- **Shale permeability**: 10 nD, 100 nD, 1000 nD
- **Shale porosity**: 5%
- **Fracture options**:
  - No fractures,
  - Hydraulic fractures (Type I)
  - Type III/IV fracture systems (in progress for Phase II)
- **Oil: C8-C14 (pseudo-component), full property description**

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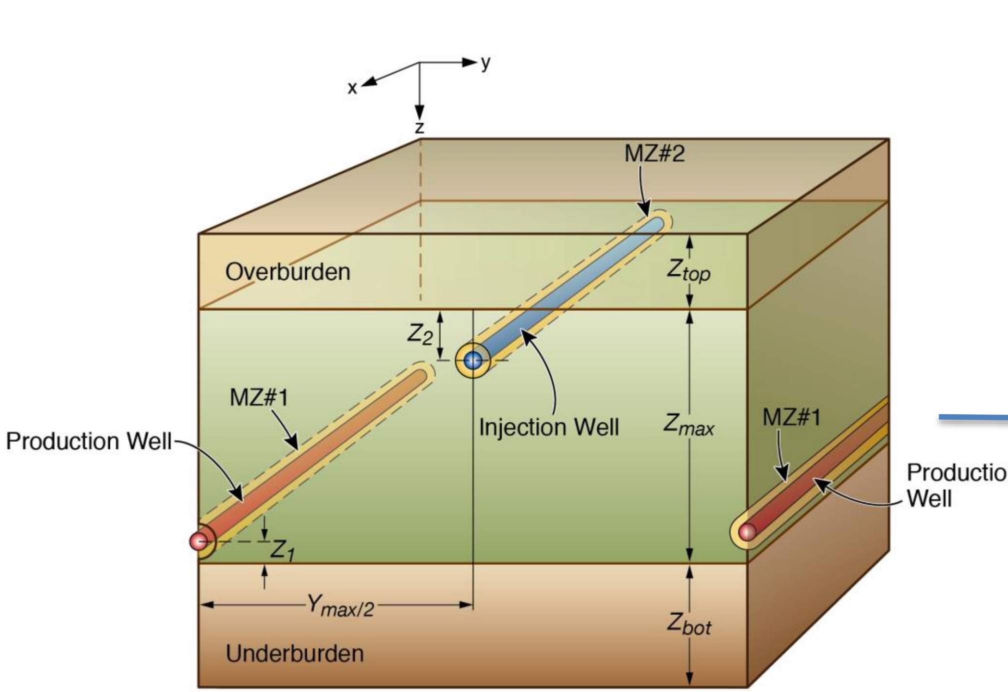
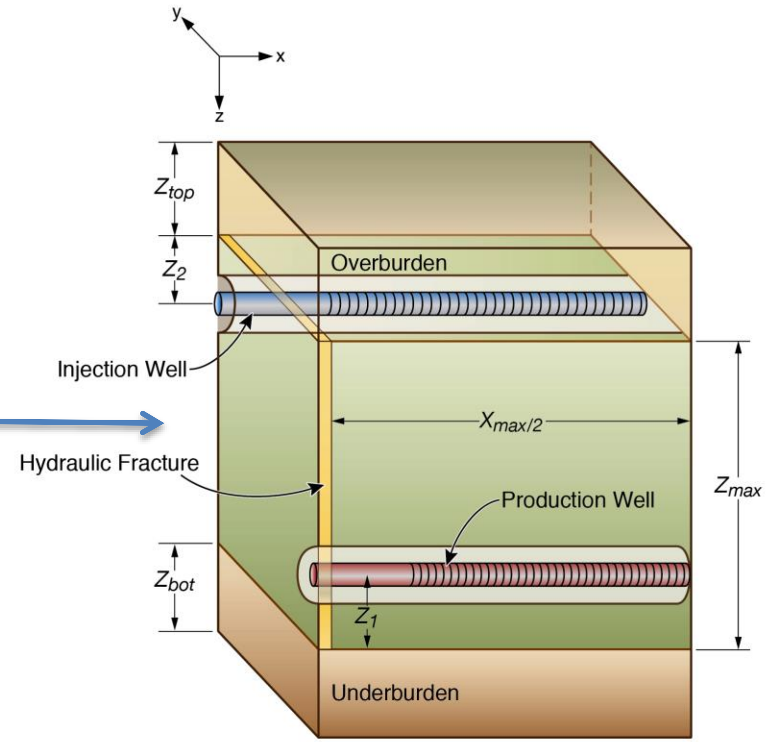
Task 3: Shale Oil Production: Basic Stencil



MZ#1 and MZ#2: Modified Zone



REFERENCE CASE

Z_{max} = 10 m (33 ft)

$Y_{max}/2$ = 10 m (33 ft)

Z_1 = 1 m (3.3 m)

$Z_{top} = Z_{bot} = 0$

REFERENCE CASE

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

No injection well

Z_1, Z_2 : Optimization parameter

Extremely fine discretization:

