



# Numerical Simulation Approaches for Modeling Natural Gas Hydrate Systems in Geologic Media Subject to Geomechanical Stresses

March 12, 2019

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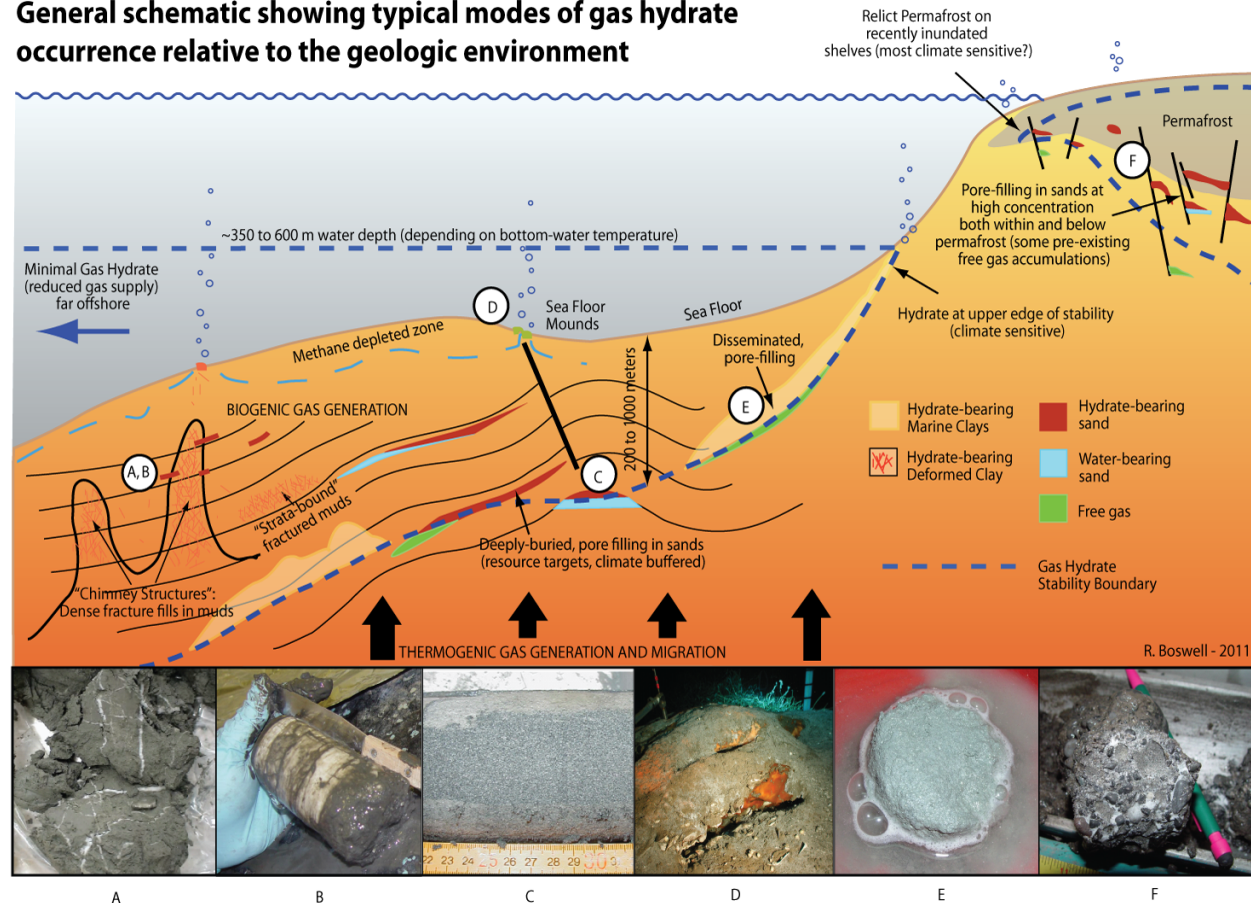


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# Modes of Natural Gas Hydrate Occurrence

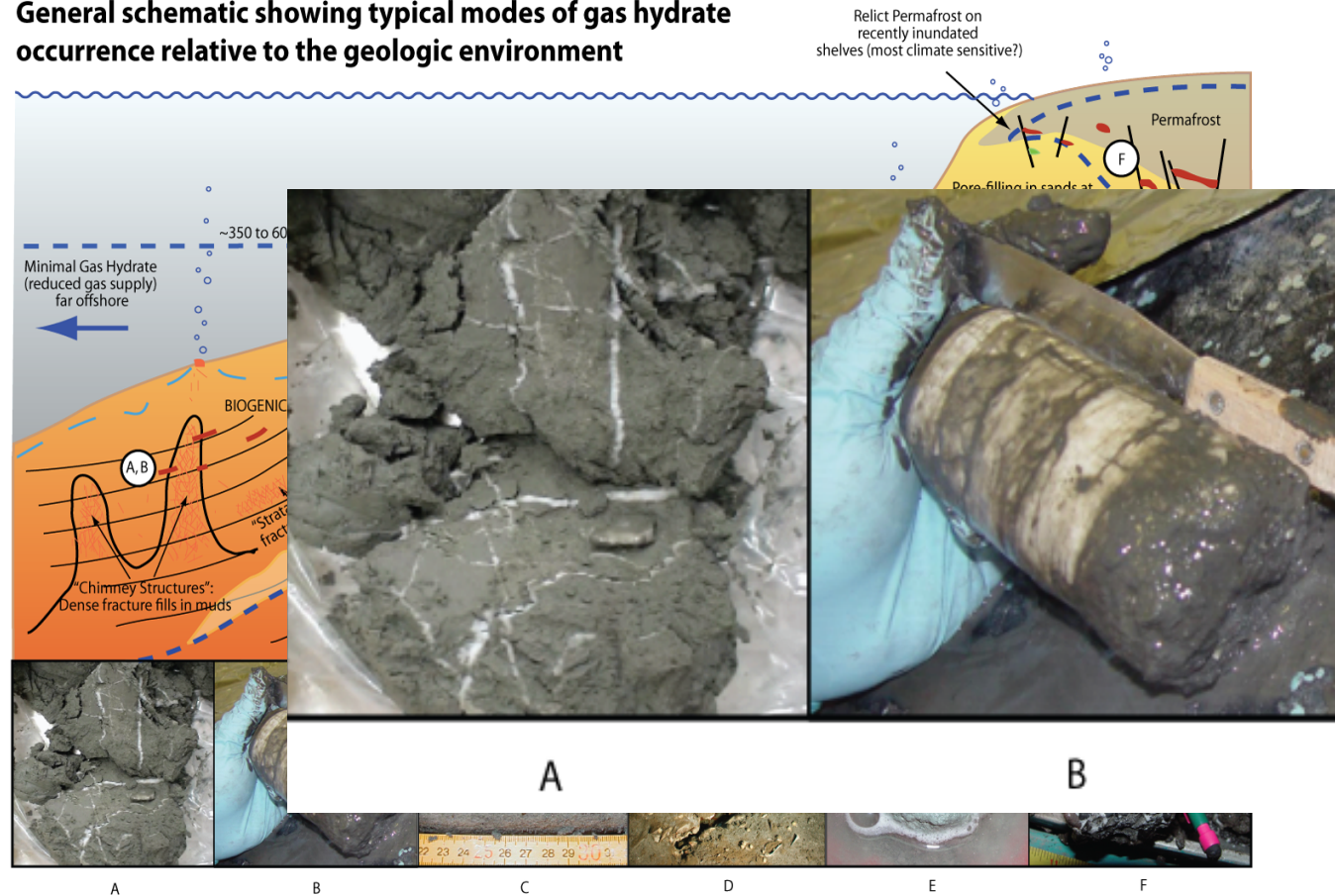
**General schematic showing typical modes of gas hydrate occurrence relative to the geologic environment**





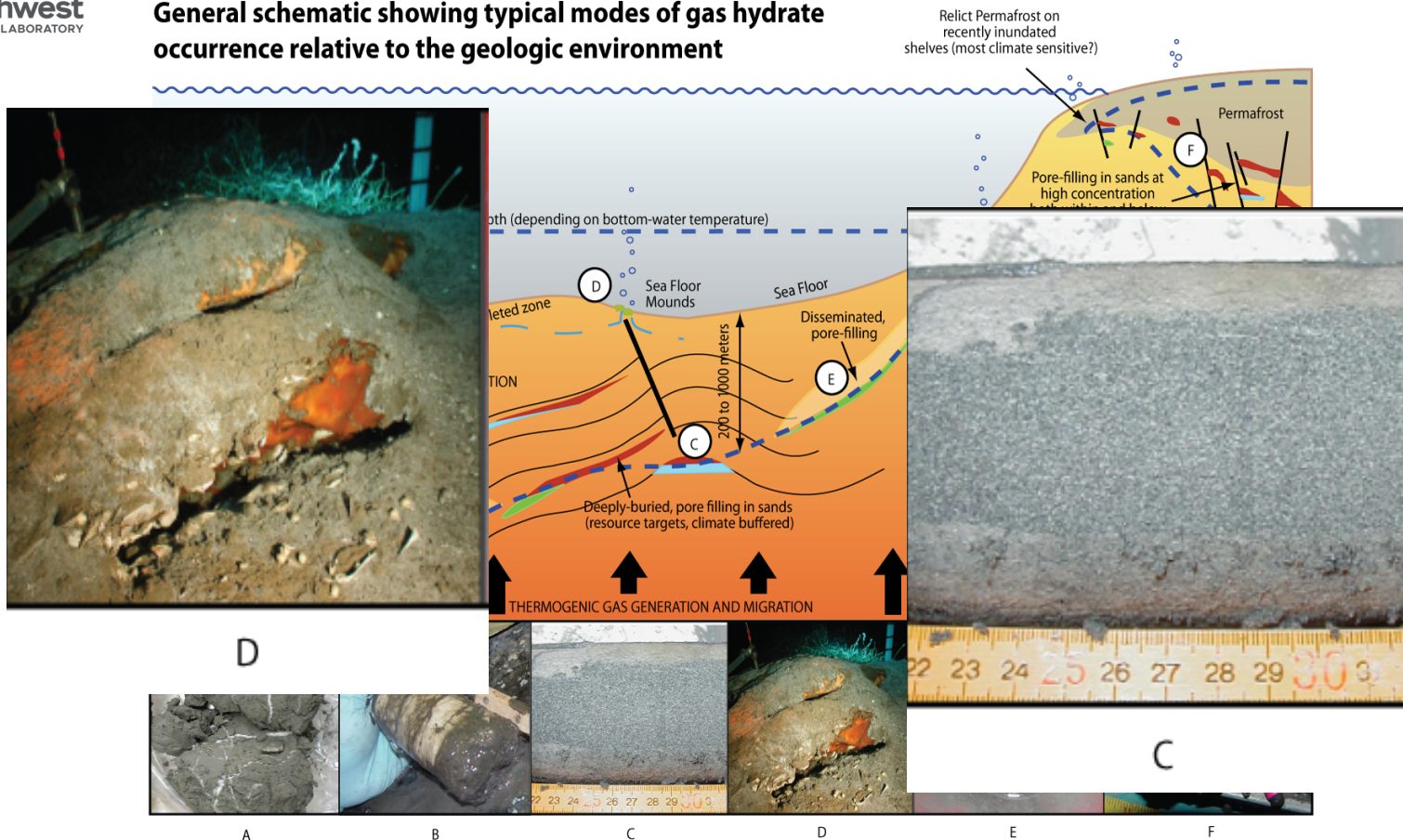
# Modes of Natural Gas Hydrate Occurrence

