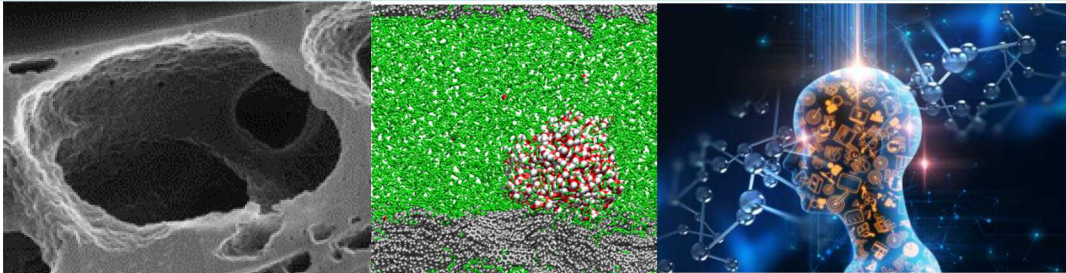




Sandia  
National  
Laboratories

SAND2018-9235PE

# Understanding Fluid Interaction and Transport in Unconventional Reservoirs: From Nanoscale to Wellbore Production



PRESENTED BY

Yifeng Wang



Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.



## Sustainability of shale oil/gas production:

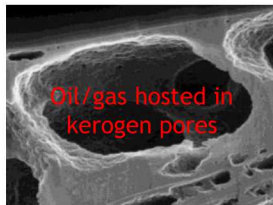
- Large variability and unexpected rapid decline in well production (up 95% reduction over first 3 years)
- New wells to be drilled to maintain the supply, with increasing cost/well
- Low recovery rates (<10%), with little known about secondary gas recovery in “brown fields” (>90% of total gas reserve!!!).
- Long-term production projection largely empirical

## Locating sweet spots, maximizing individual wellbore production while minimizing environmental impacts.

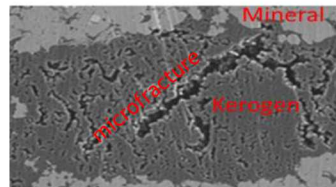
- Existing practice largely empirical.

## Limiting step of oil/gas production:

- Fluid interaction and transport in nanoporous shale matrix
- Knowledge drawn from conventional reservoirs is not applicable.
- Mechanistic understanding of oil/gas disposition and release in shale matrix is crucial for developing engineering approach to maximizing wellbore production and extending the production cycle.

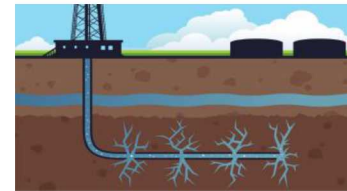


Oil/gas release from kerogen pores (Pore size: nanometer scale)

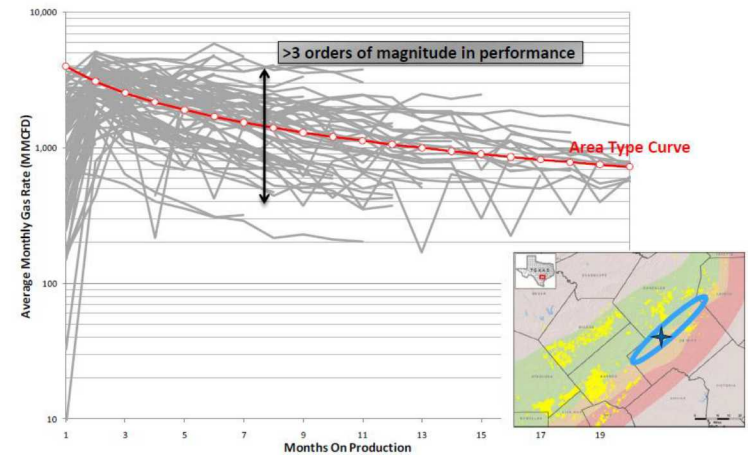


Fluids “flow” from kerogen via microfractures or connected pore networks (Channel size: micrometer scale)

Limiting step(s)

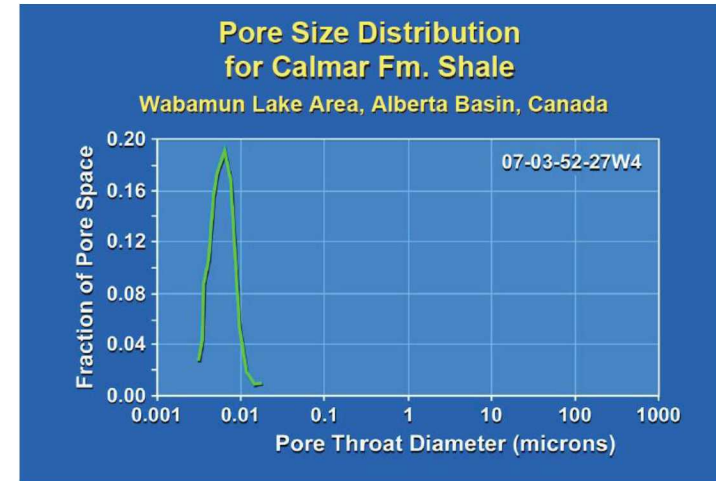


Fluids flow into hydraulic fractures then to production well (Channel size: millimeters to decimeters)