370,000-740,000 elements

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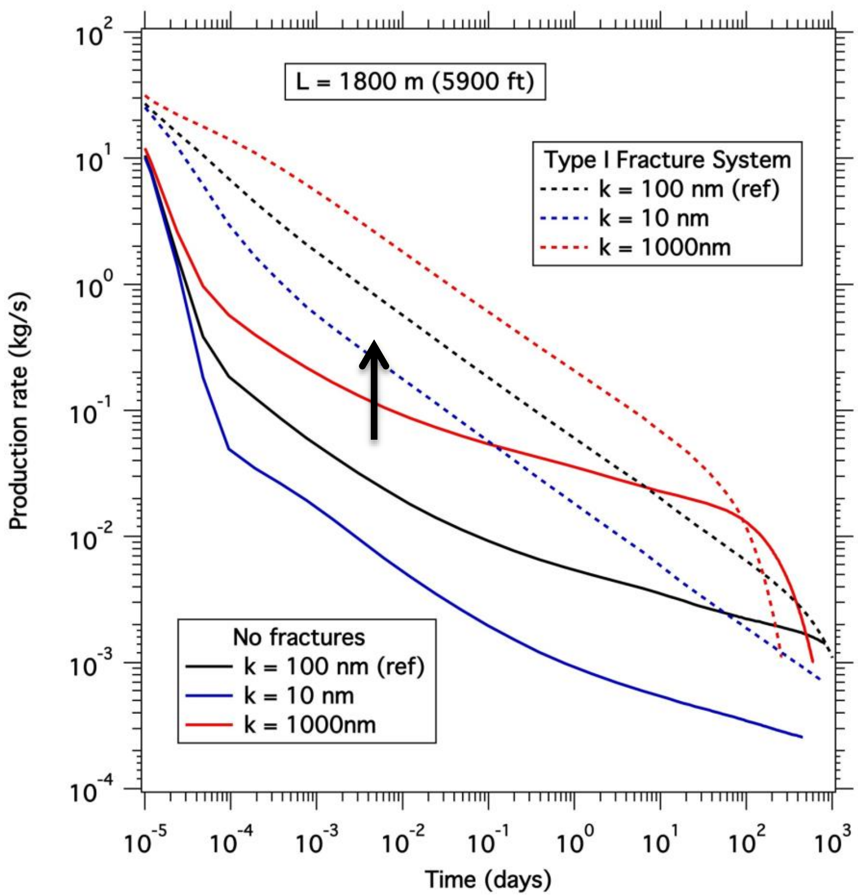
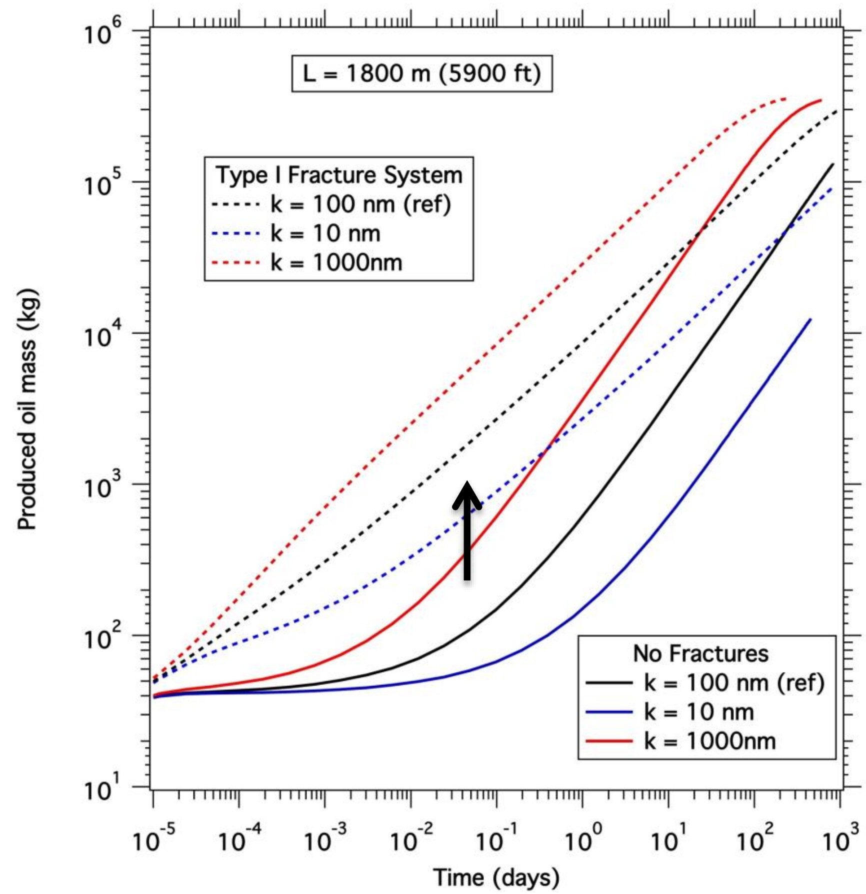
Task 3: Shale Oil Production

REFERENCE CASE



Oil Production (No injection)



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Effect of fracturing and of matrix permeability

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Task 4: Enhanced Recovery (Viscosity)

Evaluation of enhanced recovery by means of viscosity reduction

Evaluate numerically "standard" recovery strategies based on viscosity reduction:

- flooding using appropriate gases (e.g., CO_2, N_2, CH_4) and appropriate well configurations (viscosity reduction resulting from the gas dissolution)
- gas flooding due to phase changes (i.e. depressurization of **gassy oil**)
- thermal processes: viscosity reduction caused by heating

Sub-Task 4.1: *Evaluation of viscosity-reduction-based strategies using (a) standard thermodynamics and (b) "nano-pore-adjusted" thermodynamics* **(in Task 6 – Phase II activity)**

Sub-Task 4.2: *Evaluation of new viscosity-reduction-based strategies suggested from molecular simulation studies* **(in Phase II– future activity)**