**General schematic showing typical modes of gas hydrate occurrence relative to the geologic environment**



# Modes of Natural Gas Hydrate Occurrence

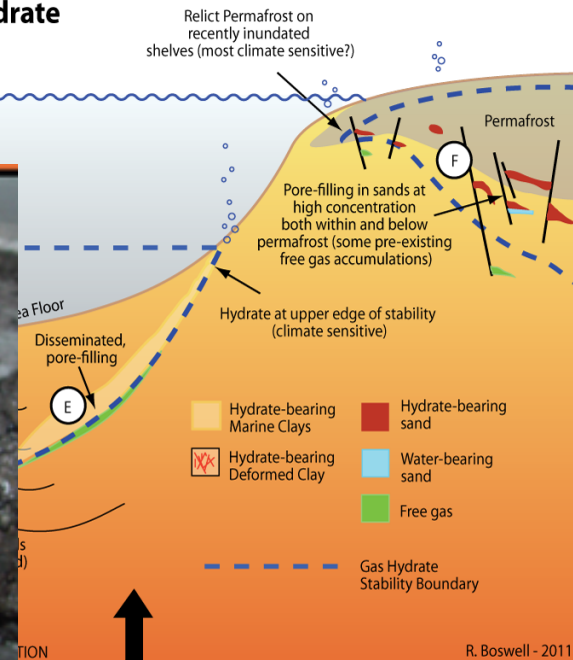
**General schematic showing typical modes of gas hydrate occurrence relative to the geologic environment**





# Modes of Natural Gas Hydrate Occurrence

**General schematic showing typical modes of gas hydrate occurrence relative to the geologic environment**



E

F



A

B

C

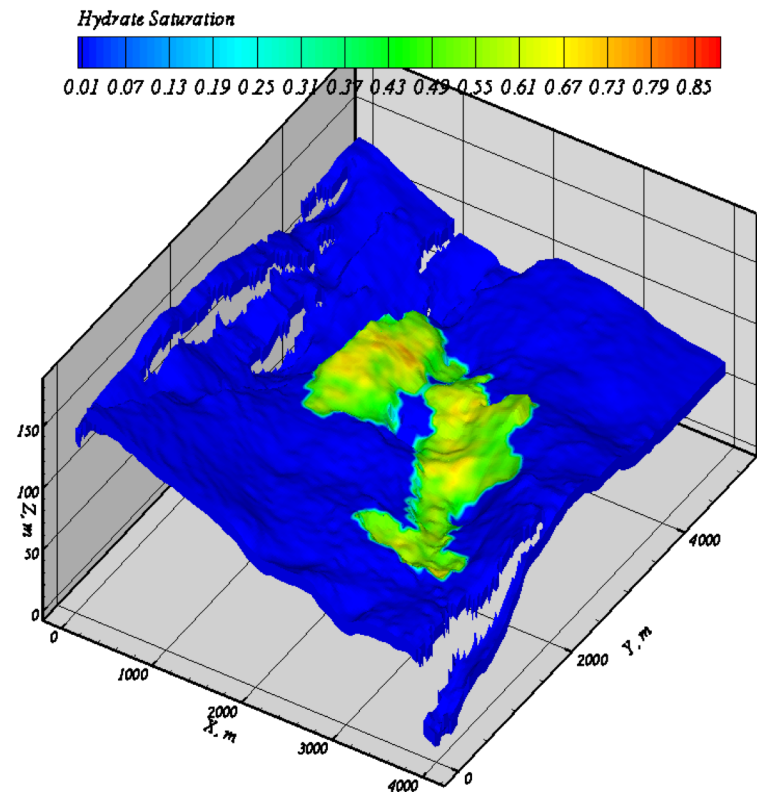
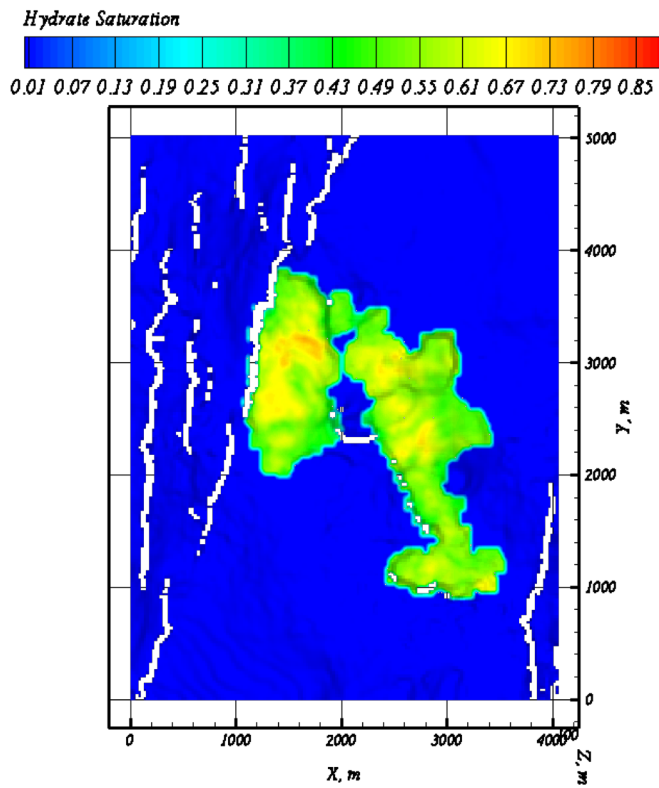
D

E

F



# Gas Hydrate Systems: Hydrate Distributions on the Alaska Northslope

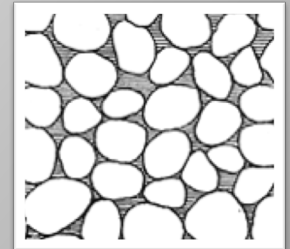


## Challenges in Modeling Natural Gas Hydrates in Geologic Environments

- Hydrate Thermodynamics
- Heat Transport
- Mobile and Immobile Phases
- Relative Permeability - Saturation – Capillary Pressure
- Kinetic Hydrate Dissolution – Formation
- Kinetic Exchange of Guest Molecules
- Potential for Three-Phase Hydraulics
- Phase Appearances – Disappearances – Transitions
- Coupled Geomechanics
- Hydrate Dependent Mechanical Properties
- Hydrate Dependent Porosity and Permeability
- Nonlinearities Abound
- Phase Equilibria

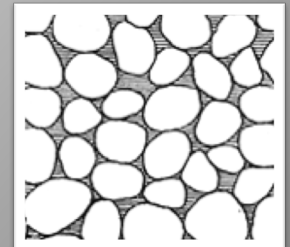
### *Pore Space Occupancy*

Aqueous  
Gas  
Nonaqueous Liquid  
Gas Hydrate  
Ice



### *Hydrate-Matrix Structure*

Encrustation  
Cementation  
Matrix-Supporting  
Pore-Filling





## An International Effort to Compare Gas Hydrate Reservoir Simulators: IGHCCS1

- Five benchmark and field-scale problems focused on gas hydrate production via depressurization and thermal stimulation
- Proceedings of the 6th International Conference on Gas Hydrates (ICGH 2008), Vancouver, British Columbia, Canada, July 6-10, 2008.
- 11 International Participants
  - University of Akron
  - Lawrence Berkeley National Laboratory
  - National Energy Technology Laboratory
  - University of West Virginia
  - U.S. Geological Survey
  - Ryder Scott Company, Petroleum Consultants
  - Japan Oil Engineering Company, Ltd.
  - National Institute of Advanced Industrial Science and Technology
  - Pacific Northwest National Laboratory
  - University of Tokyo
  - Fekete Associates Inc.



Photo: Bill Lawson  
Email: [bill-lawson@utulsa.edu](mailto:bill-lawson@utulsa.edu)





## 2<sup>nd</sup> International Gas Hydrate Code Comparison Study: IGHCCS2

- Five benchmark and challenge problems focused on gas hydrate production via depressurization and thermal stimulation with geomechanical coupling
- Principal Investigators
  - Mark White, Pacific Northwest National Laboratory
  - Tim Kneafsey, Lawrence Berkeley National Laboratory
  - Yongkoo Seol, National Energy Technology Laboratory
- 23 International Participants
- Problem Champions
- NETL EDX System
- Regularly scheduled teleconferences for code descriptions, problem development, solution comparisons, and scientific discussions
- Current focus on benchmark problems





## 2<sup>nd</sup> International Gas Hydrate Code Comparison Study: IGHCCS2



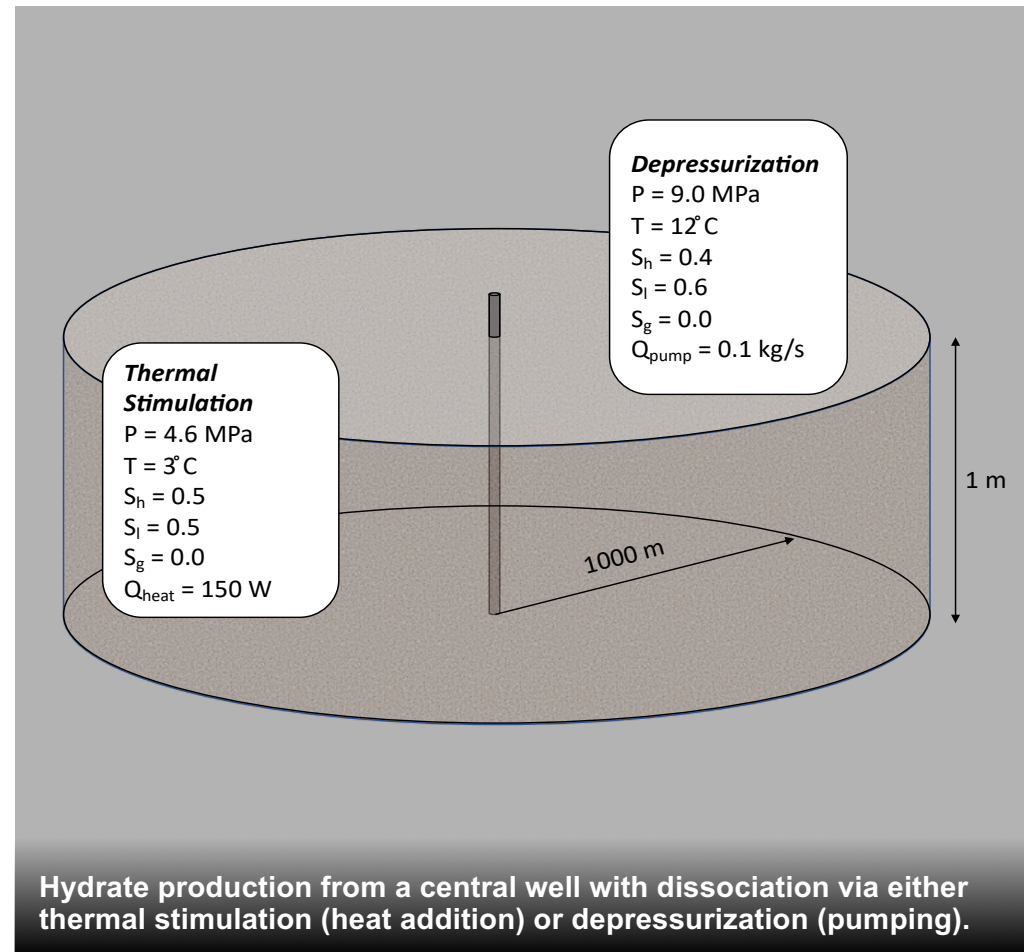
## Benchmark Problem 1 Similarity Solutions: Hydrate Dissociation in a Radial Domain