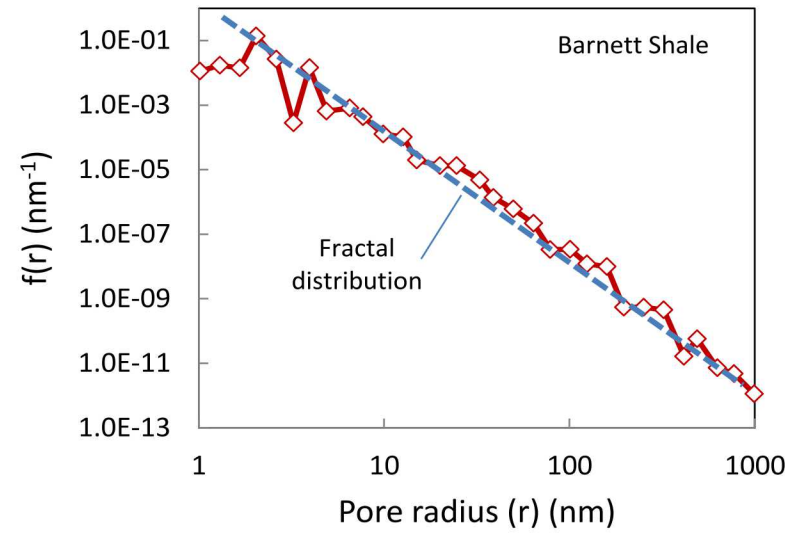


Robertson (2013)

# Shale as a nanocomposite material

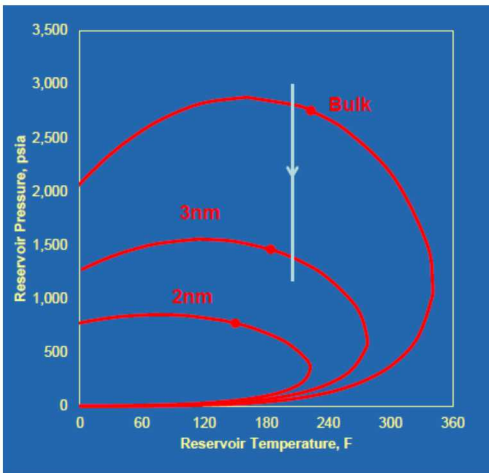


Bachu & Bennion (2006)

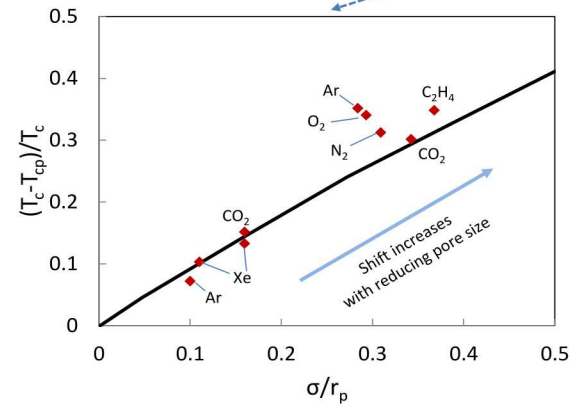


Clarkson et al. (2012)

# Effects of nanopore confinement



Akkutlu, 2013

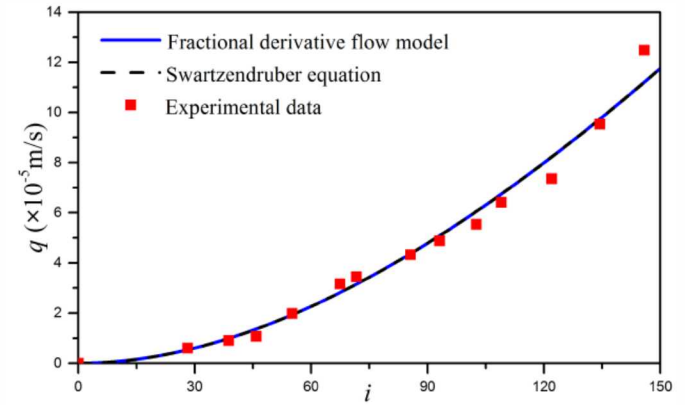
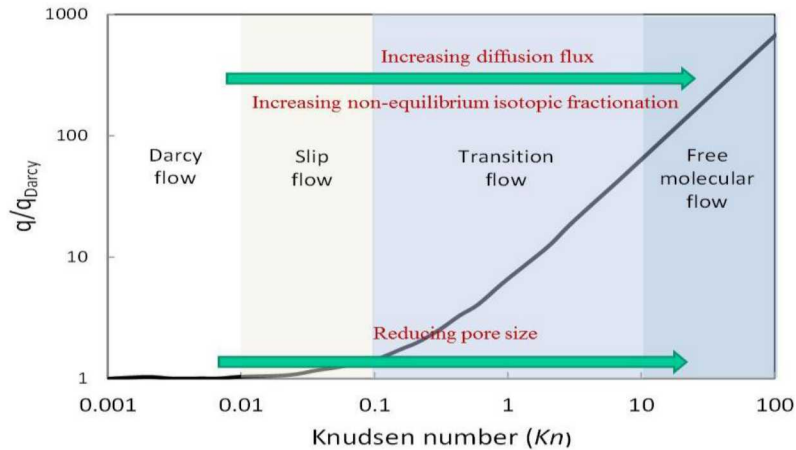


Wang (2014); Zarragoicochea and Kuz (2004)

**Rule of thumb:** Chemical species under nanoconfinement behave drastically differently from those unconfined (i.e., those in bulk phase). Nanoconfinement modifies:

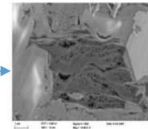
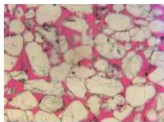
- Thermodynamic properties
- Kinetic properties
- Transport properties
- Others

# Emergent transport properties in nanopores: Isotopic fractionation



Zhou et al. (2018)

Conventional  
reservoir



Shale formation

SPE 124253 (2009)

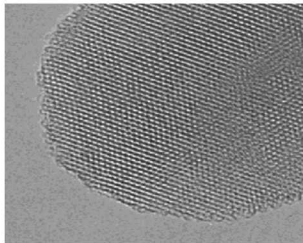
$$k_{app} = \frac{2r}{3RT} \left( \frac{8RT}{\pi M} \right)^{1/2} + \left[ 1 + \left( \frac{8\pi RT}{M} \right)^{1/2} \frac{\mu}{pr} \left( \frac{2}{\alpha} - 1 \right) \right] \frac{cr^2}{8\mu}$$