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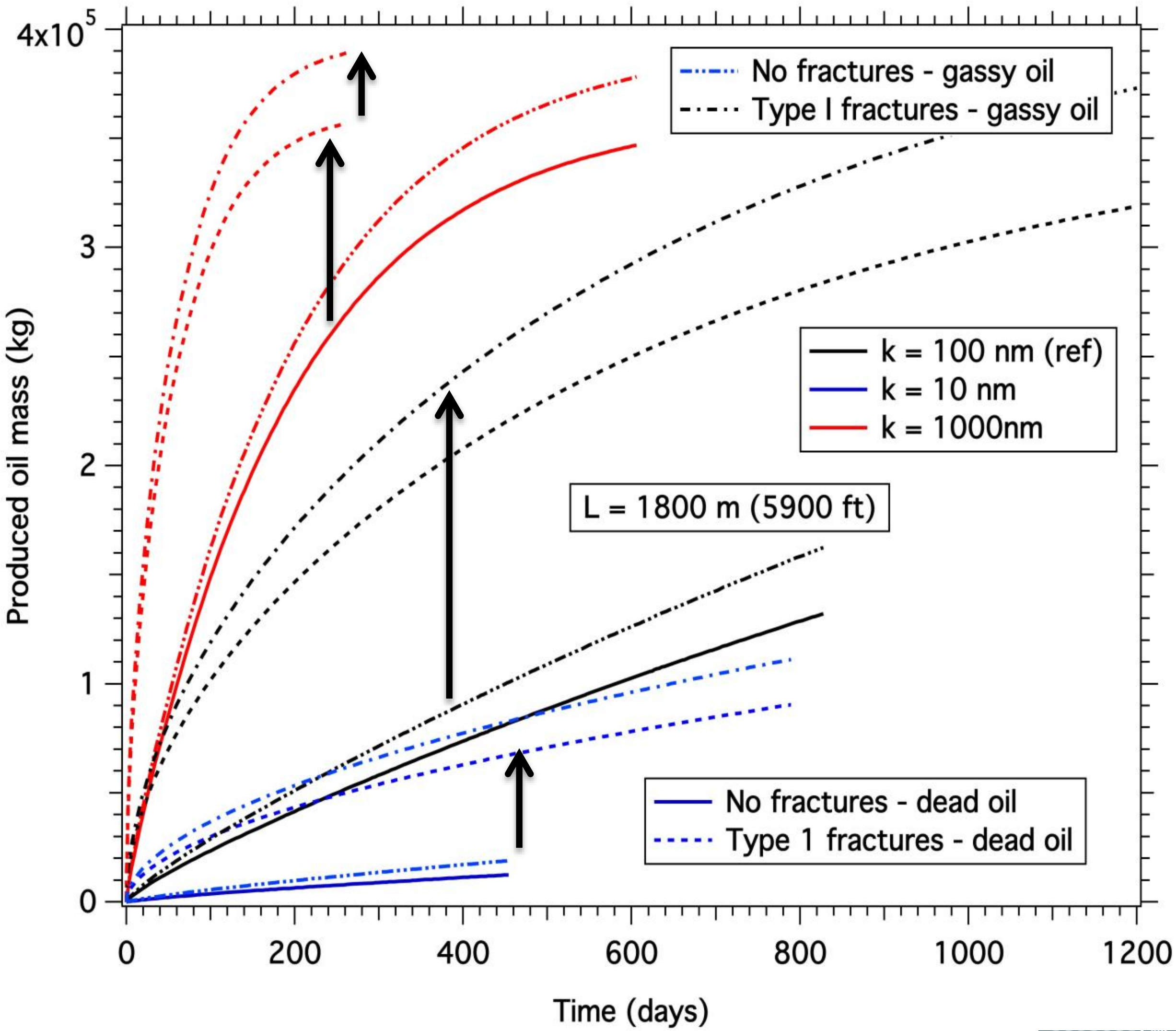
Task 3 & 4: Shale Oil Production

Effect of dissolved gas

Effect of fracturing and of matrix permeability, too



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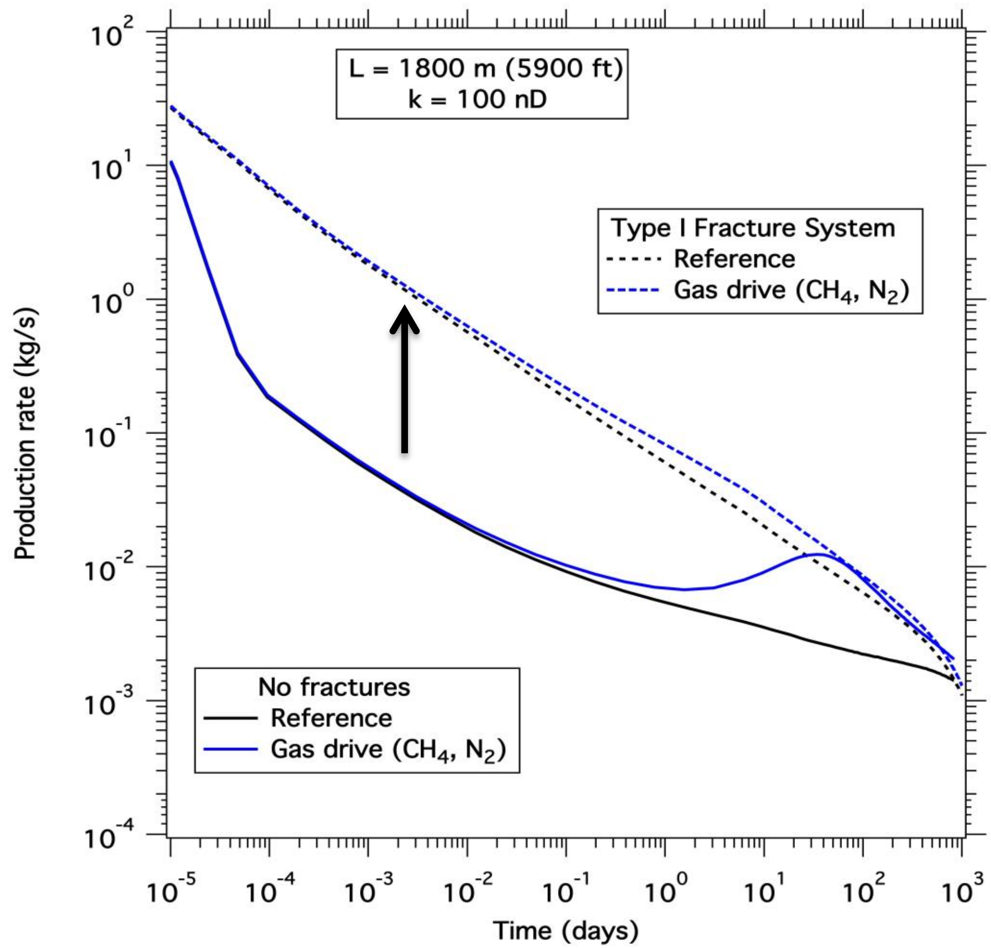
Task 3 & 4: Shale Oil Production

REFERENCE CASE

Displacement process: gas drive

No discernible difference between N_2 and CH_4 (latter not affecting the oil properties); re-evaluating basic equations