### *Problem Champion*

Mark White<sup>1,\*</sup>

<sup>1</sup>Pacific Northwest National  
Laboratory

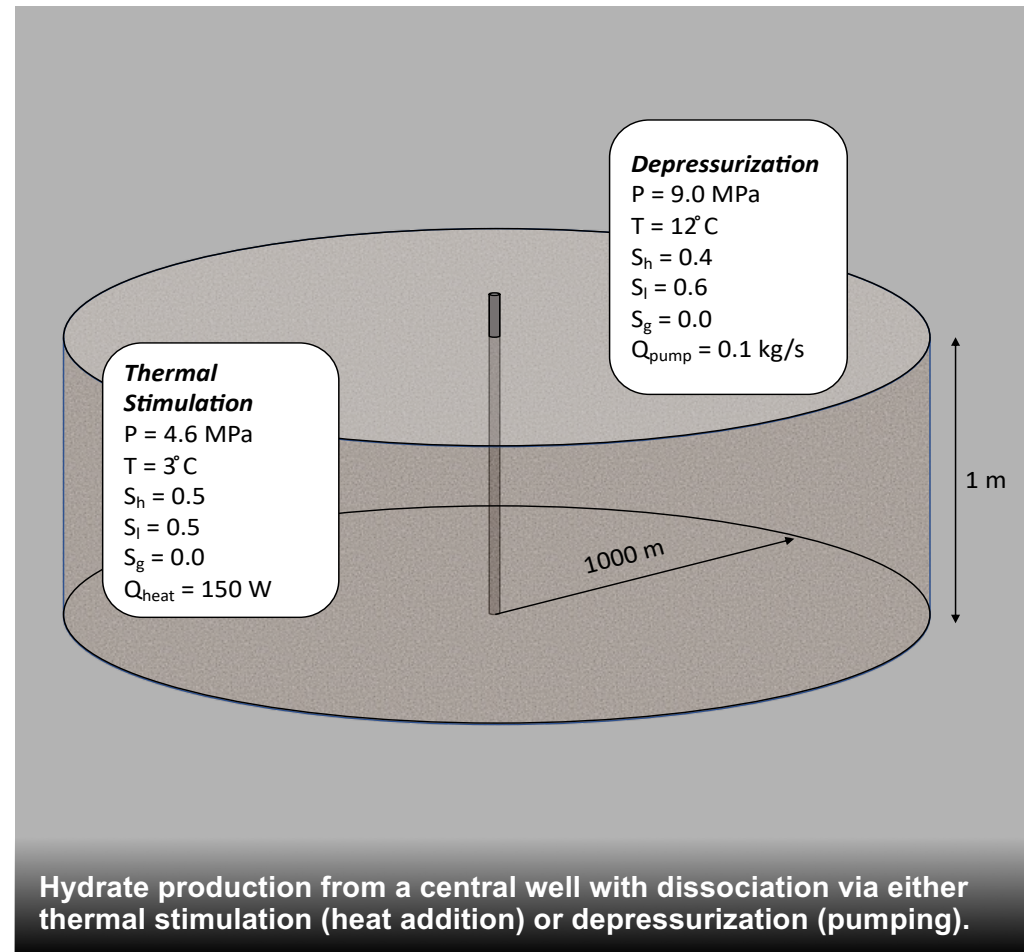
\*mark.white@pnnl.gov





### Problem Notes

- Similarity solution
- No geomechanics
- 1D radial flow
- Fine discretization near well
- Secondary hydrate formation away from well
- No ice formation
- Two-phase pumping during depressurization



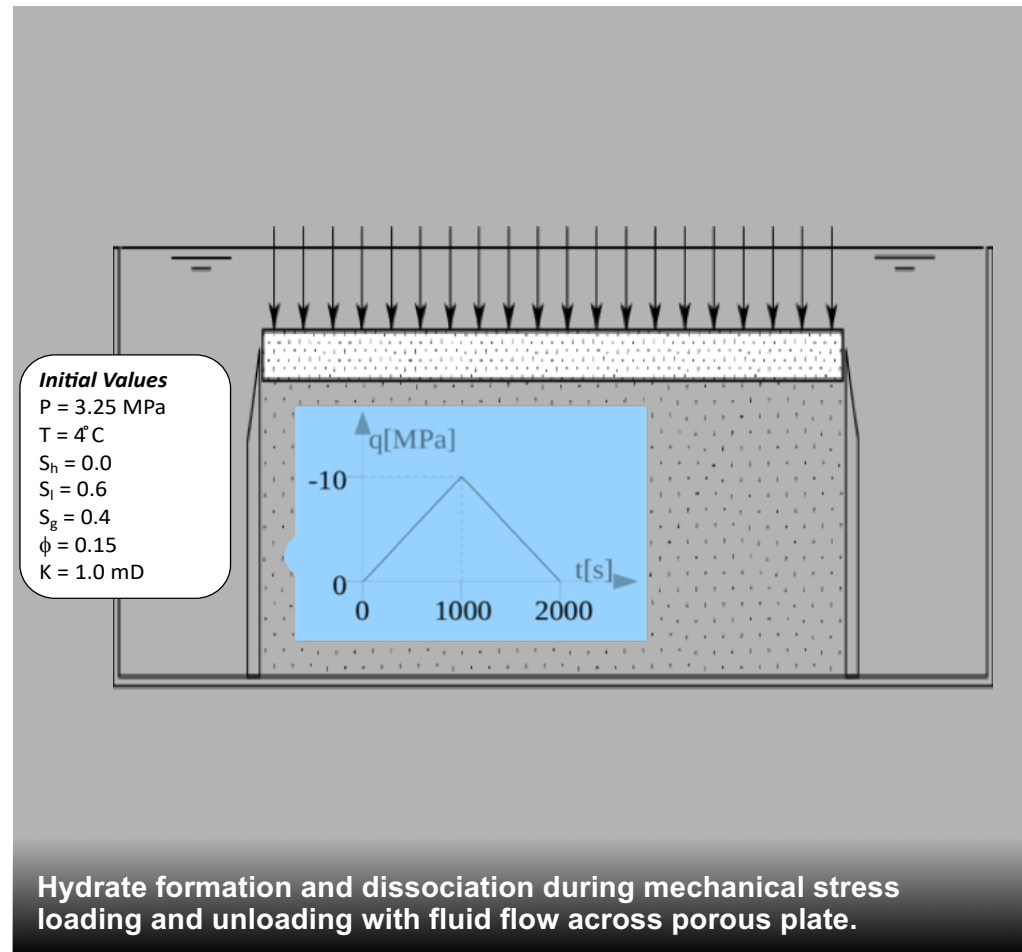
## Benchmark Problem 2 Extended Terzaghi Problem

### *Problem Champion*

Shubhangi Gupta<sup>1,\*</sup>

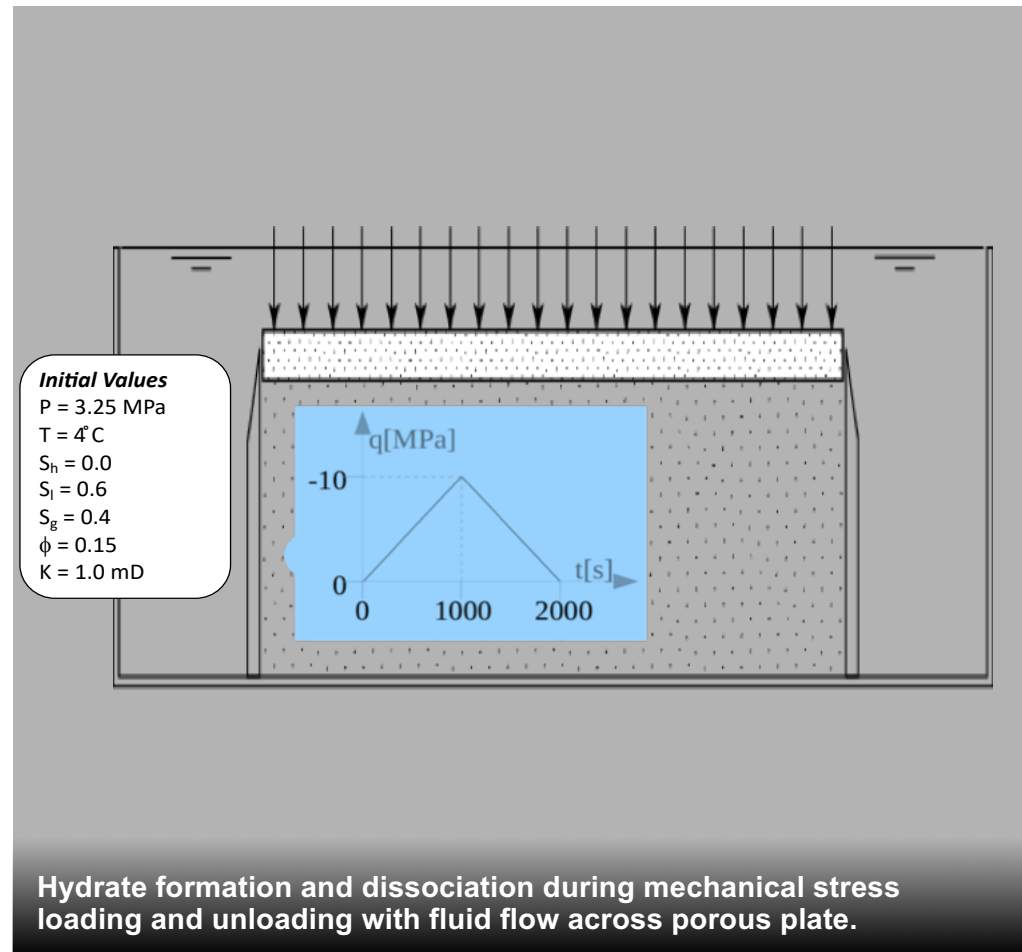
<sup>1</sup>GEOMAR Helmholtz Center  
for Ocean Research Kiel

\*sgupta@geomar.de



## Problem Notes

- 1D vertical domain
- Coupled flow, heat transport, thermodynamics, and geomechanics
- Without hydrate formation via higher initial temperature
- Variation with hydrate saturation dependent shear modulus
- Variation with rapid hydrate formation/dissociation kinetics





