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#### **Special Section:**

Gas Hydrate in Porous Media: Linking Laboratory and Field Scale Phenomena

### **Key Points:**

- · A fully coupled consistent/dependable approach to tackle problems involving HBS with a novel kinetic law to model phase transformations
- An analytical solution related to gas production via radial depressurization from a confined HBS reservoir at steady state conditions
- · Modeling of a lab test simulating gas production from a heterogeneous HBS specimen involving hydrate dissociation and ice formation/thawing

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# **Coupled Numerical Modeling of Gas Hydrate-Bearing** Sediments: From Laboratory to Field-Scale Analyses

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Abstract Methane hydrates are ice-like compounds made of gas methane and water. Hydrates are stable under low-temperature and high-pressure conditions constraining their occurrence in sediments to marine and permafrost settings. A shift from the stability condition triggers an endothermic hydrate dissociation with the associated release of gas and water, impacting (among others) on sediment pore pressure, temperature, and deformations. Therefore, the behavior of hydrate-bearing sediments (HBS) is controlled by strongly coupled thermo-hydro-chemo-mechanical actions. The analysis of available data from past field and laboratory experiments and the optimization of future field production studies require a formal and robust numerical framework able to capture the complex behavior of this type of soil. In this paper we used a fully coupled thermo-hydro-mechanical framework to study different problems involving HBS, from laboratory experiments involving natural hydrate samples to gas production tests. We also develop an analytical solution for the case of gas production via radial depressurization from a confined HBS reservoir. The analyses show the complexity of the thermo-hydro-mechanical phenomena associated with this type of system and contribute to better understand the behavior of HBS.

# 1. Introduction

Methane hydrates are solid compounds formed by methane molecules trapped in water molecule cage-like structures. The formation and stability of methane hydrates require relatively high pressures and low temperatures typically found in subpermafrost and marine settings. A shift from the stability conditions induces hydrate dissociation releasing gas and water, triggering profound changes in sediment fluid pressure, temperatures, and stresses. Hydrate concentration is generally gas limited, except near high gas flux conduits. Methane hydrates are a valuable potential energy resource (e.g., Boswell, 2009; Rutqvist & Moridis, 2007; Soga et al., 2006). Hydrate-bearing sediments (HBS) play a critical role on the evolution of various natural processes and the performance of engineered systems. For example, hydrate dissociation can trigger large-scale seafloor instabilities (Briaud & Chaouch, 1997; Chatti et al., 2005; Jamaluddin et al., 1991; Kayen & Lee, 1991). Furthermore, uncontrolled release of methane will exacerbate global warming (Dickens et al., 1997).

Pronounced expansion of the pore fluid within sediments during hydrate dissociation will cause either large fluid flux if free-draining conditions prevail or high fluid pressure if the rate of pore pressure dissipation is lower than the rate of hydrate dissociation. In intermediate drainage conditions, the excess pore fluid pressure will depend on the initial volume fraction of the phases, the rate of dissociation relative to the rate of mass transport, heat diffusion, and sediment compliance. In turn, pore pressure variations will induce changes in effective stress, impacting on sediment properties and mechanical behavior. Therefore, hydrates stability conditions combine with sediment behavior to produce a strong thermo-hydro-mechanical (THM) coupled response in HBS.

Several model and numerical solution frameworks have been proposed to study the main features of HBS behavior (e.g., Ahmadi et al., 2004; Cheng et al., 2013; Davie & Buffett, 2001; Fang, 2009; Gamwo & Liu, 2010; Kimoto et al., 2007, 2010; Kwon et al., 2008; Liang et al., 2010; Liu & Yu, 2013; Moridis, 2014; Nazridoust & Ahmadi, 2007; Rempel & Buffett, 1997, 1998; Ruan et al., 2012; Sultan et al., 2004; White, 2008; Xu & Germanovich, 2006; Xu & Ruppel, 1999). In some of these models, the sediment response is disregarded or handled with simple approaches (e.g., a rigid sediment is adopted in Nazridoust & Ahmadi, 2007, an elastic porous medium in Kwon et al., 2008, and a nonlinear 1-D compression law in Garg et al.,

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2008). HM coupled isothermal models with more appropriate (mechanical) sediment representation include developments by Klar et al. (2010). Other hydrate simulators focus on fluid flow and phase changes (e.g., Chen et al., 2017; White & McGrail, 2006). Helmig (1997) focused on numerical modeling techniques when dealing with multiphase flow and transport processes in the subsurface.