Need for supporting lab studies – inadequate physics

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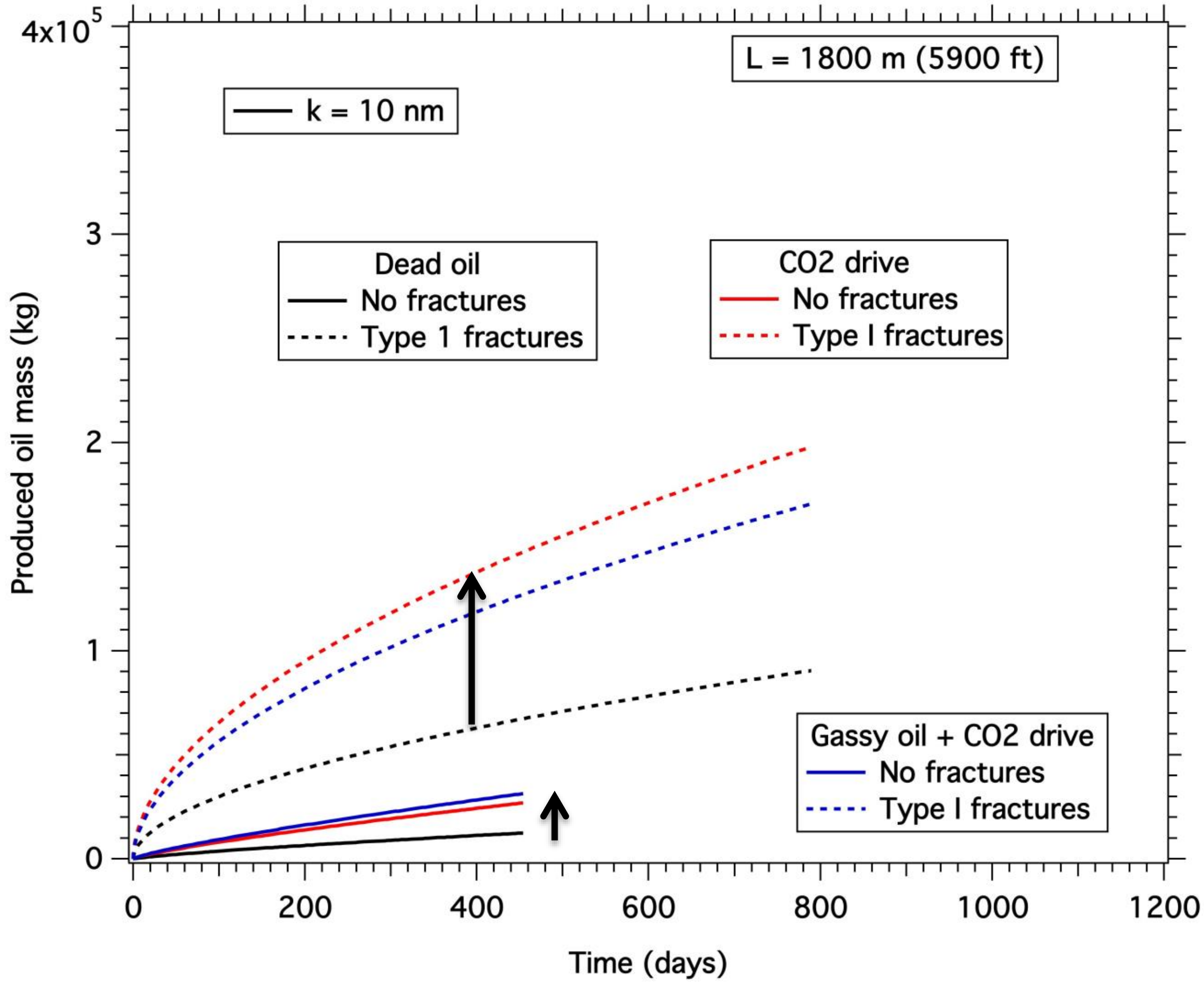
Task 3 & 4: Shale Oil Production

CO_2 Case 1: 10nD
Dead oil,
CO_2 drive,
gassy oil+CO_2 drive



Displacement process: gas drive vs. phase changes

Significant effects

New CO_2 properties module

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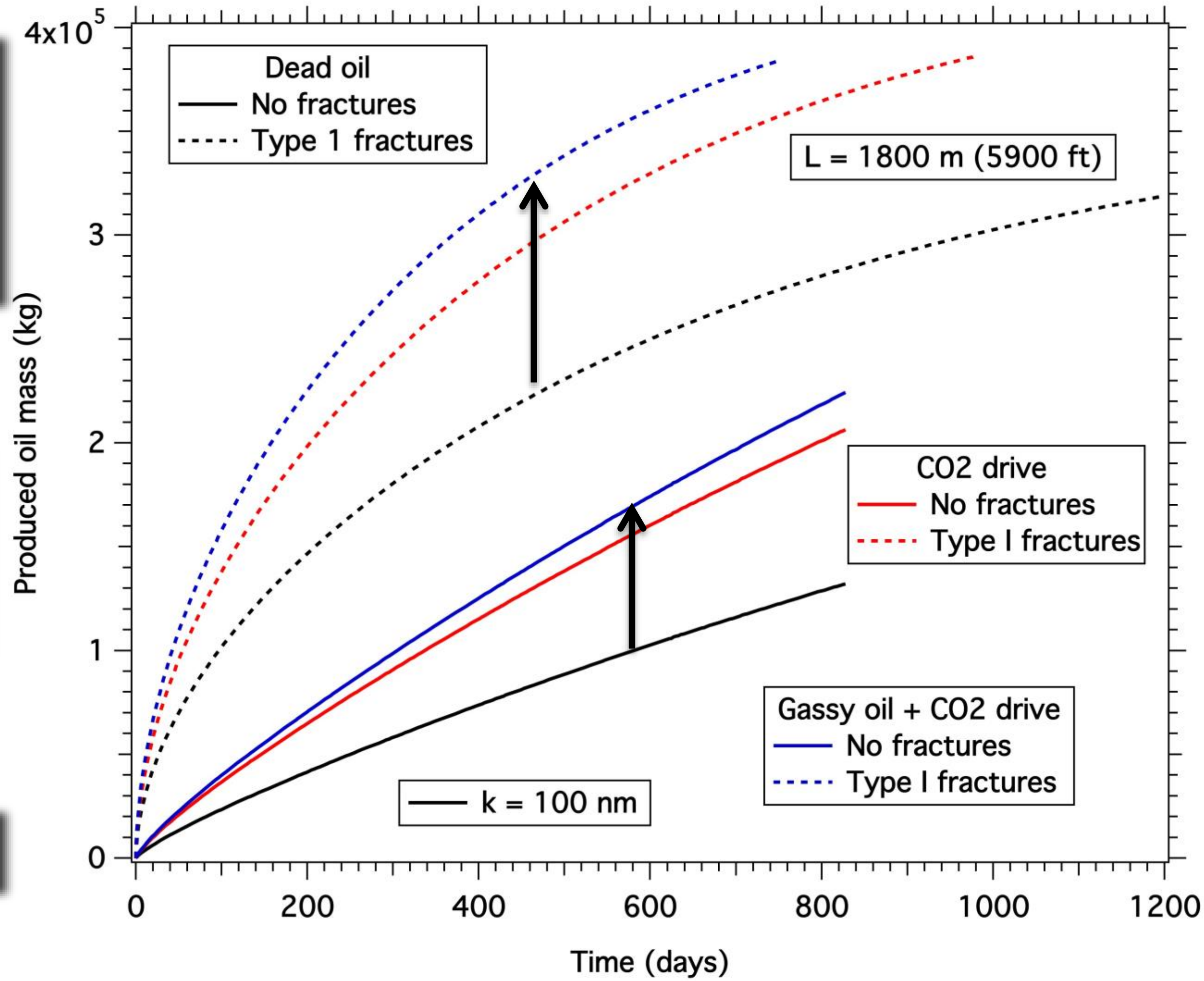
Task 3 & 4: Shale Oil Production