## Benchmark Problem 3 Radial Production

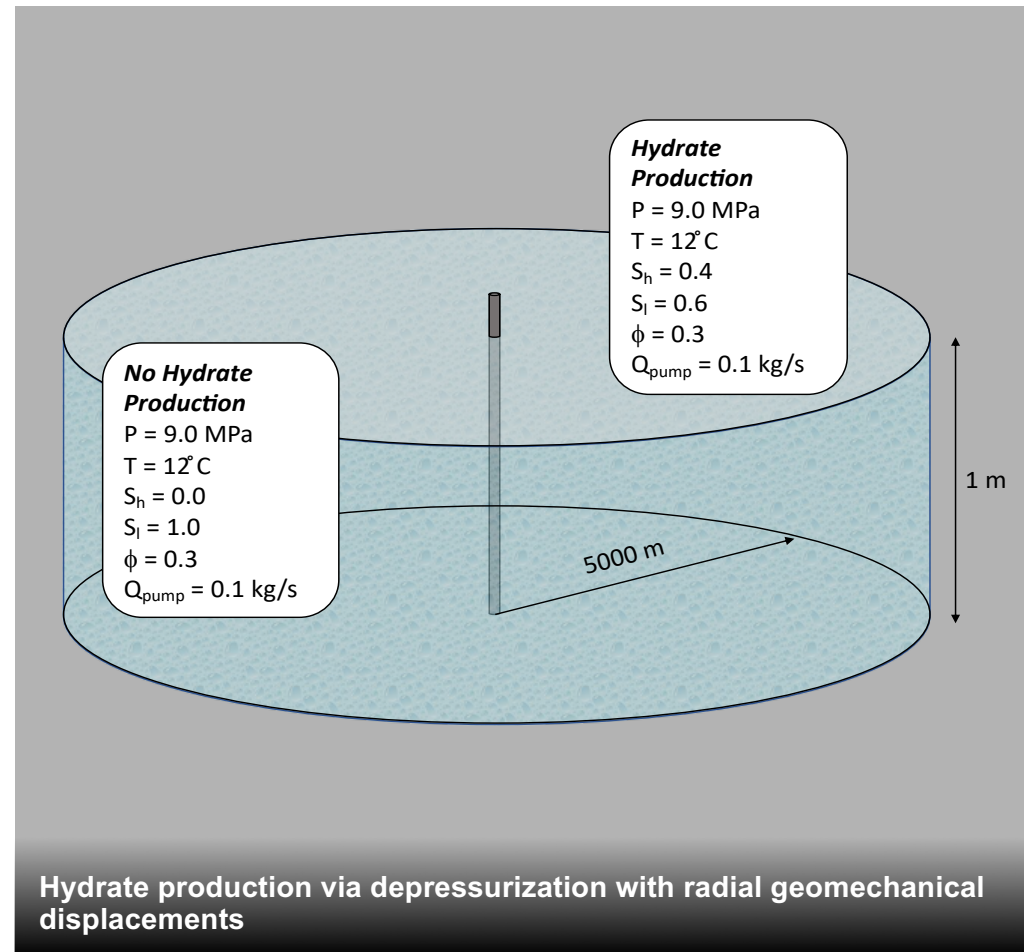
### *Problem Champions*

Matthew Reagan<sup>1,\*</sup>

Alejandro Queiruga<sup>1</sup>

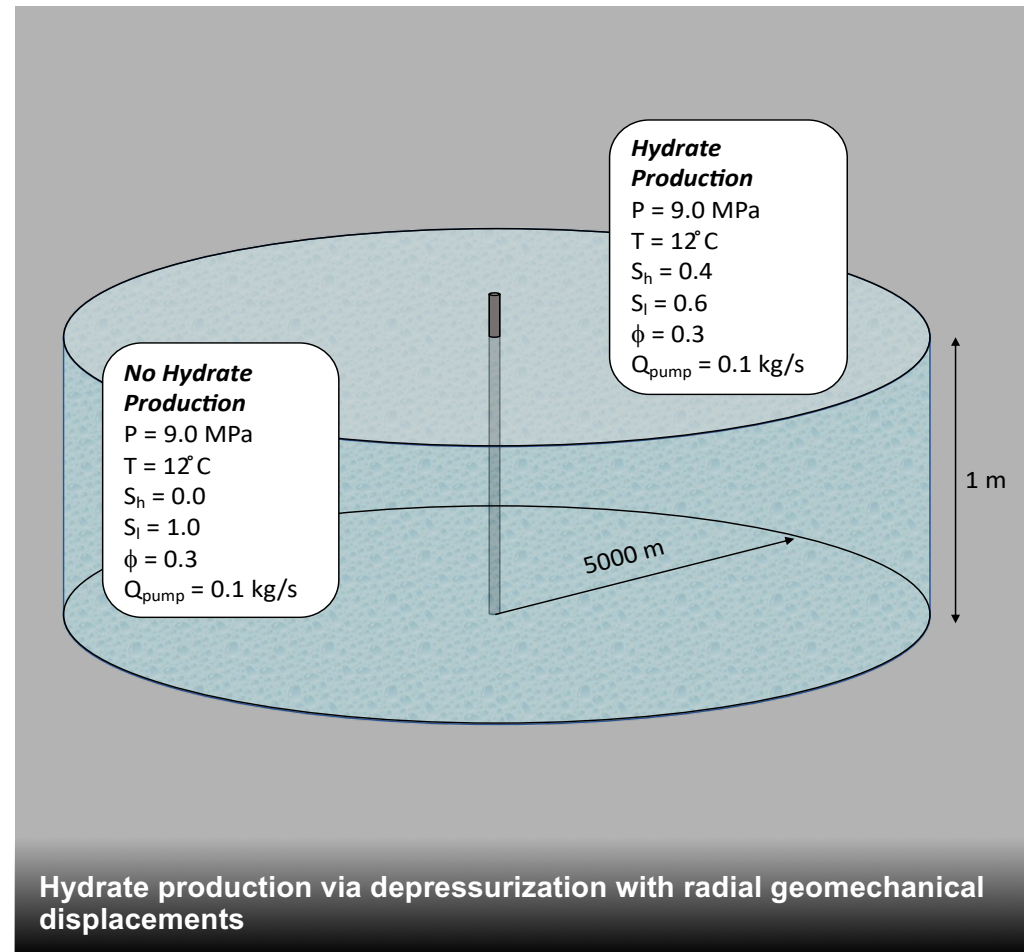
<sup>1</sup>Lawrence Berkeley National  
Laboratory

\*mtreagan@lbl.gov



## Problem Notes

- Radially symmetric domain
- No hydrate production
  - Coupled flow and geomechanics
  - Comparison to analytical solution
- Hydrate production
  - Coupled flow and geomechanics
  - No analytical solution
- Constant traction on top
- Rollers on bottom



## Benchmark Problem 4 Nankai Trough

### Problem Champions

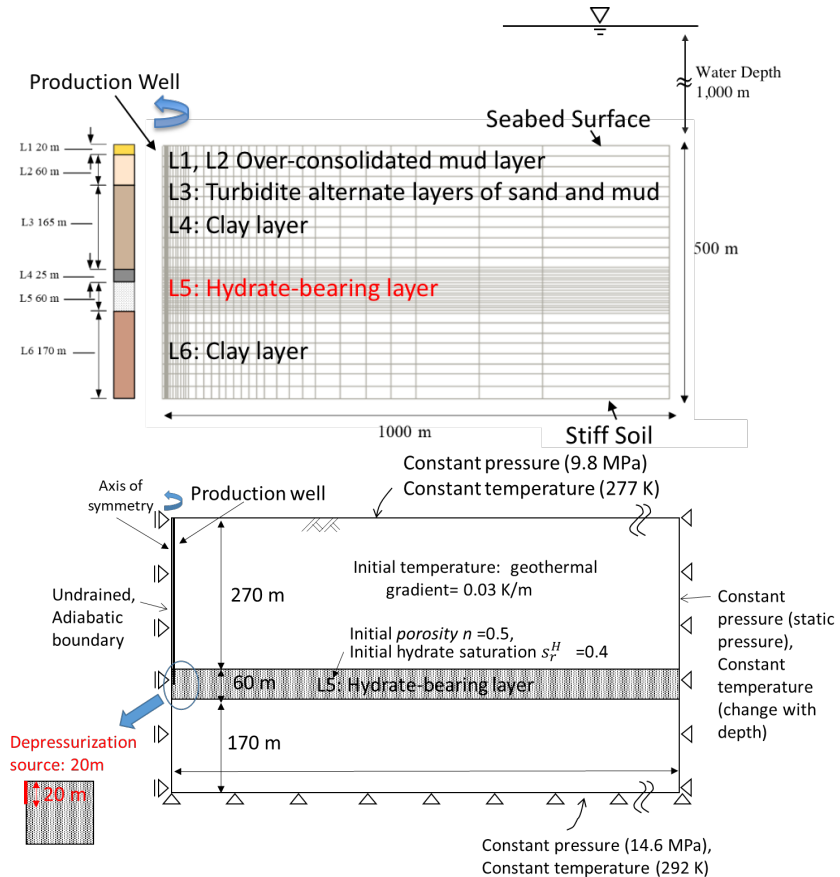
Sayuri Kimoto<sup>1,\*</sup>

Catherine Yonkofski<sup>2</sup>

<sup>1</sup>Kyoto University

<sup>2</sup>Pacific Northwest National Laboratory

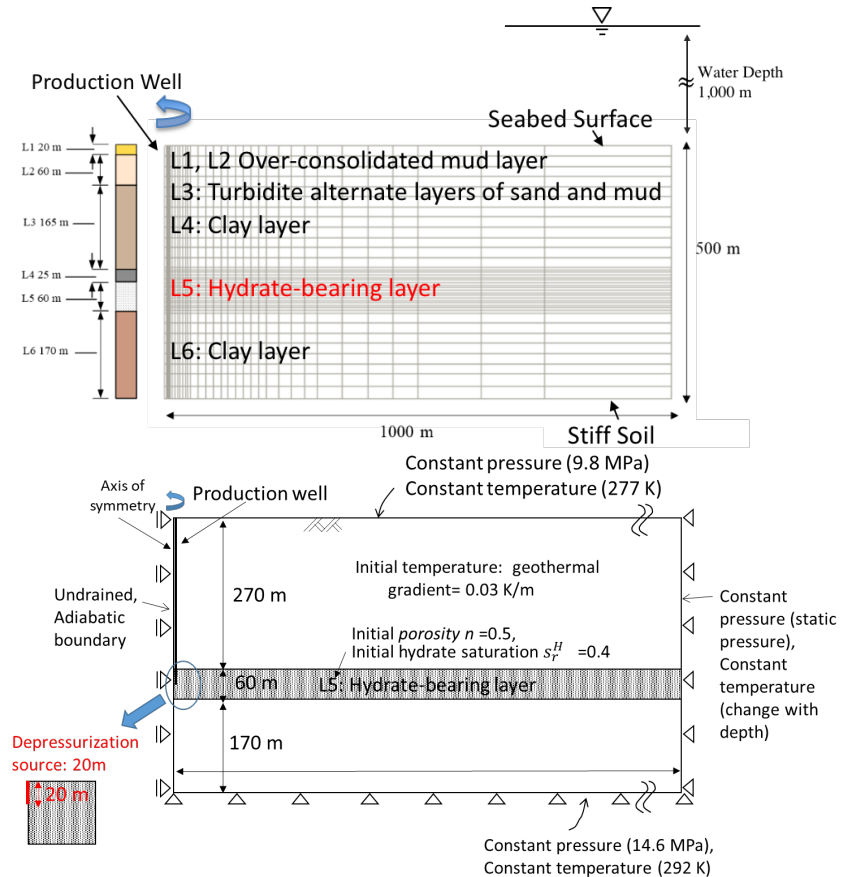
\*kimoto.sayuri.6u@kyoto-u.ac.jp



Hydrate production via depressurization from gas hydrate bearing sediments in the Nankai Trough, Japan

### Problem Notes

- 2D radially symmetric domain
- 6 sediment layers with 1 hydrate-bearing layer
- Water depth of 1,000 m
- Shear modulus dependent on hydrate saturation
- Production yields vertical displacements
- Initial geothermal, vertical effective stress, and horizontal effective stress gradients



Hydrate production via depressurization from gas hydrate bearing sediments in the Nankai Trough, Japan