M - Molecular weight

Mass dependent transport

Wang (2018)

# Capabilities for nanogeochemical and nanofluidic studies at SNL



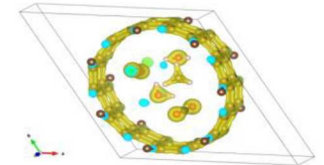
Synthesis of nanoporous materials



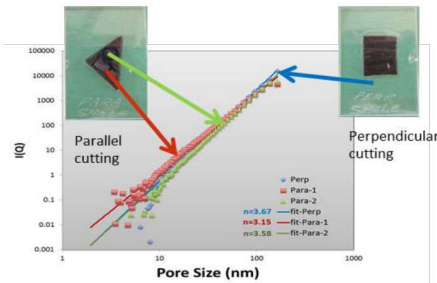
Isolation of kerogen from Mancos shale



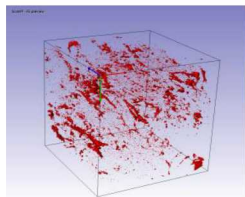
Pioneering work in nanogeochemistry. Access to DOE Center of Integrated Nanotechnology



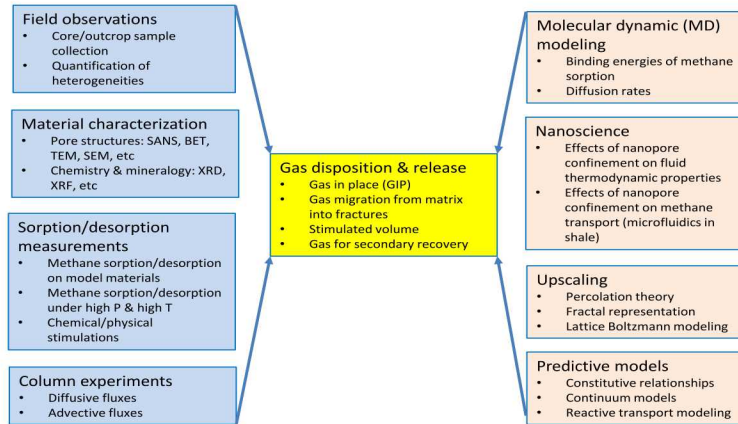
Density functional theory (DFT) modeling



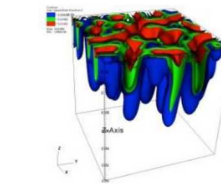
Pore structure characterization



Pore structure characterization (FIB)

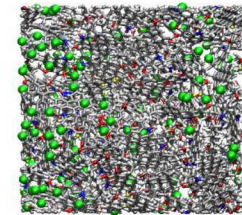


High pressure/high temperature sorption/desorption measurements

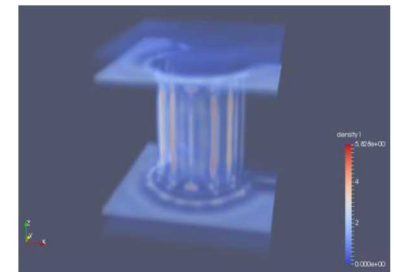


<http://www.pflotran.org/applications.html>

PFLOTRAN: Reactive transport modeling



Molecular dynamics (MD) simulation



TRAMANTO: Classical Density Functional Theory

# Fundamental Understanding of CH<sub>4</sub>-CO<sub>2</sub>-H<sub>2</sub>O Interactions in Shale Nanopores under Reservoir Conditions (PI: Yifeng Wang)

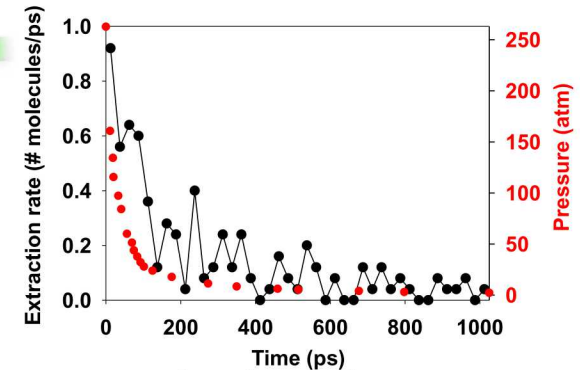
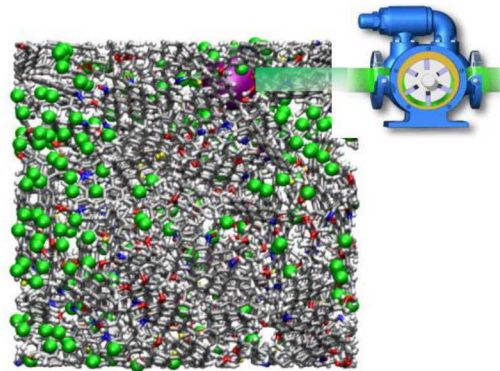


## Project Description

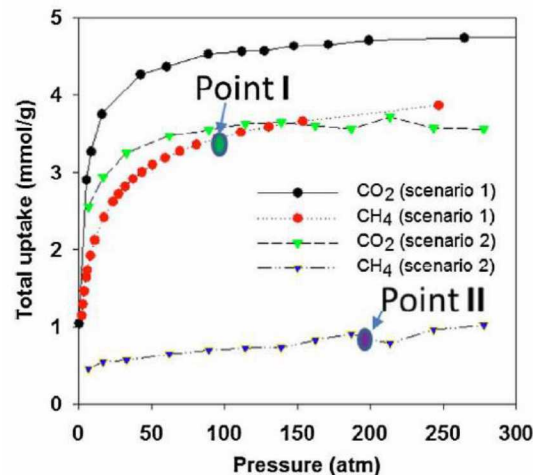
- This project aims to obtain a fundamental understanding of CH<sub>4</sub>-CO<sub>2</sub>-H<sub>2</sub>O interactions in shale nanopores under high-pressure and high temperature reservoir conditions and integrate this understanding into reservoir engineering for efficient shale gas recovery and subsurface carbon sequestration.