CO_2 Case 1: 100nD
Dead oil,
CO_2 drive,
gassy oil+CO_2 drive

Displacement process: now gas drive in both cases

Significant effects



New CO_2 properties module

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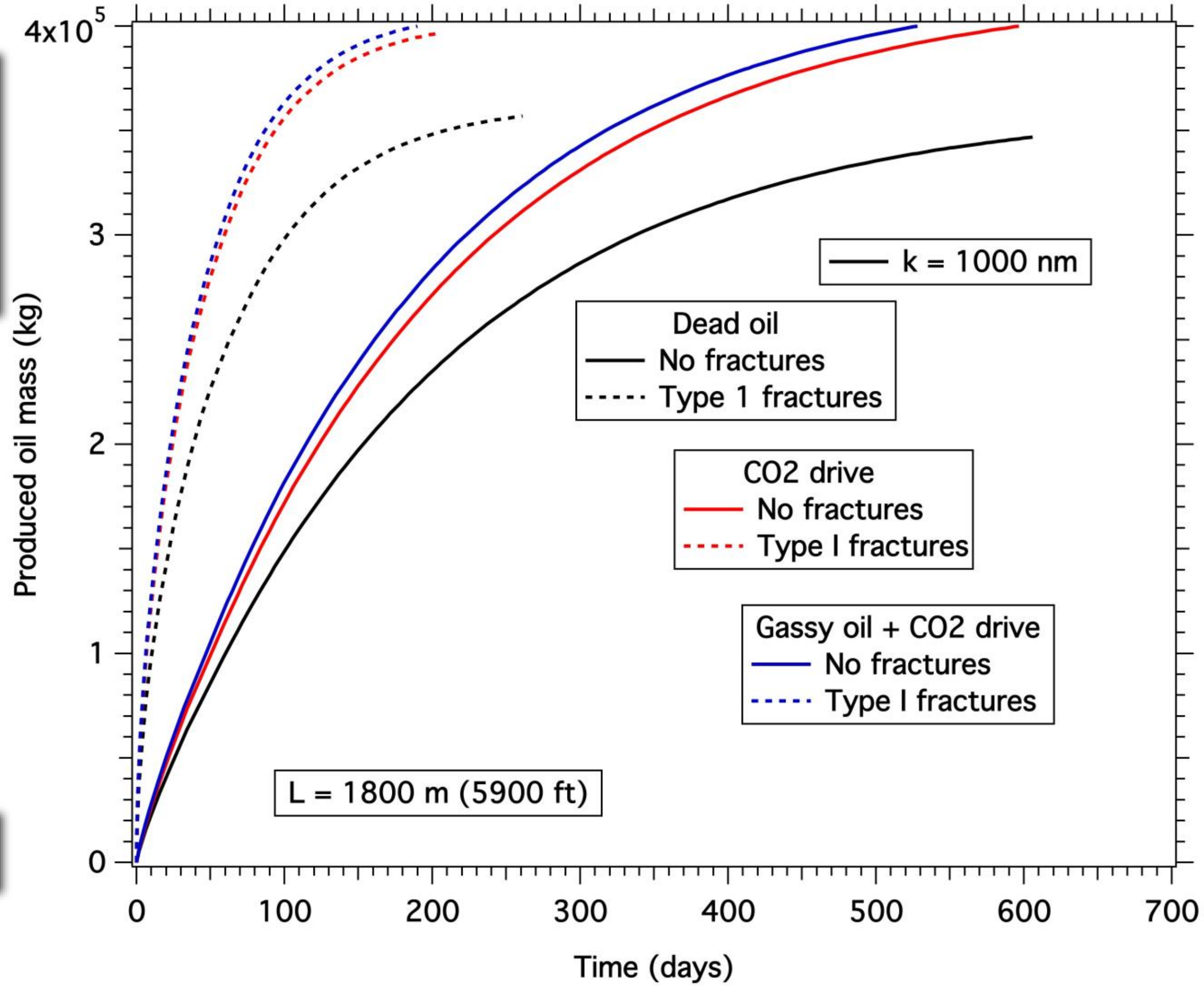
Task 3 & 4: Shale Oil Production

