Pore-scale Simulations On The Impacts Of Hydrate Production Approaches On Gas And Water Transport In Hydrate-bearing Sediments

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Outline

• Background and motivation
• Lattice Boltzmann (LB) method
  - LB model for multiphase reactive transport processes
    ▪ Model verification
    ▪ Simulation study on relative permeability estimation during hydrate dissociation
• Conclusion
Gas hydrates resource
- Hydrates are crystalline compounds composed of gas molecules trapped in a lattice of water molecules
- Stable under low temperature and high pressure
- Over 3000 trillion cubic meters

Production challenges associated with permeability changes
- Gas surge in production
- Excessive water production
- Economic feasibility

Background and motivation

(Wikipedia: Methane hydrate)  
(Boswell et al., 2009)  
(Ren, X. et al., 2020)
Essential physicochemical processes during hydrate dissociation

- Dissociation reaction of methane hydrate: $\text{CH}_4 \cdot 5.75\text{H}_2\text{O} \rightarrow \text{CH}_4 \uparrow + 5.75\text{H}_2\text{O}$
  - Triggered by changes in temperature/pressure conditions
  - Endothermic, self-inhibition reaction

- Evolution of pore structure during dissociation
- Fluids transport through the interconnected network of pores
- Heat transfer from artificial heat source/ sensible heat in adjacent layers
Methodology selection

- Lattice Boltzmann simulation for reactive transport and permeability estimation
  - Flexibility in boundary conditions treatment
    - Handle complex pore geometries
    - Capture pore scale interactions between fluids and solids
  - Reliable numerical stability
  - Ease of implementation and efficient parallelization

Molecular Dynamics molecule movement → Simplified kinetic models → LB method particle distributions → averaged fluid quantities → N-S equation macroscopic quantities
Lattice Boltzmann model

- Multiphase hydrodynamic LB model
  - Phase field multiphase model \cite{Jacqmin, D, et al., 1999}
    - Derived by minimizing the Gibbs free energy of the multiphase system to predict phase interface evolutions
    - Applies the advection-diffusion form of equation to describe the evolution of phase index
    - Introduces diffuse interfaces between different phases to achieve a smooth transition of physical properties
  - Phase field LB model \cite{Geier, M., et al. 2015}
    - Phase index distribution
      \[
      h_i(x + e_i \Delta t, t + \Delta t) = h_i(x, t) - \frac{h_i(x, t) - \bar{h}_i^{eq}(x, t)}{\tau_i} + S_i^\phi(x, t) \Delta t
      \]
    - Pressure distribution
      \[
      f_i(x + e_i \Delta t, t + \Delta t) = f_i(x, t) - \frac{f_i(x, t) - \bar{f}_i^{eq}(x, t)}{\tau_f} + S_i(x, t) \Delta t
      \]
    - Source term due to dissociation and forces \cite{Verdier, W., et al., 2020}
      \[
      S_i^\phi(x, t) = F_i^\phi_{\text{tot},i} + \dot{m}_i^\phi
      \]
      \[
      S_i(x, t) = F_{\text{tot},i} + \dot{m}_i
      \]
      - Ensure the surface tension is correctly accounted at interfaces
      - Mass source contribution to phase index
      - Body force, viscous force, surface tension
    - Mass source contribution to pressure

\[
\]
Lattice Boltzmann model

- Multiphase hydrodynamic LB model
  - Equivalent macroscopic multiphase model  
    \[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \dot{m} \]
    \[ \frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \left( \rho \vartheta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \right) + F_{\text{tot}} + \dot{m} \mathbf{u} \]

- Phase index equation (Allen-Cahn equation)
  \[ \frac{\partial \varphi}{\partial t} + \nabla \cdot (\varphi \mathbf{u}) = \nabla \cdot \left( M_{\varphi} \left( \nabla \varphi - \frac{4}{W} \varphi (1 - \varphi) \mathbf{n} \right) \right) + \frac{\dot{m} \varphi}{\rho} \]

- Volume diffusive term

Hydrodynamic equations

(Allen, S. M., et al., 1979)

(Allen, M., et al. 2015)
Lattice Boltzmann model

- Heat transfer LB model
  - Heat transfer equation
    
    Temperature distribution
    \[
    g_i(\mathbf{x} + c \mathbf{e}_i \Delta t, t + \Delta t) = g_i(\mathbf{x}, t) - \frac{1}{\tau_{g,k}} [g_i(\mathbf{x}, t) - g_i^{eq}(\mathbf{x}, t)] + \Delta t F_i
    \]

  - Heat source due to latent heat of dissociation and conjugate condition treatment (Karani et al., 2015) (Moridis, 2012)
    \[
    F_i = \omega_i (S_{\text{conj}} + S_{\text{latent}})
    \]

  - Equivalent macroscopic heat transfer equation (Karani et al., 2015)
    \[
    \rho h \frac{\partial T}{\partial t} + \nabla \cdot (\rho h \mathbf{u} T) = \nabla \cdot (k \nabla T) + S_{\text{latent}}
    \]

- Geometry alteration model (volume of pixel) (Kang et al., 2006)
  \[
  V_{s}(t + \Delta t) = V_{s}(t) - AV_{m}S_{\text{reaction}}
  \]
Multiphase transport model verification