## Major Accomplishments and/or Deliverables (10 journal publications)

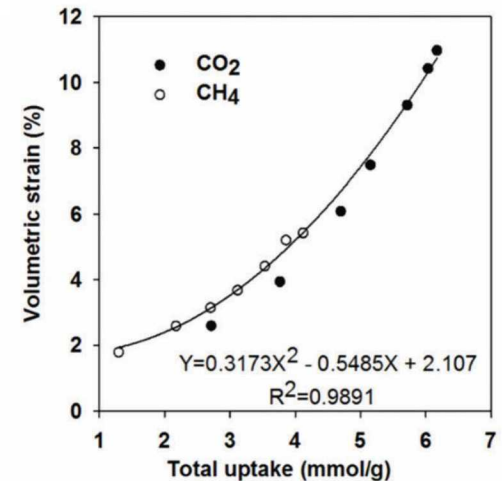
- Significant portion of CH<sub>4</sub> can adsorb to clay minerals.
- Wellbore production decline could be attributed to nanoscale gas disposition and migration in kerogen nanopores.
- Complex interactions may exist among CH<sub>4</sub>-CO<sub>2</sub>-H<sub>2</sub>O components in kerogen nanopores.
- Existing kerogen models are inadequate in representing actual kerogen structures.



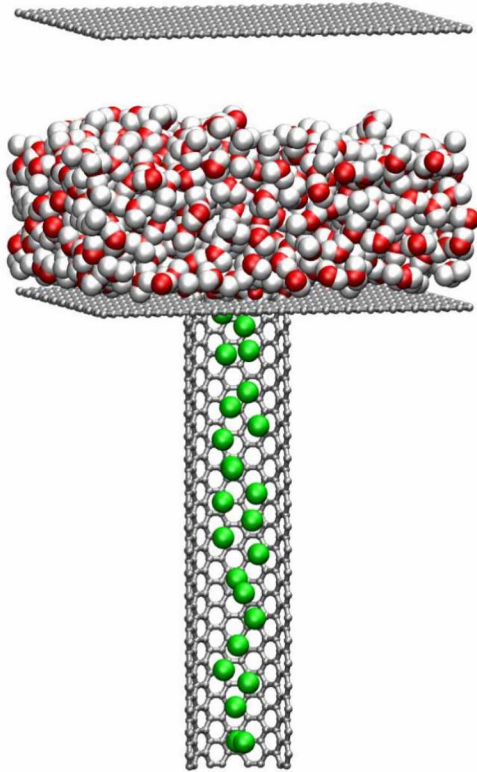
Molecular dynamics simulations show two stages of methane release from kerogen: A fast advective release of compressed free gas is followed by a slow diffusion of adsorbed gas (Scientific Reports, 2016, 6, 28053).



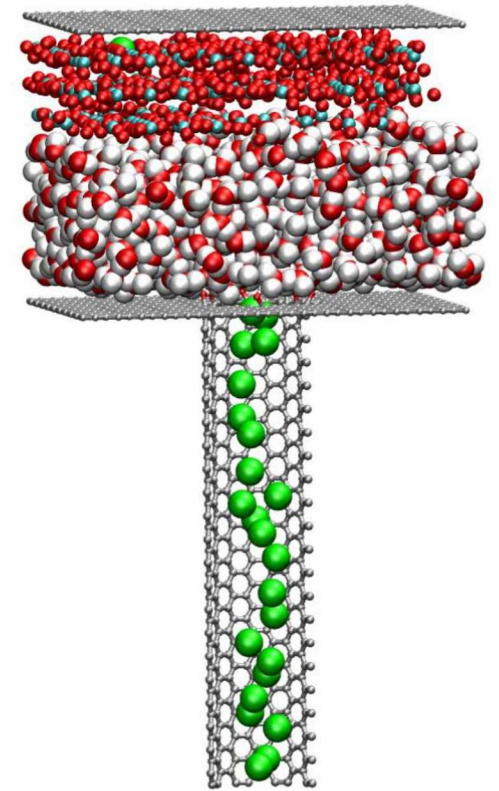
Preferential sorption of CO<sub>2</sub> by kerogen over CH<sub>4</sub> (Fuel, 2018, 220, 1-7)



Volumetric strain of kerogen as a function of gas pressure and total gas uptake (Phys. Chem. Chem. Phys., 2018, 20, 12390-12395)