CO_2 Case 1: 1000nD
Dead oil,
CO_2 drive,
gassy oil+CO_2 drive

Displacement process: gas drive, earlier depletion

Significant effects



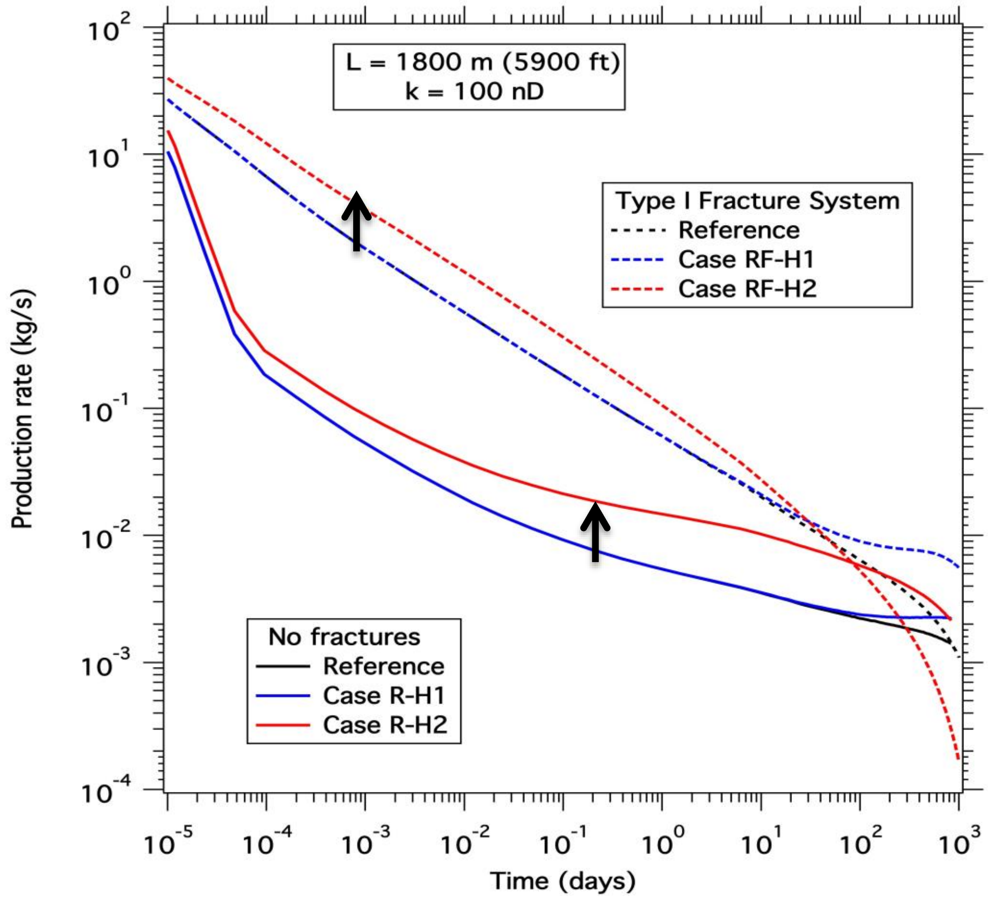
Task 3 & 4: Shale Oil Production

REFERENCE CASE

Thermal processes:
H1: Heating at t = 0
H2: Heating at t = - 30 d

Sealed injection well, circulating steam

Timing is important: early heating effective, heating at time of production ineffective (study continues)



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Task 7: Enhanced Recovery (Stimulation)

Evaluation of enhanced liquids recovery by means of increased reservoir stimulation, well design and well operation scheduling

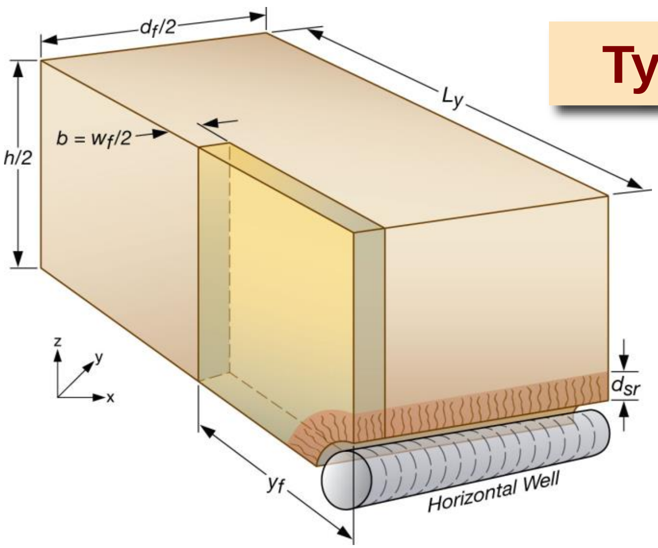
Evaluate numerically the effects of enhanced reservoir stimulation (e.g., using 20-25 stimulated wells per section) on the recovery of liquids:

- Additional fracture formation (primary, secondary, natural)
- Evaluate the performance of improved/appropriate well designs
- Evaluate the effects of appropriate operation scheduling/sequencing

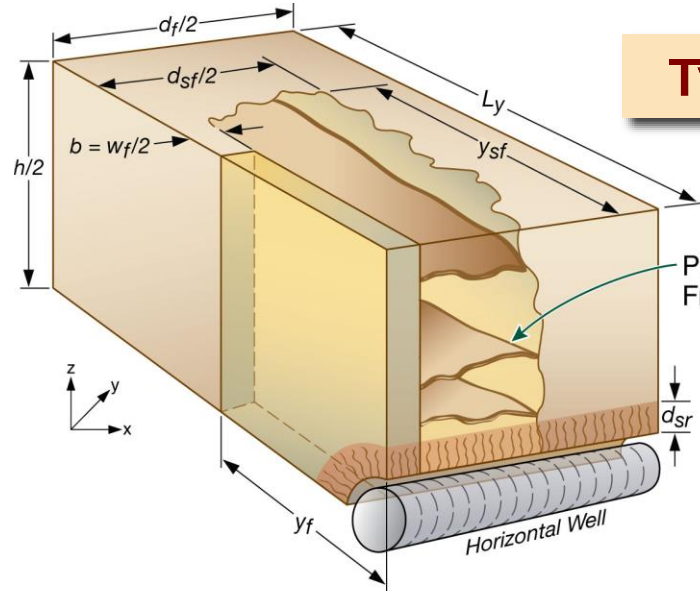
As in Tasks 3 and 4: Sensitivity analyses to determine the parameters and conditions controlling the liquids production in the various production strategies