## Benchmark Problem 5 Isotropic Consolidation with Hydrate Dissociation

### Problem Champions

Shun Uchida<sup>1,2,\*</sup>

Xuerui Gai<sup>1</sup>

Jeen-Shang Li<sup>1,3</sup>

Eugene Myshakin<sup>1</sup>

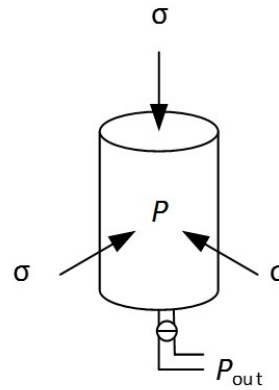
Yongkoo Seol<sup>1</sup>

<sup>1</sup>NETL

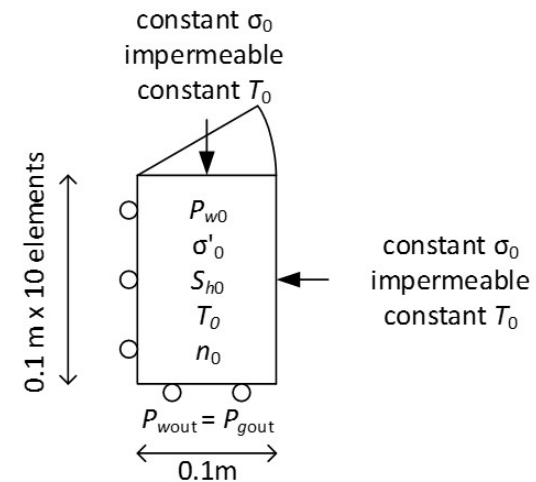
<sup>2</sup>Rensselaer Polytechnic

<sup>3</sup>University of Pittsburgh

\*uchids@rpi.edu



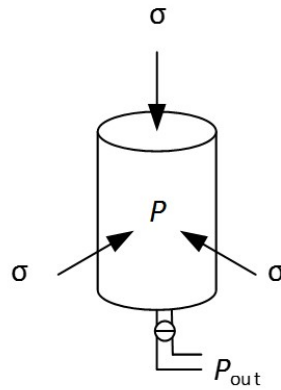
- $\sigma$  is constant throughout.
- Initial  $P$  is larger than  $P_{out}$ .
- Open the valve and let pore water drain.
- With time,  $P$  reaches to  $P_{out}$ .
- Volume of water out = soil volume reduction



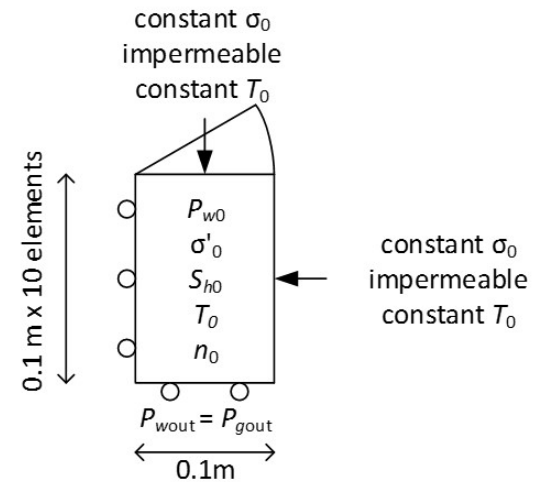
Depressurization induces isotropic consolidation, leading to volumetric deformation

### Problem Notes

- Axisymmetric domain with 10 grid cells/elements
- Important to know how each hydrate simulator handles volumetric deformation as well as hydrate dissociation
- To see how each simulator couples flow and volumetric deformation
- To see how each simulator couples hydrate dissociation and deformation



- $\sigma$  is constant throughout.
- Initial  $P$  is larger than  $P_{out}$ .
- Open the valve and let pore water drain.
- With time,  $P$  reaches to  $P_{out}$ .
- Volume of water out = soil volume reduction



Depressurization induces isotropic consolidation, leading to volumetric deformation

## Coupled THMC Modeling Approach in STOMP-HYDT-KE



- Conservation of mobile component mass

$$\frac{\partial}{\partial t} \int_{V_n} \left[ \sum_{\gamma=l,n,g} (\phi \rho_\gamma s_\gamma \omega_\gamma^i) \right] dV_n = \int_{\Gamma_n} [\mathbf{F}^i \cdot \mathbf{n}] d\Gamma_n + \int_{V_n} \left[ \sum_{\gamma=l,n,g} (\omega_\gamma^i m_\gamma) \right] dV_n$$

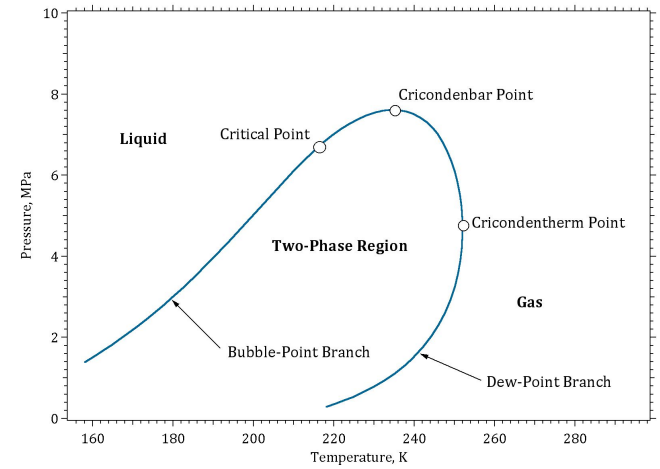
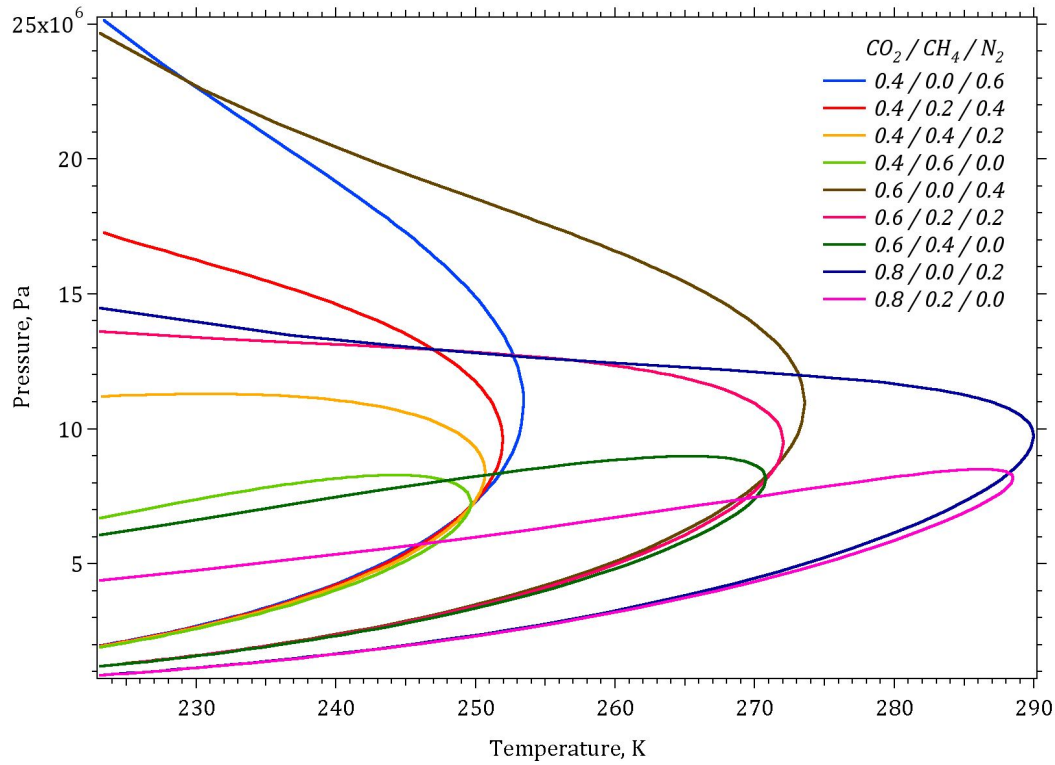
$$\int_{V_n} \left[ \sum_{\gamma=l,n,g} -K_e M^i A_h (\phi_m^i - \phi_h^i) - \left\{ \begin{array}{l} K_f \phi_m^i M^i A_h (P_m^v - P_h^v) / P \text{ for } P_m^v > P_h^v \\ K_d \phi_h^i M^i A_h (P_m^v - P_h^v) / P \text{ for } P_h^v > P_m^v \end{array} \right\} \right] dV_n; \text{ for } i = CH_4, CO_2, N_2$$

- Conservation of hydrate component mass

$$\frac{\partial}{\partial t} \int_{V_n} [\phi \rho_h s_h \omega_h^i] dV_n =$$

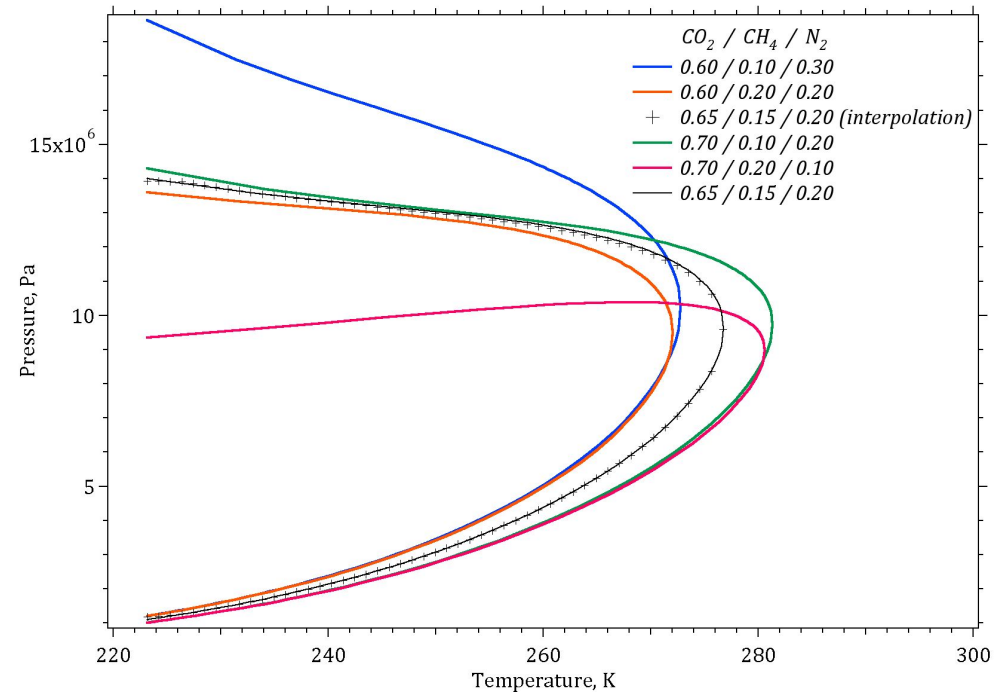
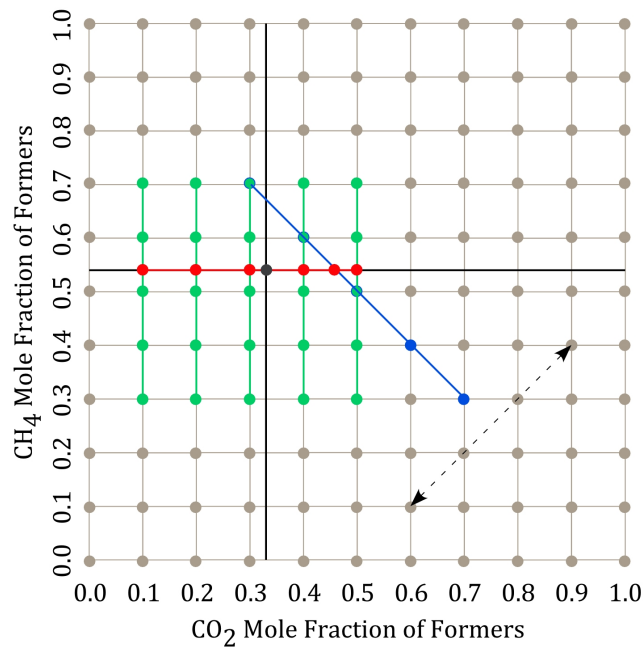
$$\int_{V_n} \left[ K_e M^i A_h (\phi_m^i - \phi_h^i) + \left\{ \begin{array}{l} K_f \phi_m^i M^i A_h (P_m^v - P_h^v) / P \text{ for } P_m^v > P_h^v \\ K_d \phi_h^i M^i A_h (P_m^v - P_h^v) / P \text{ for } P_h^v > P_m^v \end{array} \right\} \right] dV_n; \text{ for } i = CH_4, CO_2, N_2$$