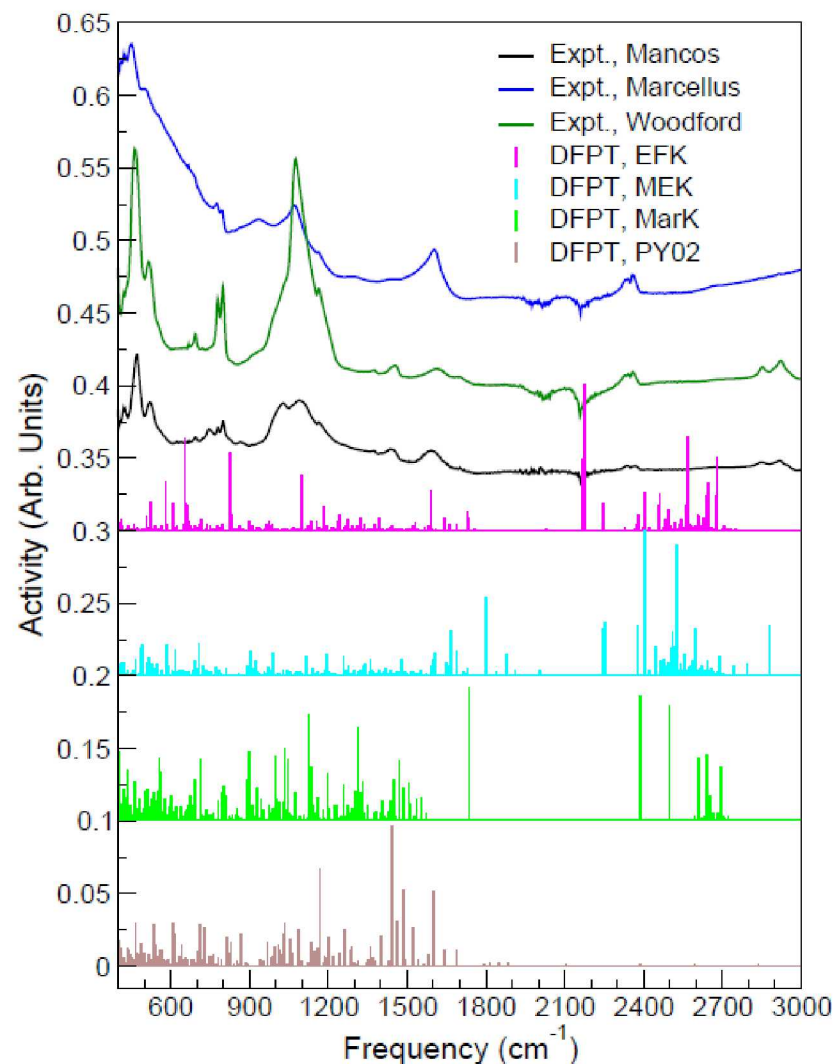
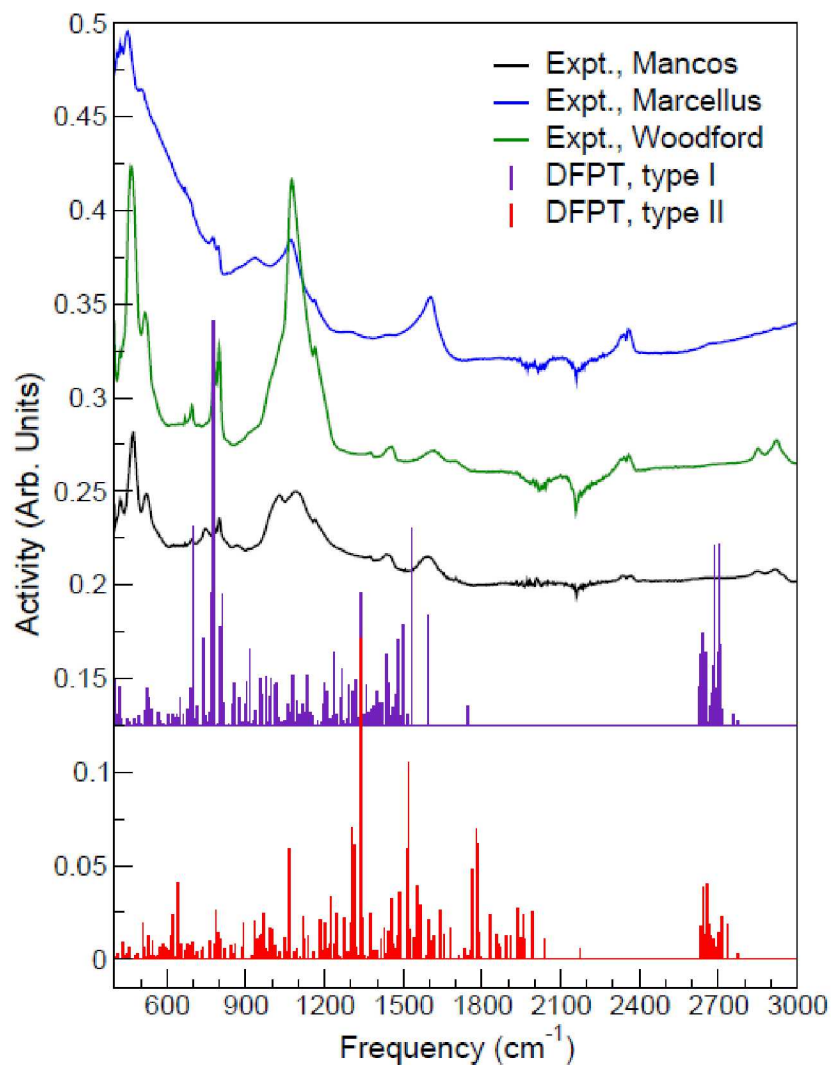
**Water effect**