- Verification on hydrodynamic processes
  - Multiphase flow in porous medium  
  
  \[ \frac{t}{t_{bt}} = 0.088 \]
  \[ \frac{t}{t_{bt}} = 0.224 \]
  \[ \frac{t}{t_{bt}} = 0.349 \]
  \[ \frac{t}{t_{bt}} = 0.478 \]

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\[ t_{bt} = 0.740 \]
\[ t_{bt} = 0.869 \]
\[ t_{bt} = 1.01 \]

Pressure comparisons

(Aursjø et al., 2011)
Heat transfer model verification

• Verification on heat transfer processes

Horizontal walls have fixed sinusoidal temperatures:

$$T(x, y = 0) = T(x, y = H) = \cos(\omega x), \omega = 2\pi/L$$

(Karani et al., 2015)
Simulation setup

- Evolution of pore structure defines the relative permeability \( K_r \) vs wetting-phase (water) saturation \( S_w \) relation
- Coupling between fluid transport and heat transfer plays a dominant role in pore structure evolution
- Study the coupling effects on the \( K_r - S_w \) relations on homogeneous hydrate-bearing sediment with two common distribution morphologies under different dissociation conditions

\[ S_{\text{hyd}} = 35\% \]
\[ 2.42 \text{ mm} \times 1.84 \text{ mm} \]
\[ 484 \times 368 \]
\[ P = 12 \text{ MPa} \]
\[ T = 287.75 \text{ K} \]
Simulation for gas and water transport processes

- Relative permeability estimation during hydrate dissociation
  - Baseline case: isothermal LB simulation on fluid transport
  - Pore structure evolution during dissociation is modeled by assumed evolution patterns
  - Boundary conditions
    - Periodic boundary condition on outer boundaries
    - Bounce-back boundary condition on fluid-solid interfaces
    - Wettability boundary condition on solid boundaries (water contact angle on solid interface: 0°) (Dai, S., et al., 2019)

Initialization

$S_{\text{hyd}}=20\%$

Pore filling

Grain-coating

$K_r\text{ vs }S_w$

Pore filling

Grain-coating
Simulation for gas and water transport processes

- Relative permeability estimation during hydrate dissociation
  - Thermal stimulation case: both considering latent heat and heat source
  - Top/bottom thermal intervention from hydrate-free layer was considered
  - Boundary conditions
    - Periodic boundary condition on outer boundaries
    - Bounce-back boundary condition on fluid-solid interfaces
    - Constant temperature boundary condition on top/bottom boundaries
    - Fully developed temperature boundary condition on inlet/outlet boundaries
    - Wettability boundary condition on solid boundaries

- Grain coating $K_r vs S_w$ vs $S_{hyd} = 20\%$

- Pore filling

- Gas generation during dissociation

- Simulation for gas and water transport processes
Simulation for gas and water transport processes

- $P_c$ vs $S_w$ relation comparisons for homogeneous cases
  - $P_c$ vs $S_w$ relations under different hydrate saturation
  - Boundary conditions
    - Constant pressure boundary condition on inlet boundary
    - Convective outflow boundary condition on outlet boundary

- Jamin effect
  - resistance to fluid flow through capillaries which is due to the presence of bubbles/droplets

\[
P_2 - P_1 = \frac{2\sigma_{wg}}{R_1} \\
P_2 - P_3 = \frac{2\sigma_{wg}}{R_2} \\
P_3 - P_1 = 2\sigma_{wg}\left(\frac{1}{R_1} - \frac{1}{R_2}\right)
\]

(Li et al., 2021)
Simulation for gas and water transport processes

- $K_r$ vs $S_w$ relation comparisons for homogeneous cases
  - Gas gathers in areas without hydrates, while water remains in areas with hydrates due to capillarity
    - The non-wetting phase tends to occupy larger pores, whereas the wetting phase is more likely to occupy smaller pores
    - Gas exhibits lower dynamic viscosity than water, resulting in higher mobility
    - Capillary pressure and Jamin effect are significantly decreased
  - Thermal stimulation cases show considerable improvements in $K_{rg}$ values but little decrease in $K_{rw}$

Simulation for gas and water transport processes
Conclusion

- Concluding remarks
  - Uniform dissociation in baseline model obscures the formation of hydrate-free zone, making capillarity impact and Jamin effect on fluid transport dependent solely on $S_{\text{hyd}}$
  - The coupling of mass and heat transfer typically results in the creation of a hydrate-free zone, causing the redistribution of fluid under capillary effects, which significantly impacts the $K_r - S_{\text{hyd}}$ relation
  - Gas is prone to occupy the hydrate-free zone under capillary force as the non-wetting phase, leading to a significant increase in $K_{r,g}$ values compared to those obtained from baseline models
  - Considerable deviations can be found by comparing the $K_r - S_w$ relations obtained from coupled and baseline models
  - Gas bubble transport in HBS is mostly impeded by the Jamin effect, which prevents the formation of a continuous gas stream. Therefore, it is crucial to mitigate this effect during production to facilitate efficient gas extraction
References

- Methane clathrate - Wikipedia
- MH21-S R&D consortium--Fundamental Technology-- (mh21japan.gr.jp)