Task 7: Types of fractured systems

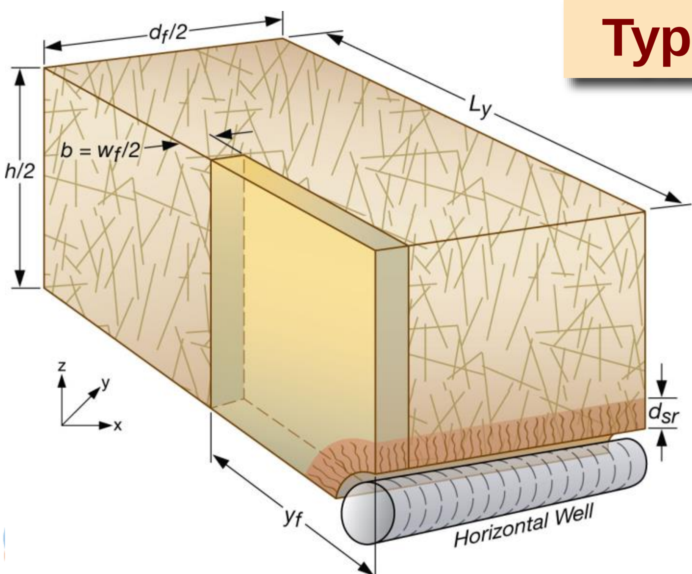
Type I



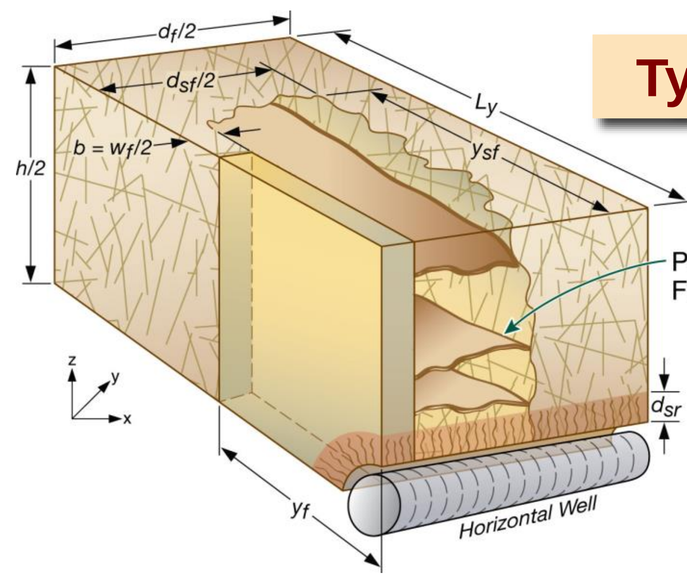
Type II



Type III



Type IV

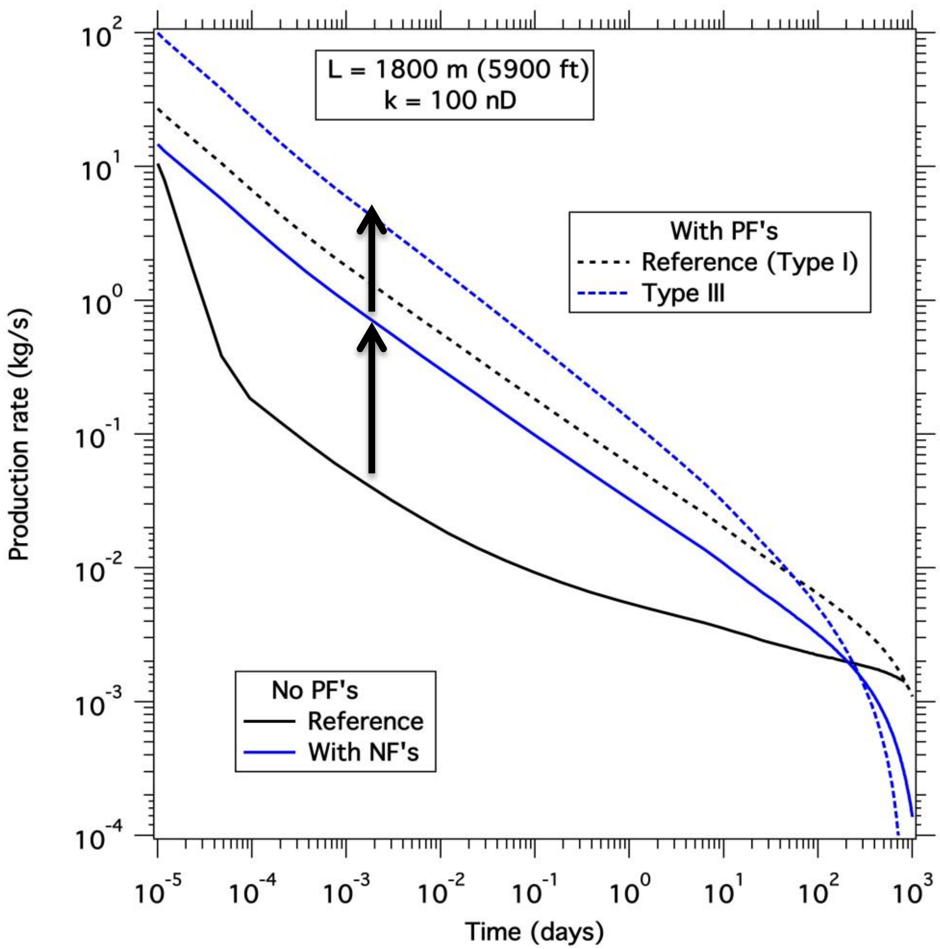


Task 7: Shale Oil Production

Example:
Effect of fracture types/distribution

Natural, primary, and/or secondary fractures

Significant impact!



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Task 6: Molecular Fluid Dynamics

Molecular Fluid Dynamics-based simulation analysis of molecular system interactions

Study the expected fluid interactions and behavior in the most promising production scenarios identified in Tasks 3 and 4, as further focused by the laboratory results in Task 5.

- Grand Canonical Monte Carlo (GCMC) simulations at constant temperature, chemical potential of the confined fluid, and pore volume
- Classical Molecular Dynamics (CMD) simulations at constant density (pressure) and temperature
- **Classical Molecular Dynamics (CMD) using reactive potentials to simulate chemical reactions (water-oil; oil-silicate; silicate-water) at interfaces**

- **Compare simulation results to nano-scale visualization studies**
- **Develop appropriate PVT relationships to incorporate into simulations**
- **Seek clues to enhanced recovery techniques**

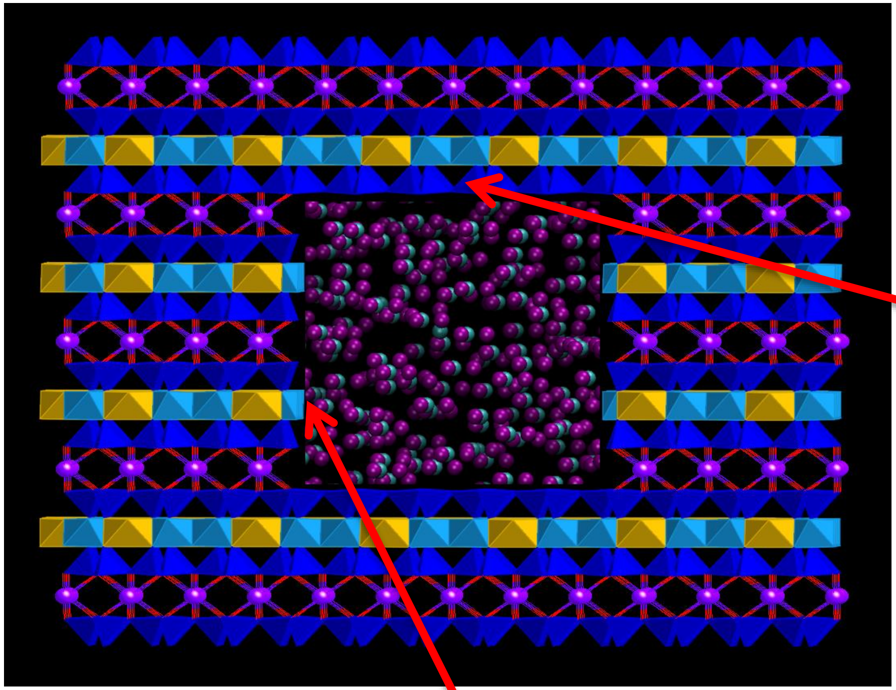
Task 6: Molecular Fluid Dynamics

Definition of domain/setup:

