A coupled thermal-hydraulic-mechanical-chemical (THMC) model for methane hydrate bearing sediments using COMSOL Multiphysics

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Keyword: Hydrate bearing sediments; Coupled THMC model; Critical state model; Gas production

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## Introduction

- The mechanical behavior of methane hydrate bearing sediment (MHBS) changes during the process of hydrate dissociation, which may induce catastrophic failures including layer collapse, sliding and damage to infrastructure.
- Most models are based on the finite differential method (FDM) or finite volume method (FVM). Few models for MHBS are based on the finite element method (FEM) even though FEM is very robust for nonlinear deformation and stress calculations.
- The coupling system of the problem examined in this study consists of governing equations and auxiliary equations. The governing equations include the conservation of energy, mass, and momentum. All these equations are derived from the local balance conditions.
- In thermodynamics-based critical state model, dilatant part can be asymmetric with contraction part. The model can predict the stress softening and dilatancy during the drained shearing process for specimens with different hydrate saturations and different hydrate accumulation habits.

# Model description

Governing Equations	
Mass conservation for gas, water and hydrate: $\alpha = g$ , w, h	$\frac{d}{dt}(\rho_{\alpha}\phi_{\alpha}) + \rho_{\alpha}\phi_{\alpha}\nabla \cdot \nu_{\alpha} = \frac{dm_{\alpha}}{dt}$ Source term : $\sum_{\alpha} \frac{dm_{\alpha}}{dt} = 0$
	No hydrate squeezing out from the skeleton: $v_s = v_h$ The relation between porosity and volume fraction: $\phi = \phi_w + \phi_g + \phi_h$
	The relation between saturation and volume fraction: $s_{\alpha} = \frac{\phi_{\alpha}}{\phi}$
	Gas density: $\rho_g = 16.042 g/mol \cdot p_g/Z/T$ $Z = 8.32 J/mol \cdot K$
Mass conservation for host sediments	$\frac{d}{dt}(\rho_{s}\phi_{s}) + \rho_{s}\phi_{s}\boldsymbol{\nabla}\cdot\boldsymbol{\nu}_{s} = 0$
Momentum conservation for the compound	$\boldsymbol{\nabla} \cdot \left(\boldsymbol{\sigma}' - \frac{s_w p_w + s_g p_g}{s_w + s_g} \boldsymbol{\delta}\right) + \left(\boldsymbol{\phi}_s \rho_s + \boldsymbol{\phi}_w \rho_w + \boldsymbol{\phi}_g \rho_g + \boldsymbol{\phi}_h \rho_h\right) \boldsymbol{g} = \boldsymbol{0}$
Momentum conservation for water(Darcy's law)	$\nabla p_w + \frac{\mu_w}{K_h k_{wr}} \boldsymbol{q}_w = \rho_w \boldsymbol{g}$
	Darcy s velocity of water: $\boldsymbol{q}_w = \boldsymbol{\varphi}_w(\boldsymbol{v}_w - \boldsymbol{v}_s)$ Water viscosity: $\mu_w = 1e - 3 kg/ms$
Momentum conservation for gas(Darcy's law)	$\boldsymbol{\nabla} p_g + \frac{\mu_g}{K_h k_{gr}} \boldsymbol{q}_g = \rho_g \boldsymbol{g}$
	Darcy's velocity of gas: $\boldsymbol{q}_g = \phi_g(\boldsymbol{v}_w - \boldsymbol{v}_s)$
	Gas viscosity: $\mu_g = \frac{\mu_W}{1051 - 3.31T}$
Energy conservation for the compound	$\sum_{\alpha} (\phi_{\alpha} \rho_{\alpha} c_{T\alpha}) \frac{dI}{dt} - \nabla \cdot \sum_{\alpha} (\phi_{\alpha} K_{T\alpha}) \nabla T + \nabla \cdot (\rho_{w} c_{Tw} q_{w} T) + \nabla \cdot (\rho_{g} c_{Tg} q_{g} T) = -\Delta H R_{h}$
	Heat capacity: $c_{Tw} = 4.02 + 0.000577 \cdot T$ , $c_{Tg} = 1.24 + 0.00313 \cdot T$ , $c_{Ts} = 0.8J/gK$ , $c_{Th} = 2.11/gK$
	Heat conductivity: $k_{Tw} = 0.556W/mK$ , $k_{Tg} = 0.0335W/Mk$ , $k_{Ts} = 3.92W/mK$ , $k_{Th} = 0.394W/Mk$