Two basic numerical strategies can be adopted to solve the system of coupled partial different equations that govern the behavior of HBS: (i) simultaneous solution (also called fully coupled approach), where all the governing equations are concurrently advanced in time and (ii) sequential solution (or partitioned approach), where the time-integration process is carried out over each governing equation separately (keeping the variables of the other fields frozen) with the interactions between the different field equations conducted following different strategies (e.g., Felippa & Park, 1980; Kim et al., 2011; Mainguy & Longuemare, 2002; Rutqvist & Moridis, 2007). Sequential approaches can be based on linking existing simulation codes (or modules) for the different physics by introducing an interface between them to exchange information at, for example, time step or iteration levels. Sequential schemes often restrict computations to one-way coupled analysis, where one can investigate (e.g., the effects of pressure changes on mechanical behavior but cannot consider the influence of sediment strains on the multiphase flow).

Rutqvist and Moridis (2007) and Rutqvist (2011) proposed a thermo-hydro-mechanical and chemical (THMC) framework for HBS that combines the TH computer code TOUGH+HYDRATE with the mechanical software FLAC using a one-way sequentially coupled scheme. Kim et al. (2012) extended this approach for a two-way coupling scheme. Chemo-thermo-mechanical analyses related to ground deformation and gas production using a viscoplastic model are presented in Kimoto et al. (2007, 2010). Klar et al. (2013) proposed a THM explicitly coupled formulation for HBS. Gupta et al. (2015) present a hydro-geomechanical coupled model for HBS systems. The flow and geomechanical models are solved using an iterative coupling strategy based on the Gauss-Seidel scheme. This iterative coupling scheme was able to solve the coupled problem as rigorously as a fully coupled approach when iterates to full convergence. Gupta et al. (2016) extended their work by developing several multirate time stepping solution schemes. Gupta et al. (2017) proposed a THMC code for HBS based on a simplified coupling concept for linking different simulators. Kim et al. (2009) study four different operator-splitting techniques and discuss about their convergence and stability conditions. Recently, Dana and Wheeler (2018) demonstrated that the fixed stress split iterative scheme converge numerically when analyzing the coupled flow and deformation Mandel's problem with transverse isotropy. Ajayi et al. (2018) discussed several aspects to be considered when modeling methane production from HBS.

In this paper we analyze different problems involving HBS. The fully coupled multiphysic program CODE\_BRIGTH (Olivella et al., 1996) was intensively modified to deal with HBS. The proposed approach establishes couplings between the different physics (e.g., through the corresponding balance and constitutive equations) and the nonlinear system of partial different equations is solved simultaneously, in a fully coupled manner, via the Newton Raphson scheme. The finite element (FE) method is adopted for the spatial discretization, while finite differences are used for the temporal discretization via an (unconditionally stable) implicit scheme that incorporates an automatic time stepping algorithm (CODE\_BRIGHT Manual, 2018). We use a novel pseudo-kinetic law to describe the rate of hydrate dissociation/formation. We take into consideration potential ice formation. We partially validate our approach analyzing the controlled depressurization lab test of a natural HBS specimen. We propose a new analytical solution for analyzing gas production from a confined hydrate reservoir at steady state conditions. We also use this analytical solution to partially verify our numerical code.

# 2. Theoretical Framework

To simulate the behavior of HBS we consider balance equations, constitutive equations, equilibrium restrictions, and phase transformations. This set of equations describe mathematically the key THM processes anticipated in this type of sediment: (i) methane and water flow driven by advective and nonadvective flows; (ii) heat transfer via conduction and phase advection; (iii) heat of phase transformation (i.e., methane dissociation/formation and ice thawing/formation); and (iv) deformable sediment. This set of coupled phenomena is analyzed next, following the FE CODE\_BRIGHT framework and numerical platform (Olivella et al., 1996).



**Figure 1.** Hydrate-bearing sediment. (a) Solid, liquid, gas, and hydrate may be found forming the sediment. (b) Components can be grouped into phases and species.

#### 2.1. Phases Properties and Partial Saturations

We assume an HBS consisting of a granular skeleton with pores that can be partly filled with liquid, gas, hydrate, or ice. We consider three species—methane, water, and mineral—that are distributed in the adopted phases as indicted in Figure 1. The ice phase is modeled because water-to-ice transformation may take place during fast depressurization. Observations related to phase composition and mass densities are discussed next. Figure 1b summarizes phases and species, and Table 1 lists key thermal properties of species and phases.

*Solid* and *ice* are single species phases. Minerals form the grains of the solid phase, and ice is made of pure water. Their densities are assumed constant.

*Hydrate* is made of water and methane. The hydration number  $\chi$  controls the amount of water in methane hydrates (CH<sub>4</sub> $\chi$ H<sub>2</sub>O). From the atomic masses  $\alpha = \chi/(0.89 + \chi)$ , where  $\alpha$  is the water/methane mass fraction ( $\alpha = m_w/m_h$ ). In the case of Structure I,  $\chi = 5.75$  and  $\alpha = 0.866$ . Hydrates found in nature often involve higher hydration numbers (e.g., Handa, 1988).