- **Novel geometry exposes basal plane and edges to flow**
- **Novel use of reactive potentials**

- **Two methodologies for flow:**
- (a) enhanced flow-direction-oriented gravitational forces
- (b) fluid flow with constrained laminar velocity profile
- **Use the LAMMPS program on NERSC supercomputers**

- **OIL**: (a) C8 alkanes or (b) alkane with substituent species
- **Water**: H_2O with dissolved oils; clay pore solution inorganics
- **Pore structure:** from micro-CT studies/TEM when available



Basal plane silica sites

Edge sites with Al and Mg (oxide-like) chemistry

The initial clay tunnel/pore simulation cell. Central water molecules are red (H_2) and green (O_2). Flow direction into the figure. 12000 atoms; 4 x 5 x 5 nm; pore 1.5 x 1.5 x 5 nm

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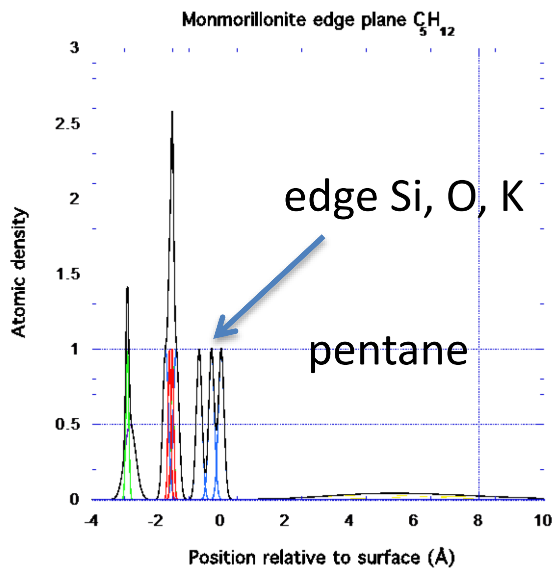
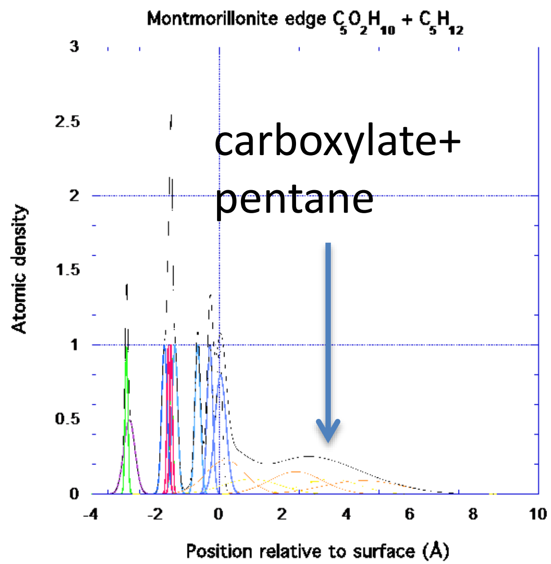
Task 6: Molecular Fluid Dynamics

- Interactions of fluid with clay surfaces depend on fluid composition; carboxylics bind to oil and edges, slowing near edge flow
- Interactions of basal plane much different from edges in terms of reactivity

Addition of carboxylate to aqueous phase binds pentane to the edges of montmorillionite. Results not observable without reactive potentials.





Phase II work: Install flow to all simulations; enlarge system to 80K atoms (ca. 10 x 10 x 10 nm; pore to 3 x 3 x 10 nm)

- Study flow characteristics for various P,T solution compositions
- Test effect on flow of varied aqueous phase chemistry
- Evaluate possible extension to 10^6 atoms using reactive potentials

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Accomplishments to Date

(Phase I Simulation tasks)

- Development and testing of T+MCMP: shale oil/gas all-purpose simulator
- Evaluation of production enhancement via:
  - Gas injection
  - Viscosity reduction
  - Fracture extent/type
- First MD/MFD simulations of molecular/pore-scale surface phenomena

- Work on hold until Phase II commences

Future Activities– Phase II

- Continuation of simulation studies
  - Completion of sensitivity studies
  - Inclusion of more complex fractured systems
  - Assessment of optimal combinations of methods
  - Translation of results of upscaling studies (lab, MFD) into numerical simulator (completion of code development)
  - Updating effects of gas dissolution on gas viscosity and critical oil saturation (based on the lab studies)
  - Studies involving multi-component oils (Bakken or Eagle Ford analogs)
- Transport and geomechanical fate of proppants (new task!)
- Coordination with laboratory and visualization tasks

Synergy Opportunities

- 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

Gantt Chart

Budget Period	#1			#2		
Quarter	Q1	Q2	Q3	Q4	Q5	Q6
Task 1: Project Management and Planning	X					
Task 2: Definition of metrics and methodology for screening production strategies	X					
Task 3: Evaluation of enhanced liquids recovery using displacement processes			X			
Task 4: Evaluation of enhanced liquids recovery by means of viscosity reduction			X			
Task 5: Multi-scale laboratory studies of system interactions						X
Task 6: Molecular simulation analysis of system interactions					X	
Task 7: Evaluation of enhanced liquids recovery by means of increased reservoir stimulation, well design and well operation scheduling						X
Task 8: Evaluation of combination methods and of new strategies						X

Phase I completed. The budget is exhausted at this time--effort much more demanding than expected. Phase II commencing soon.

Organization Chart

George Moridis, PI

- **Laboratory Studies**
  Tim Kneafsey, Sharon Borglin, Jonathan Ajo-Franklin, Marco Voltolini
- **Reservoir Modeling**
  George Moridis, Matthew Reagan
- **Fundamental Molecular Studies**
  Glenn Waychunas