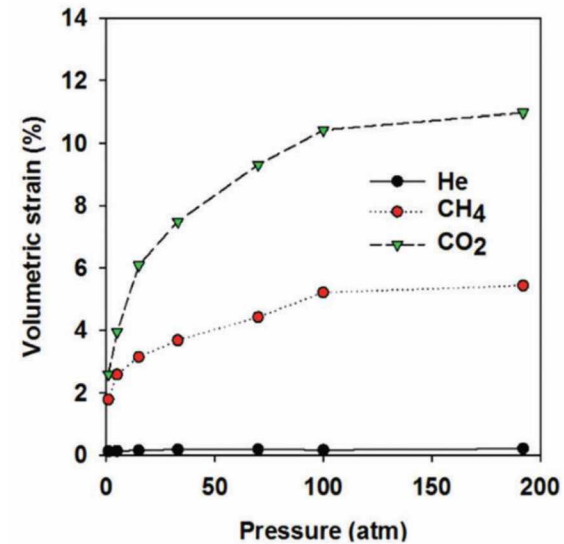
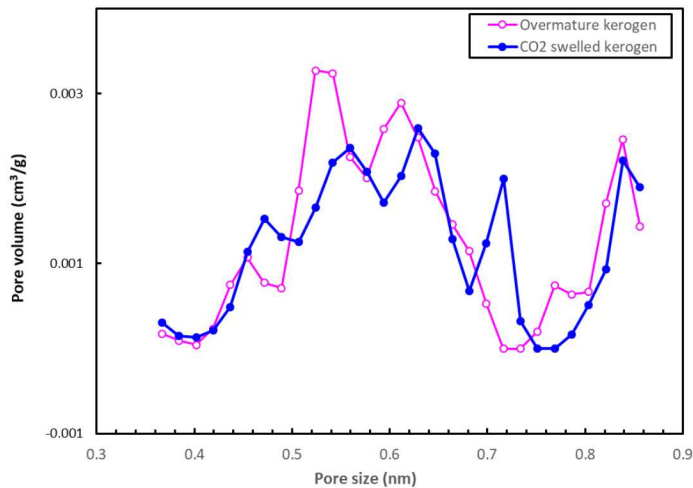
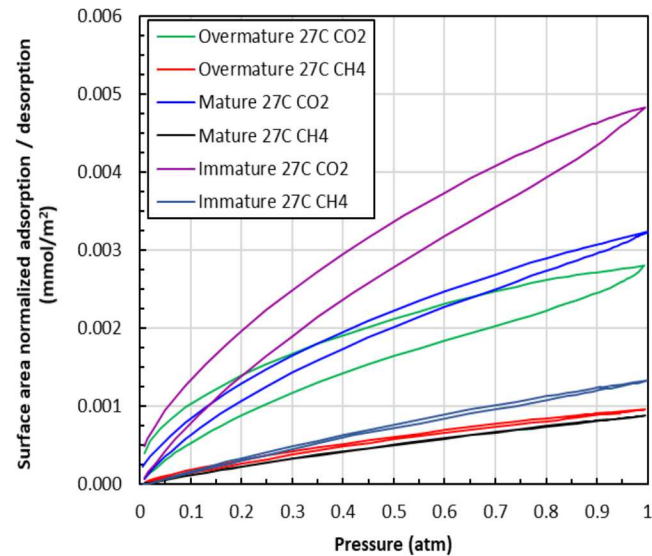
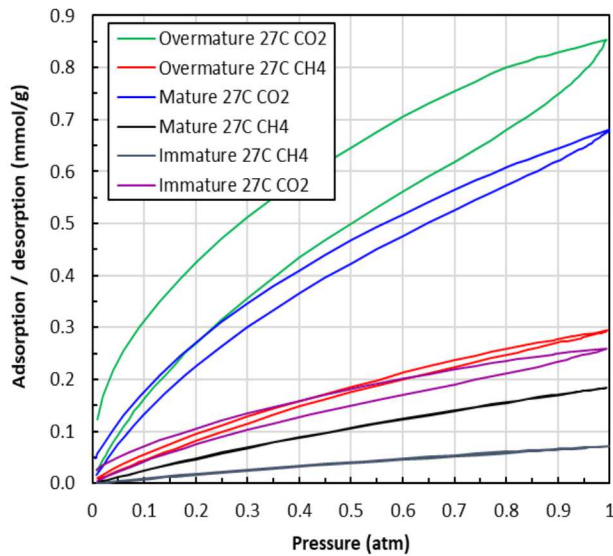
Assume that water thin films block the pore entrance.

$\text{CO}_2$  invades through water and replaces  $\text{CH}_4$  in the nanopore.

# Are the existing kerogen models adequate?

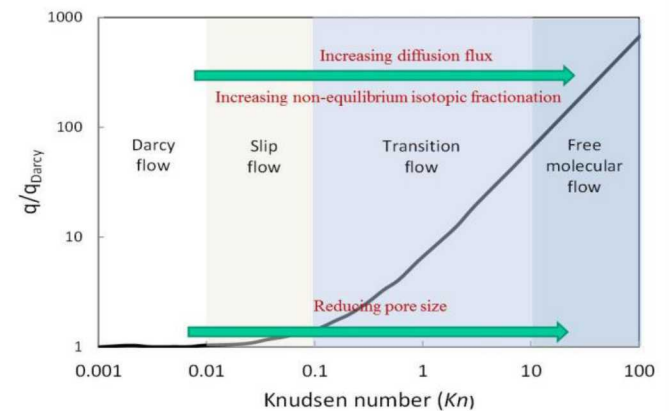
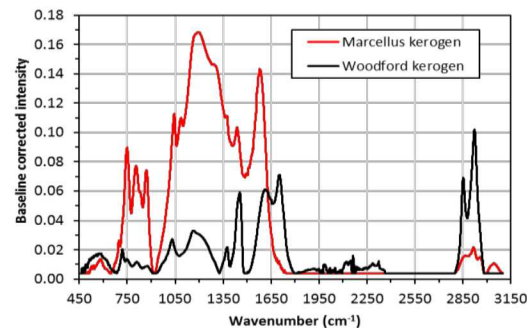
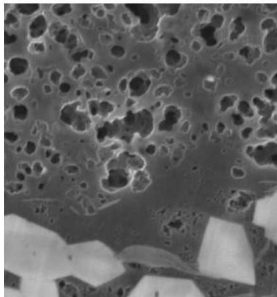
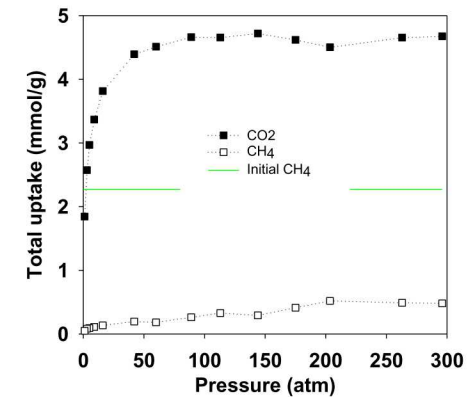
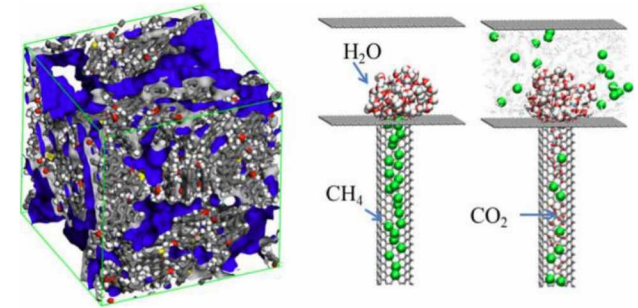