*Liquid* water and dissolved methane are the two components of the liquid phase. The solubility of methane in water is always very low; for example, at pressure liquid  $P_{\ell} = 10$  MPa and temperature T = 280 K, the mass fraction of CH<sub>4</sub> in water is  $m_m/m_w \sim 1.4 \times 10^{-3}$ . In free-hydrate systems the solubility of CH<sub>4</sub> in water



Specific Energy and memorina nursport—Selected hepresentative values						
	Specific	Transport				
Species and phases	Expression	Specific heat-latent heat	Thermal conductivity			
Water—vapor	$e_{g}^{w} = L_{evap} + c_{wv}(T - T_{o})$	$L_{evap} = 2257 J/g$ $c_{wv} = 2.1 J \cdot g^{-1} \cdot K^{-1}$	$0.01 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$			
Water—liquid	$e_{\rm w} = c_{\rm wl}(T - T_{\rm o})$	$c_{\rm wl} = 4.2  {\rm J} \cdot {\rm g}^{-1} \cdot {\rm K}^{-1}$	$0.58  \text{W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$			
Water—ice	$e_{\rm ice} = L_{\rm fuse} + c_{\rm wice}(T - T_{\rm o})$	$L_{\text{fuse}} = 334 \text{ J/g}$	2.1 W·m <sup><math>-1</math></sup> ·K <sup><math>-1</math></sup>			
Methane gas	$e_m = c_m(T - T_o)$	$c_{\text{wice}} = 2.1 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ $c_m = 1.9 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1} \text{ V} = \text{const}$ $c_m = 2.5 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1} \text{ P} = \text{const}$	$0.01 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$			
Hydrate <sup>(1)</sup>	$e_h = L_{diss} + c_h(T - T_o)$	$L_{\rm diss} = 339  {\rm J/g}$	$0.5 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}$			
Mineral	$e_{\rm s}=c_{\rm s}(T-T_{\rm o})$	$c_h = 2.1 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1}$ $c_s = 0.7 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1} \text{ quartz}$ $c_s = 0.8 \text{ J} \cdot \text{g}^{-1} \cdot \text{K}^{-1} \text{ calcite}$	8 W·m <sup>-1</sup> ·K <sup>-1</sup> quartz 3 W·m <sup>-1</sup> ·K <sup>-1</sup> calcite			

Table 1

Specific Energy and Thermal Transport—Selected Representative Values<sup>a</sup>

*Note*. The sign of the latent heat is adopted to capture endothermic-exothermic effects during phase transformation. <sup>a</sup>Table from Sanchez and Santamarina (2016).

Source: CRC handbook and other general databases. (1) Waite, http://woodshole.er.usgs.gov/operations/hi\_fi/index. html; Handa, 1986.

 $(mol/m^3)$  tends to increase with pressure and decrease with temperature. The opposite is true when hydrates are present (Sun & Duan, 2007). While the contribution of methane dissolution in water to mass transport can be disregarded for gas production studies, we keep it (governed by the Henry's law) in view of potential related studies such as formation of hydrates from dissolved CH<sub>4</sub>.

We assume that the liquid density  $\rho_{\ell}$  is a function of  $P_{\ell}$  (MPa) and T (K) through:

$$\rho_{\ell} = \rho_{\ell o} \left( 1 + \frac{P_{\ell}}{B_{\ell}} \right) \left[ 1 - \beta_{T\ell} \left( \frac{T - 277K}{5.6} \right)^2 \right] \qquad 272K < T < 300K, \tag{1}$$

where  $\rho_{\ell o} = 0.9998 \text{ g/cm}^3$  is the reference liquid density at T = 277 K and at atmospheric pressure,  $B_{\ell} = 2000 \text{ MPa}$  is the liquid bulk stiffness, and  $\beta_{T\ell} = 0.0002 \text{ K}^{-1}$  is the coefficient of liquid thermal expansion. This equation properly captures the thermal expansion liquid experiences below and above T = 277 K.

Taber (1929) postulated that unfrozen water may be present in soils under freezing conditions. Tice et al. (1988) confirmed experimentally the presence of unfrozen water at temperature even as low as -15 °C. The formulation proposed herein is capable of considering cryogenic suction effects and the presence of unfrozen water at freezing temperature. However, hereafter we initially disregard the existence of unfrozen water, assuming that the liquid water is transformed into ice at freezing temperature.