# Equation of State Phase Envelopes for the Mobile Phases



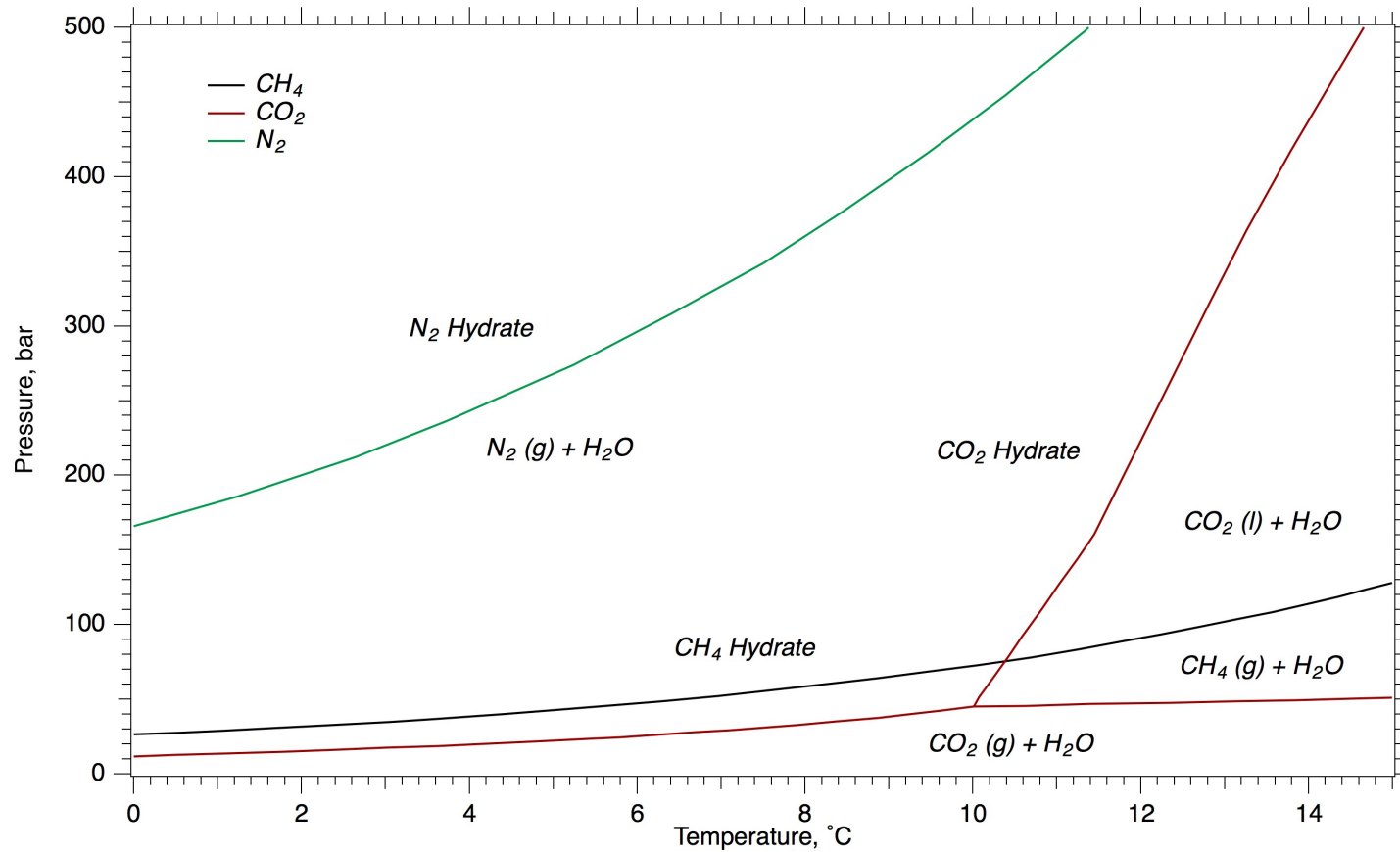


# Tabular Interpolation Scheme

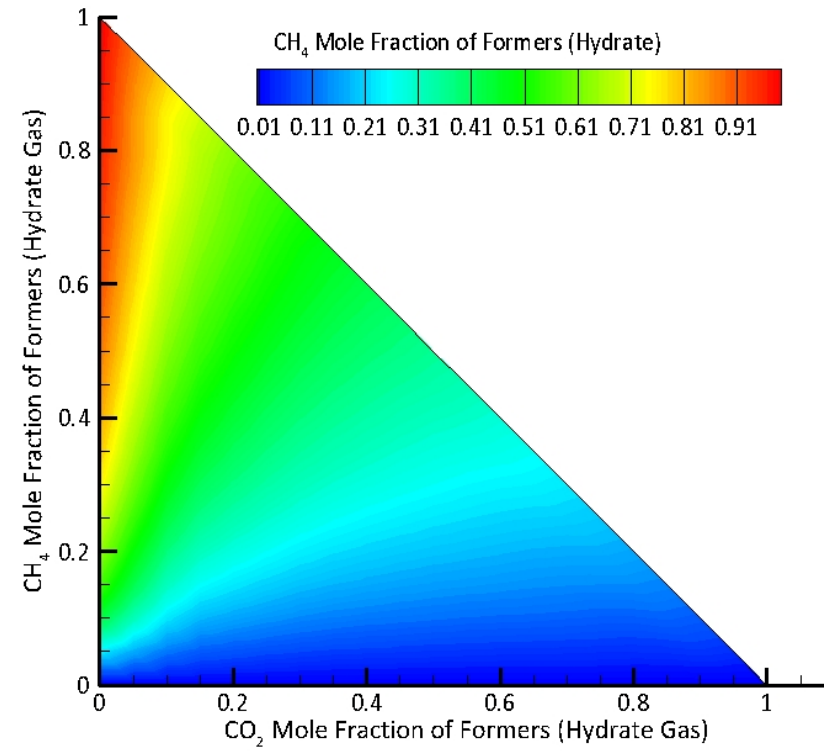
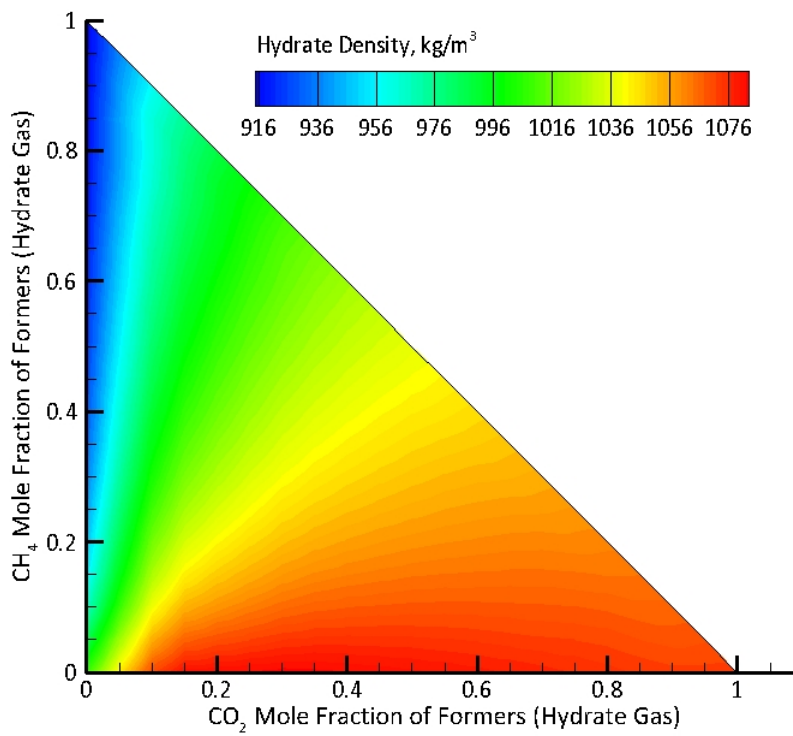


$$T_{tab} = T_{tab}^{cricondenthern} \left[ \frac{T}{T_{mix}^{cricondenthern}} \right] \text{ for } T < T_{mixture}^{cricondenthern} \quad P_{tab} = P \left[ \frac{P_{tab}^{upper} - P_{tab}^{lower}}{P_{mix}^{upper} - P_{mix}^{lower}} \right] + P_{tab}^{lower} \text{ for } P_{mix}^{lower} < P < P_{mix}^{upper}$$

# Gas Hydrate Systems – Hydrate Phase Equilibria



# Gas Hydrate Systems – Ternary Hydrate Properties from Tables



## Gas Hydrate Systems – Phase Conditions and Primary Variables



Phase Condition #10 Series  $s_h = 0.0, s_n + s_g = 0.0, s_\ell + s_i = 1.0$

Energy	$T$	Temperature
Water Mass	$P$	Pressure
Mobile CO <sub>2</sub> Mass	$P_v^{CO_2}$	CO <sub>2</sub> Vapor Pressure
Mobile CH <sub>4</sub> Mass	$P_v^{CH_4}$	CH <sub>4</sub> Vapor Pressure
Mobile N <sub>2</sub> Mass	$P_v^{N_2}$	N <sub>2</sub> Vapor Pressure
Hydrate CO <sub>2</sub> Mass	$M_h^{CO_2}$	Hydrate CO <sub>2</sub> Mass
Hydrate CH <sub>4</sub> Mass	$M_h^{CH_4}$	Hydrate CO <sub>2</sub> Mass
Hydrate N <sub>2</sub> Mass	$M_h^{N_2}$	Hydrate CO <sub>2</sub> Mass
Salt	$y_\ell^S$	Brine Mass Fraction of Total Salt



## Gas Hydrate Systems – Phase Conditions and Primary Variables



Phase Condition #20 Series  $s_h = 0.0, s_n + s_g > 0.0, s_\ell + s_i < 1.0$

Energy	$T$	Temperature
Water Mass	$s_\ell + s_i$	Aqueous + Ice Saturation
Mobile CO <sub>2</sub> Mass	$z_m^{CO_2}$ or $P$	CO <sub>2</sub> Mole Fraction or Pressure
Mobile CH <sub>4</sub> Mass	$z_m^{CH_4}$ or $P$	CH <sub>4</sub> Mole Fraction or Pressure
Mobile N <sub>2</sub> Mass	$z_m^{N_2}$ or $P$	N <sub>2</sub> Mole Fraction or Pressure
Hydrate CO <sub>2</sub> Mass	$M_h^{CO_2}$	Hydrate CO <sub>2</sub> Mass
Hydrate CH <sub>4</sub> Mass	$M_h^{CH_4}$	Hydrate CO <sub>2</sub> Mass
Hydrate N <sub>2</sub> Mass	$M_h^{N_2}$	Hydrate CO <sub>2</sub> Mass
Salt	$y_\ell^S$	Brine Mass Fraction of Total Salt