# Sorption-Desorption Hysteresis and Chemo-Mechanical Coupling (?)





- Xiong, Y., Wang, Y. & Olivas, T. (2015) Experimental Determination of P-V-T-X Properties and Sorption Kinetics in the CO<sub>2</sub>-CH<sub>4</sub>-H<sub>2</sub>O System under Shale Gas Reservoir Conditions: Part One, P-V-T-X Properties, Sorption Capacities and Kinetics of Model Materials for CO<sub>2</sub>-CH<sub>4</sub> Mixtures to 125°C, **High Temperature Aqueous Chemistry**, HiTAC-II Workshop, Heidelberg, April 16, 2015.
- Ho, T. A., Criscenti, L. J. & Wang, Y. (2016) Nanostructural control of methane release in kerogen and its implications to wellbore production decline. **Scientific Reports** 6, 28053; doi: 10.1038/srep28053.
- Weck, P. F., Kim, E. & Wang, Y. (2016) van der Waals forces and confinement in carbon nanopores: Interaction between CH<sub>4</sub>, COOH, NH<sub>3</sub>, OH, SH and single-walled carbon nanotubes. **Chem. Phys. Lett.** 62, 22-26.
- Cristancho, D., Akkutlu, I.Y., Criscenti, L.J., Wang, Y. (2016) Gas storage in model kerogen pores with surface heterogeneities, **SPE-180142-MS**, DOI: 10.2118/180142-MS.
- Wang, Y. (2017) On subsurface fracture opening and closure. **J. Petrol. Eng.** 155, 46-53.
- Wang, Y. (2018) From nanofluidics to basin-scale flow in shale: Tracer investigations, In: **Shale Subsurface Science and Engineering** (in press, book chapter)
- Weck, P. F. Kim, E., Wang, Y. et al. (2017) Model representation of kerogen structures: An insight from the density functional theory. **Scientific Reports**, 7, DOI:10.1038/s41598-017-07310-9.
- Ho, T. A., Greathouse, J. A., Wang, Y., and Criscenti, L. J. (2017) Atomistic structure of mineral nano-aggregates from simulated compaction and dewatering. **Scientific Reports**, 7, 15286.
- Ho, T. A., Wang, Y., Criscenti, L. J. & Xiong, Y. (2017) Differential retention and release of CO<sub>2</sub> and CH<sub>4</sub> in kerogen nanopores: Implications to gas extraction and carbon sequestration. **Fuel**, 220, 1-7.
- Ho, T. A. Wang, Y. and Criscenti, L. J. Chemo-mechanical coupling in kerogen gas adsorption/desorption. **PCCP** (in press).
- **Book:** Wang, Y., **Nanogeochemistry: Emergent Properties of Nano-Scale Mineral Phases and Confined Fluids**, Elsevier (in preparation)

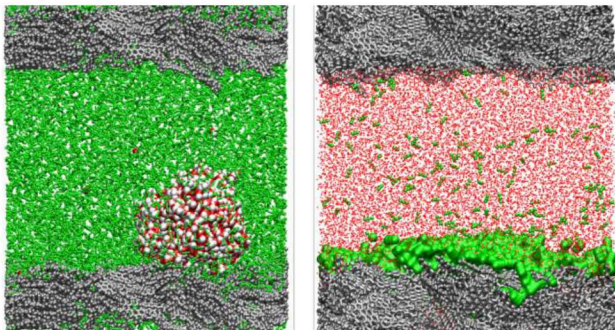
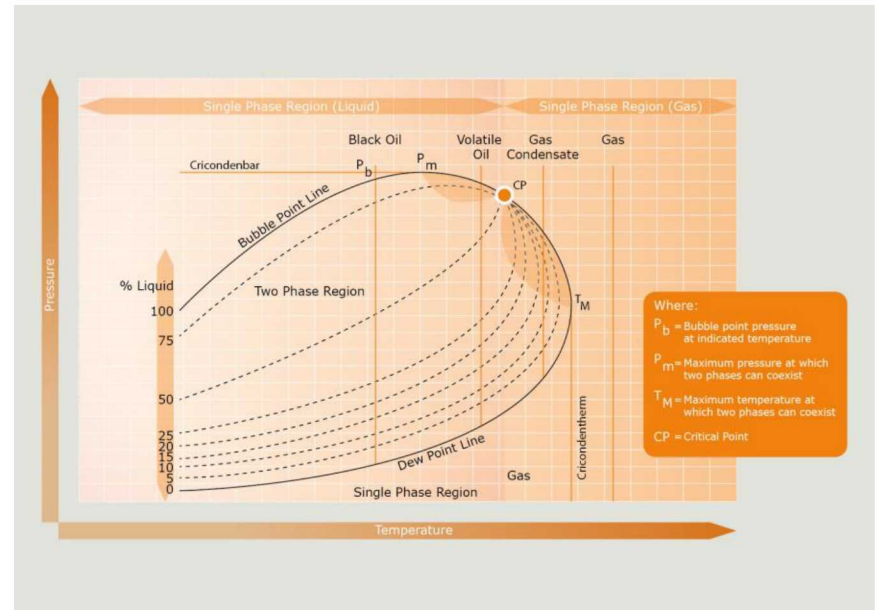