Auxiliary equation	
Capillary model	van Genuchten model: $p_{\rm c} = p_g - p_w = p_0 (s_e^{-\frac{1}{a}} - 1)^{1-a}$ , $a = 0.52$ , $p_0 = 10  {\rm kPa}$
Stress-strain relationship	$d\boldsymbol{\sigma}' = \left(\boldsymbol{D}^{\boldsymbol{e}} - \frac{\boldsymbol{D}^{\boldsymbol{e}}: \boldsymbol{d} \otimes \frac{\partial f}{\partial \boldsymbol{\sigma}'}: \boldsymbol{D}^{\boldsymbol{e}}}{\frac{\partial f}{\partial \boldsymbol{\sigma}'}: \boldsymbol{D}^{\boldsymbol{e}}: \boldsymbol{d} + H}\right): d\boldsymbol{\varepsilon} + \left(\boldsymbol{\chi} \boldsymbol{D}^{\boldsymbol{h}}: \boldsymbol{\varepsilon}^{\boldsymbol{e}} - \frac{\boldsymbol{D}^{\boldsymbol{e}}: \boldsymbol{d} \left(\frac{\partial f}{\partial p_{cc}'} \boldsymbol{\zeta} \omega(\boldsymbol{s}_{h}^{m})^{\omega-1} \boldsymbol{\chi} + \frac{\partial f}{\partial p_{cd}'} \boldsymbol{\xi} w(\boldsymbol{s}_{h}^{m})^{w-1} \boldsymbol{\chi}\right)}{\frac{\partial f}{\partial \boldsymbol{\sigma}'}: \boldsymbol{D}^{\boldsymbol{e}}: \boldsymbol{d} + H}\right) d\boldsymbol{s}_{h}$
	Hardening law: $H = \frac{\partial f}{\partial p'_{cc}} \omega m p'_{cc} + \frac{\partial f}{\partial p'_{cd}} w m p'_{cd} - \frac{\partial f}{\partial p'_{cs}} \frac{(1+e_R)p'_{cs}}{\lambda - \kappa} D + \frac{\partial f}{\partial R} u ln R  \boldsymbol{d} $
	Flow rule: $\boldsymbol{d} = \left( D \frac{\partial p'}{\partial \sigma'} + \frac{\partial q}{\partial \sigma'} \right)$
	Yield surface: $f = \frac{\left(p' - R\left(\frac{1}{2}\gamma(p'_{cc} + p'_{cd} + p'_{cs}) - \left(1 - \frac{\gamma}{2}\right)p'_{cc}\right)\right)^2}{\left((1 - \gamma)p' + R\frac{1}{2}\gamma(p'_{cd} + p'_{cs}) + Rp'_{cc}\right)^2} + \frac{q^2}{\left((1 - \alpha)Mp' + \alpha M\rho' R + RMp'_{cc}\right)^2} = 1,$
	Model parameters: $m = 2$ , $\xi = 20$ MPa, $w = 1.4$ , $\zeta = 0.5$ MPa, $\omega = 1.2$ , $\kappa = 0.02$ , $u = 200$ , $M = 1.37$ , $\nu = 1.2$ , $\alpha = 1$ , $\lambda = 0.2$
Reaction kinetics	Reaction rate per mol: $R_{\rm h} = \phi_h A_{hs} K_{d0} \exp(\frac{\Delta E_d}{ZT}) < p_{eq} - p_g >$
	Specific area: $A_{hs} = 0.1 \cdot 1/\mu m$ Dynamic coefficient: $K_{d0} = 1.24 \times 10^5 \ mol/m^2 \cdot Pa \cdot s$
	Reaction activation energy: $\Delta E_d = -78300$ J/mol
	Phase equilibrium pressure: $p_{eq} = \exp\left(39.08 - \frac{8520}{T}\right)$
Permeability	$K_i = K_{i0} \left(\frac{e}{e_0}\right)^{\beta} (1 - S_h)^N$
	Water relative permeability: $k_{\rm w} = s_e^b \left[ 1 - \left( 1 - s_e^{\frac{1}{a}} \right)^a \right]^2$
	Water relative permeability: $k_{\rm g} = (1 - s_e)^c \left(1 - s_e^{\frac{1}{a}}\right)^{2\alpha}$
Variation in Density	Water density: $\frac{1}{\rho_w} \frac{d\rho_w}{dt} = \frac{1}{B_w} \frac{dp_w}{dt} - \beta_w \frac{dT}{dt}$
	Gas density: $\frac{1}{\rho_g} \frac{d\rho_g}{dt} = \frac{1}{B_g} \frac{dp_g}{dt} - \beta_g \frac{dT}{dt}$
	Bulk modulus: $B_w = 2$ GPa , $B_g = p_g$ Theorem 1 emerges $P_w = (12.41 \text{ m} \text{ m} 2717) \times 10^{-6}$
	$p_w = (13.41 \cdot I - 3/1) \times 10^{\circ},  \beta_a = 1/1$

# Model Verification

The hydrate dissociation experiment data produced by Masuda *et al.* (1999) were used to verify the performance of the coupled THMC code.



Fig. 1 Draft of the numerical model for the specimen



Fig. 2 Comparison between the amount of gas production from simulation and experiment

Fig. 3 Comparison between temperatures in simulations and experiments

#### Comparison of simulations with different codes



heat injection

depressurization

## Performance of the mechanical model

We used the data published by Masui et al. (2006; 2007), Hyodo et al. (2013a; 2013b) to examine the performance of the proposed constitutive model.



#### Simulation of hydrate production by depressurization

We used the data published by Masui et al. (2006; 2007), Hyodo et al. (2013a; 2013b) to examine the performance of the proposed constitutive model.



### Conclusions

The accuracy of the model was verified by carefully comparing the simulated results to some triaxial test data available in the literature. The accuracy of the fully coupled THMC model without the mechanical part was validated by the gas production test data provided by Masuda et al. (1999). The performance of the code was similar to that of other simulators reported in the past.

The effect of full coupling compared with semi-coupling was investigated by simulating methane gas extraction by the depressurization method. Results showed that the changes in pressure, temperature, and hydrate saturation in the semi-coupled model were faster than those in the fully coupled model. The main reason for the difference was due to the volume change deformation, which influences the water and gas permeability and prolongs the pore pressure equalization diffusion process.

A case study of gas extraction from a heterogeneous hydrate layer system by depressurization was analyzed using the fully coupled model. Compared with a homogeneous model, a continuous heat supply from the layer without hydrate prohibited the temperature drop in the hydrate-dissociated layer due to hydrate dissociation, guaranteeing continuous gas production. Different mechanical properties of the different layers resulted in local shear stress and strain found at the interface between the hydrate layer and the layer without hydrates.