## Gas Hydrate Systems – Phase Conditions and Primary Variables



Phase Condition #30 Series  $s_h > 0.0, s_n + s_g > 0.0, s_\ell + s_i < 1.0$

Energy	$T$	Temperature
Water Mass	$s_\ell + s_i$	Aqueous + Ice Saturation
Mobile CO <sub>2</sub> Mass	$z_m^{CO_2}$ or $P$	CO <sub>2</sub> Mole Fraction or Pressure
Mobile CH <sub>4</sub> Mass	$z_m^{CH_4}$ or $P$	CH <sub>4</sub> Mole Fraction or Pressure
Mobile N <sub>2</sub> Mass	$z_m^{N_2}$ or $P$	N <sub>2</sub> Mole Fraction or Pressure
Hydrate CO <sub>2</sub> Mass	$\varphi_h^{CO_2}$ or $s_h$	CO <sub>2</sub> Mole Fraction of Former
Hydrate CH <sub>4</sub> Mass	$\varphi_h^{CH_4}$ or $s_h$	CH <sub>4</sub> Mole Fraction of Former
Hydrate N <sub>2</sub> Mass	$\varphi_h^{N_2}$ or $s_h$	N <sub>2</sub> Mole Fraction of Former
Salt	$y_\ell^S$	Brine Mass Fraction of Total Salt

## Gas Hydrate Systems – Phase Conditions and Primary Variables



Phase Condition #40 Series  $s_h > 0.0, s_n + s_g = 0.0, s_\ell + s_i < 1.0$

Energy	$T$	Temperature
Water Mass	$P$	Pressure
Mobile CO <sub>2</sub> Mass	$P_v^{CO_2}$	CO <sub>2</sub> Vapor Pressure
Mobile CH <sub>4</sub> Mass	$P_v^{CH_4}$	CH <sub>4</sub> Vapor Pressure
Mobile N <sub>2</sub> Mass	$P_v^{N_2}$	N <sub>2</sub> Vapor Pressure
Hydrate CO <sub>2</sub> Mass	$\varphi_h^{CO_2}$ or $s_h$	CO <sub>2</sub> Mole Fraction of Former
Hydrate CH <sub>4</sub> Mass	$\varphi_h^{CH_4}$ or $s_h$	CH <sub>4</sub> Mole Fraction of Former
Hydrate N <sub>2</sub> Mass	$\varphi_h^{N_2}$ or $s_h$	N <sub>2</sub> Mole Fraction of Former
Salt	$y_\ell^S$	Brine Mass Fraction of Total Salt

## Gas Hydrate Systems – Phase Transition Example



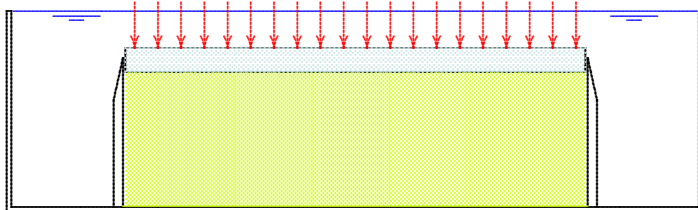
Phase Condition #10 Series  $s_h = 0.0, s_n + s_g = 0.0, s_\ell + s_i = 1.0$

- Assume a hydrate phase exists (common approach!)
- Compute a hydrate equilibrium pressure  $P_h^{eq} = \text{func}[T, \phi_h^{CO_2}, \phi_h^{CH_4}, \phi_h^{N_2}]$
- Compute the vapor pressure of formers  $P_v = P_v^{CO_2} + P_v^{CH_4} + P_v^{N_2}$
- Compute the total gas pressure  $P_g = P_v^{CO_2} + P_v^{CH_4} + P_v^{N_2} + P_v^{H_2O}$
- *if* ( $P_v > P_h^{eq}$ ) *then* hydrate forms
- *if* ( $P_g > P_\ell + P_{entry}$ ) *then* nonaqueous gas or liquid forms

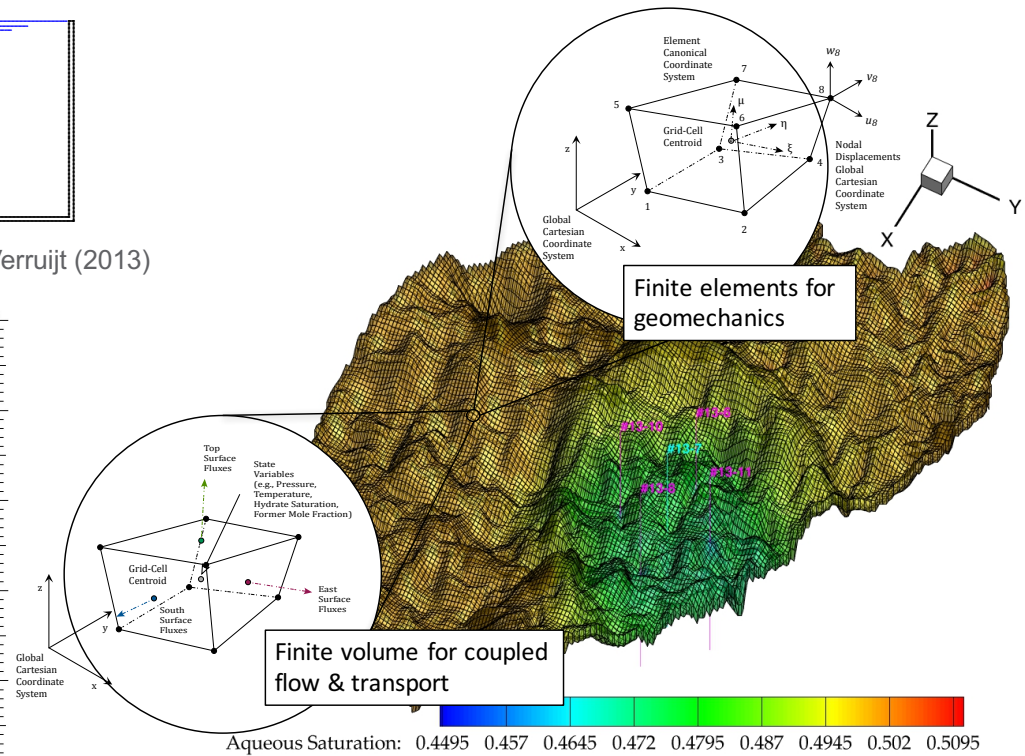
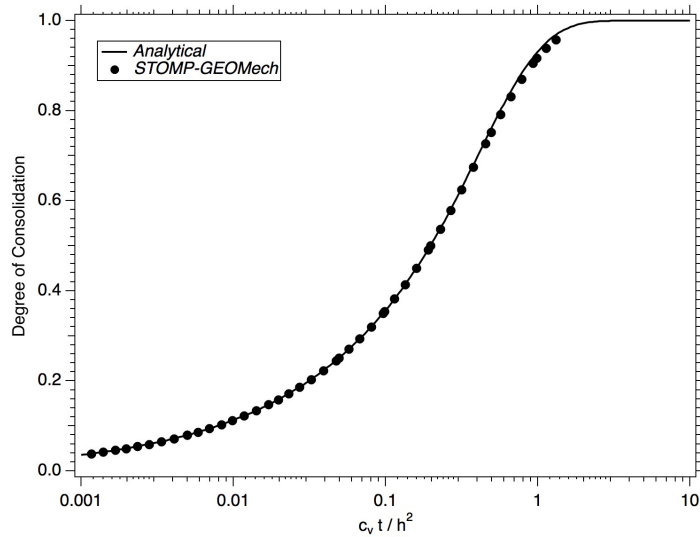
Phase Condition #30 Series  $s_h > 0.0, s_n + s_g > 0.0, s_\ell + s_i < 1.0$



# Coupling Flow and Transport with Poro-Thermo-Elastic Geomechanics



Conceptualization of the Terzaghi problem, taken from Verruijt (2013)



## Fixed Stress Sequential Coupling



### Flow and Transport Solution via Finite Volume

- Iterative Solution of Governing Equations for Flow and Transport
- Effective Permeability Function of Flow Porosity  $\phi_{flow}$  and  $S_h$
- Yielding Pore Pressure  $P_{pore}$  and Temperature  $T$

### Poros-Thermo-Elastic Geomechanics via Finite Element

- Direct Solution of the Governing Equations for Geomechanics
- Compute the Mechanical Porosity  $\phi_{mech}$
- $\phi_{mech}^{k+1} = func [\phi_{mech}^k, \Delta P_{pore}, \Delta \epsilon_V]$
- $if \left\{ \frac{\phi_{flow} - \phi_{mech}^{k+1}}{\phi_{mech}^{k+1}} > tol (e.g. 10^{-6}) \right\}$

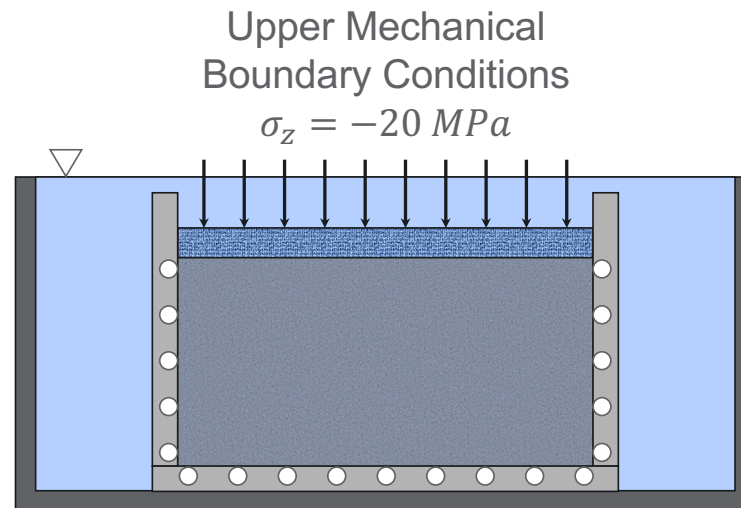


## Example of Geomechanical Coupling and Hydrate Dissociation



Side Mechanical  
Boundary Conditions  
 $u_x = 0.0 \text{ m}$

Initial Conditions  
 $T = 4^\circ\text{C}$   
 $P = 5.0 \text{ MPa}$   
 $s_h = 0.5, s_\ell = 0.5$   
 $\psi_h^{CO_2} = 0.0, \psi_h^{CH_4} = 1.0, \psi_h^{N_2} = 0.0$   
*state conditions = equilibrium*