# Understanding multi-component and multi-phase hydrocarbon fluid interaction and transport in shale matrix: From nanoscale to wellbore production (PI: Yifeng Wang)



## Project Description

This project will use an integrated experimental and modeling study as well as field observations to fundamentally understand the disposition and release of complex hydrocarbon mixtures in a nanopore network of shale matrix and their transport from low-permeability matrix to hydrofracking-induced fracture networks in various reservoir types from black oil to dry gas.



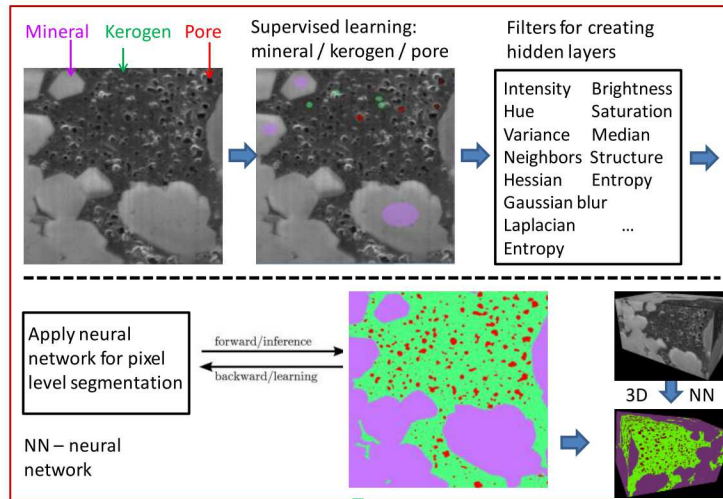
**Phase separation in nanopores controls oil/gas movement in unconventional reservoirs.**

Red and white - water; silver - kerogen; Green - CO<sub>2</sub>

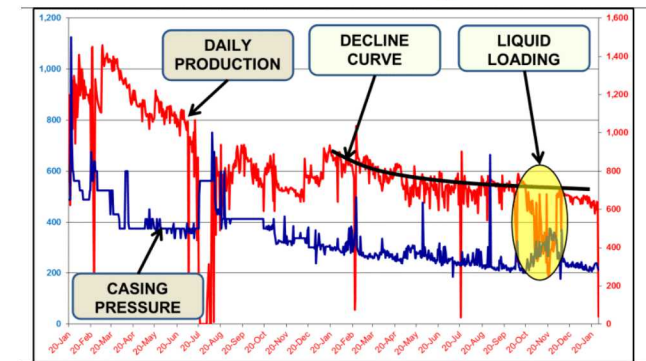
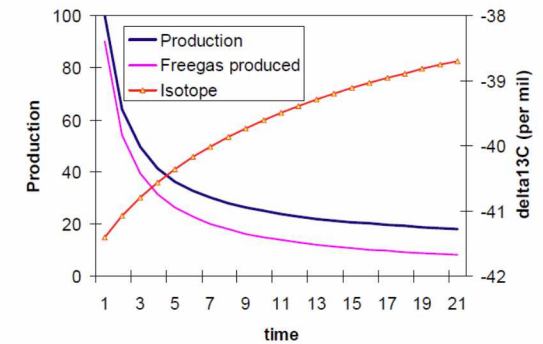
Ho et al. (2018) Nano Scale (in review)

- Expand our nanoscale understanding of fluid flows in shale matrix to wet gas and black oil reservoirs.
- Use machine learning to upscale nanoscale understanding and incorporate it into a reservoir simulator.
- Establish a scientific basis for a reliable prediction of wellbore production decline and for reservoir engineering optimization.

# Physics-based Machine-Learning (ML) for Data Integration and Process Upscaling: A gray box approach



## Using Real Time Gas Isotope to Model Gas Production Decline Curve



### 3D pore network and pore morphology

- 3D kerogen pore network
- Pore connectivity
- Pore size distribution
- Pore morphology
- Kerogen spatial distribution

### Kerogen and shale properties (measurements)

- Density
- Maturity
- CO<sub>2</sub>-CH<sub>4</sub> gas sorption
- Micro-FTIR / micro-Raman spectroscopy
- Auger Nanoprobe elemental analysis
- Nano indentation / Nano-mechanical property
- Imaging with artificial pyrolysis generated pores
- Imaging with artificial stress generated fractures
- Percolation or imbibition measurements

### Kerogen properties (MD & cDFT simulations)

- CO<sub>2</sub>-CH<sub>4</sub> gas sorption modeling
- DFT modeling infrared spectroscopy with maturity
- Atomistic modeling of stress generated fracture
- Thermal dynamic modeling of pore generation

Training dataset for deep learning

ML

- Reduced order models
- Constitutive relationships

Reservoir simulator

Production curve

## Research Team & collaborators



Name	Expertise	Role
Yifeng Wang	Nanogeochemistry	P.I., integration, reactive-transport model
Tuan Anh Ho	Molecular modeling	MD simulations
Philippe Weck	Molecular modeling	DFT and cDFT simulations
Guangping Xu	Experimental geochemistry	Material characterization, flow-through & imbibition experiments
Louise Criscenti	Geochemical modeling	MD simulations
Yongliang Xiong	High-temperature-high pressure geochemistry	Sorption-desorption measurements
Hongkyu Yoon	Lattice Boltzmann simulations	Pore network simulations
Stephen Verzi	Machine learning	Machine learning