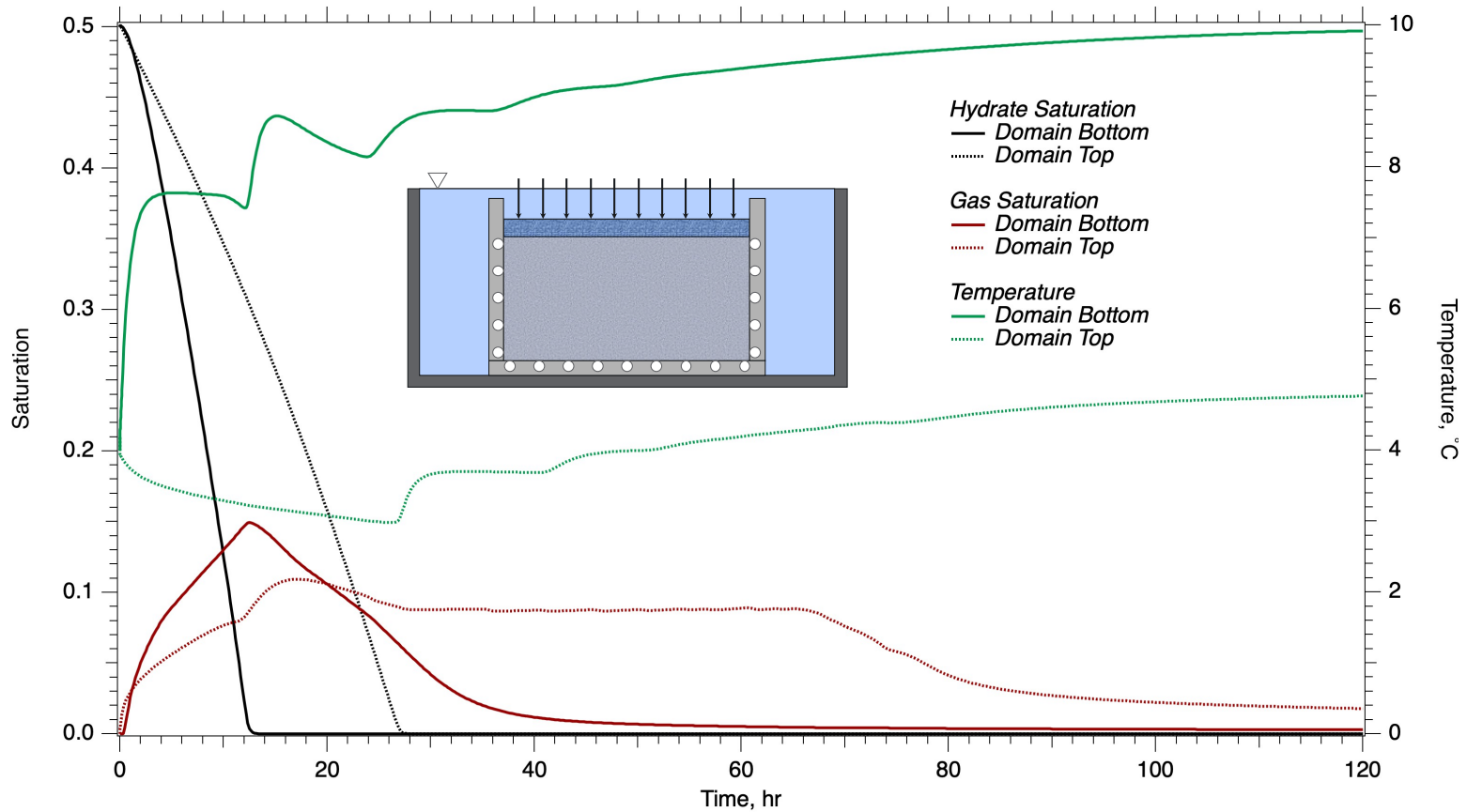
Upper Mechanical  
Boundary Conditions  
 $\sigma_z = -20 \text{ MPa}$

Bottom Mechanical  
Boundary Conditions  
 $u_z = 0.0 \text{ m}$

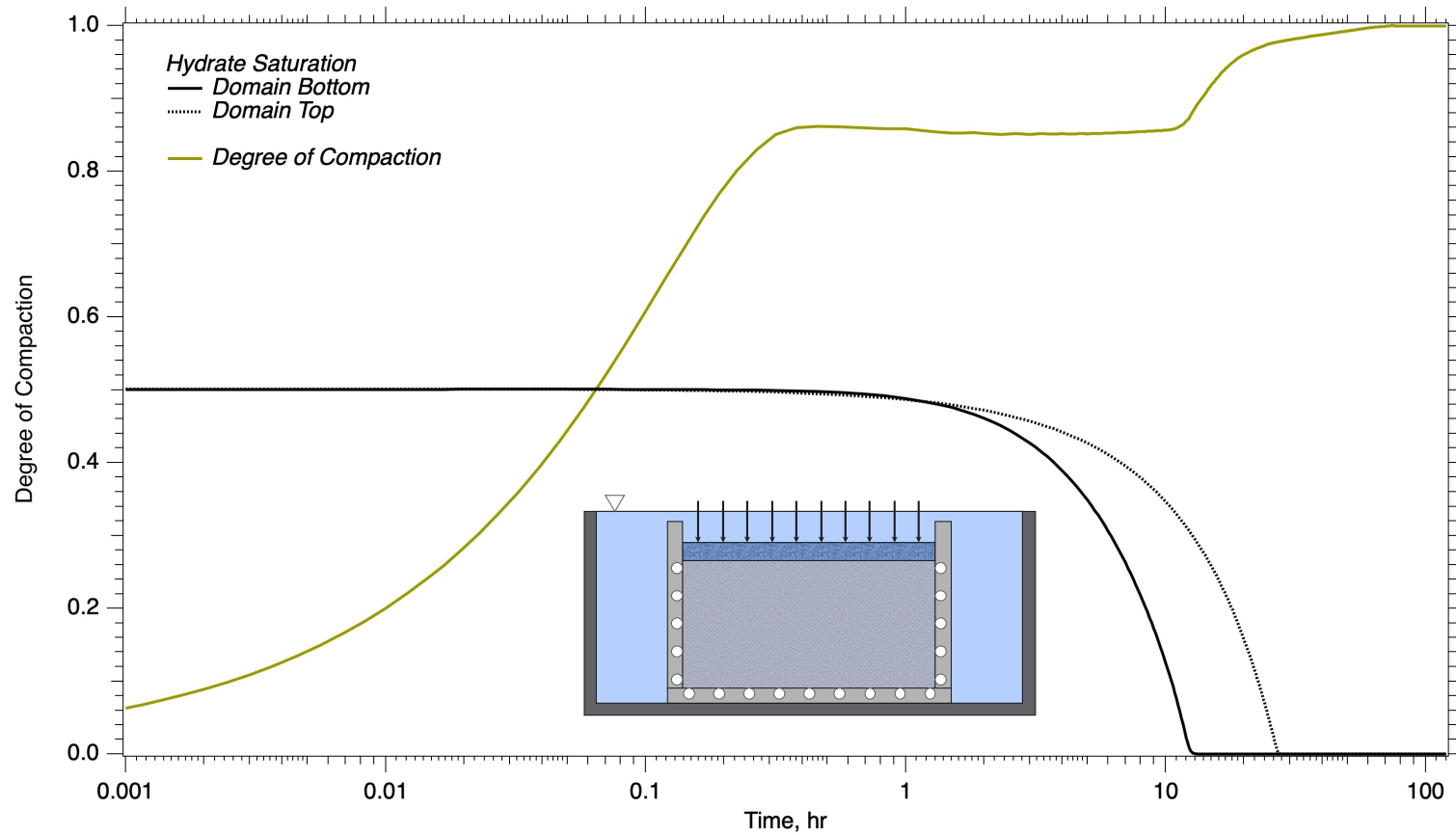
Upper Fluid Boundary  
Conditions  
 $T = 4^\circ\text{C}$   
 $P = 3.0 \text{ MPa}$   
 $s_h = 0.0, s_\ell = 1.0$

Side Fluid  
Boundary  
Conditions  
 $T = 10^\circ\text{C}$   
*no flow*

# Example of Geomechanical Coupling and Hydrate Dissociation

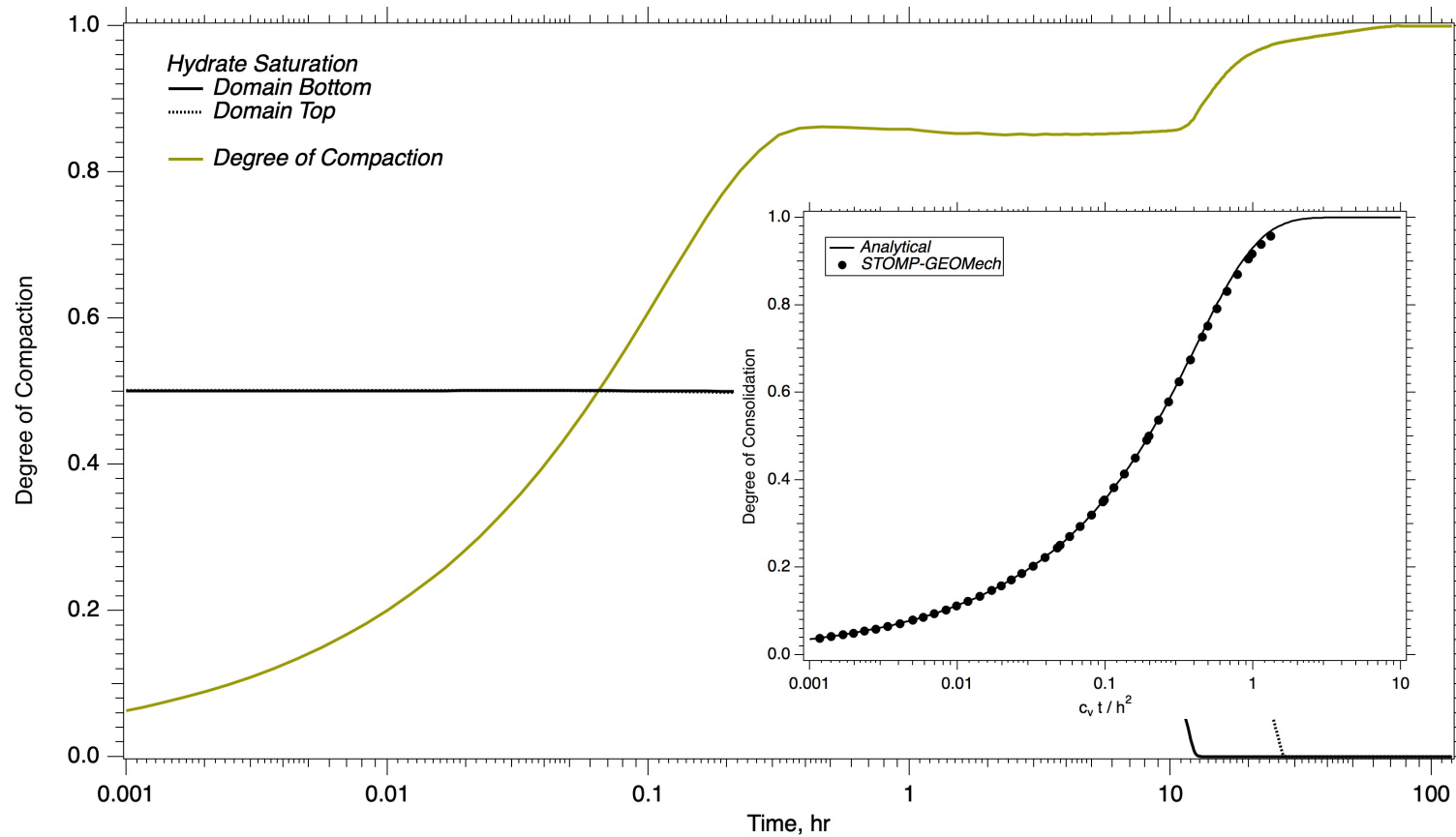


# Example of Geomechanical Coupling and Hydrate Dissociation





# Example of Geomechanical Coupling and Hydrate Dissociation





**Thank you**