*Gas* methane is the main component of the gas phase. The psychrometric law can be used to calculate the amount of water in the gas phase to conclude that the mass of water vapor in gas is very small (e.g.,  $m_w/m_g \approx 10^{-6}$  for a gas pressure of  $P_g = 10$  MPa, capillary pressure  $P_c = 0.1$  MPa, and temperature T = 280 K). The gas density depends on temperature and gas pressure. Experimental data in Younglove and Ely (1987) are used to modify the ideal gas law in the range of interest (fitted range: 270 K < T < 290 K and 0.1 MPa <  $P_q < 40$  MPa):

$$\rho_{g} = \frac{M_{m}P_{g} \times 10^{6}}{RT} \left[ 1.0 + 0.025 \frac{P_{g}}{1MPa} - 0.000645 \left( \frac{P_{g}}{1MPa} \right)^{2} \right],$$
(2)

where R = 8.314 J/(mol·K) is the gas constant and  $M_{\rm m} = 0.016042$  kg/mol the molecular mass of methane.

CODE\_BRIGHT is capable of dealing with the presence of solutes. Problems with a single solute can be handle in a fully coupled manner, as described in Olivella et al. (1994, 1996). Reactive transport problems involving multiple (*N*) interactive species are handled as described in Guimarães et al. (2007) via a sequentially coupled scheme (at Newton-Raphson iteration level) that links the THM solution with a reactive transport module.



We assume that the volume of voids is the sum of the liquid, gas, hydrate, and ice volumes; therefore, the porosity is defined as

$$\phi = \frac{V_v}{V_{total}} = \frac{V_g + V_\ell + V_h + V_i}{V_{total}},$$
(3)

where the total volume ( $V_{total}$ ) is obtained as the sum of the volumes of voids ( $V_v$ ) and solid ( $V_s$ ). The partial phases saturations are obtained as the ratio between the corresponding volume of the phases and the volume of voids (i.e.,  $S_j = V_j/V_v$ , j = I, g, h, i), such that

$$S_{\ell} + S_q + S_h + S_i = 1.$$
 (4)

#### 2.2. Balance Equations

The macroscopic balance of either mass or energy relates the rate of change per unit of volume to the flux out and in of the volume and takes into consideration external inputs as well. Mass balance equations are written for the three species: water (w), methane (m), and the mineral that makes the particles (no letter is required; it coincides with the solid). The proposed framework can also accommodate nonadvective diffusive transport of species in the phases (i.e., w in g, and m in l) as discussed in Olivella et al. (1994).

#### 2.2.1. Mass Balance: Water

The water mass per unit volume of sediment combines the water mass in four phases: liquid, gas, hydrate, and ice. The total flux of water associated with the liquid, gas, hydrate, and ice phases with respect to a fixed reference system combines the nonadvective and Darcian advective flows with respect to the soil skeleton and the whole sediment movement with velocity  $\mathbf{v}$  (m/s) relative to the fixed reference frame. Then, the mass balance of water is expressed as

$$\frac{\partial}{\partial t} \left[ \left( \theta_{\ell}^{w} S_{\ell} + \theta_{g}^{w} S_{g} + \alpha \rho_{h} S_{h} + \rho_{i} S_{i} \right) \phi \right] + \nabla \left[ \mathbf{j}_{1}^{\prime w} + \theta_{\ell}^{w} S_{\ell} \phi \mathbf{v} + \mathbf{j}_{g}^{\prime w} + \theta_{g}^{w} S_{g} \phi \mathbf{v} + \alpha \rho_{h} S_{h} \phi \mathbf{v} + \rho_{i} S_{i} \phi \mathbf{v} \right] = \mathbf{f}_{e}^{w}, \quad (5)$$

where  $\theta_l^w$  and  $\theta_g^w$  stand for the mass fraction of water per unit volume of liquid and gas phases, respectively (calculated by means of the Psychometric law). Also,  $f_e^w$  (g/[m<sup>3</sup>·s]) is the external sink/source of water per unit volume. This term allows modeling processes such as water injection at higher temperature as part of the production strategy;  $\mathbf{j}'_l^w$  and  $\mathbf{j}'_g^w$  denote the relative motion of species in the phases with respect to the solid phase, which are obtained as the sum of nonadvective and advective fluxes as follows:

$$\mathbf{j}^{\prime j}_{\ \alpha} = \mathbf{i}^{j}_{\ \alpha} + \theta^{j}_{\ \alpha} \mathbf{q}_{\alpha} \tag{6}$$

in which  $\mathbf{i}_{\alpha}^{j}$  is the nonadvective flux of the species j = w,m in the phase  $\alpha = l,g$  and  $\mathbf{q}_{\alpha}$  are the advective (Darcy's) fluxes associated with the motion of the phase  $\alpha = l,g$ .

The first term (left-hand side) in equation (5) includes the water mass exchange during hydrate formation/dissociation and ice formation/thawing when equilibrium is assumed (or pseudo-kinetic models are adopted for describing the phase transformations). Note that we assume the hydrate and ice phases move with the solid particles (equation (5), last two terms, left-hand side).

#### 2.2.2. Mass Balance: Methane

The total methane mass per unit volume of HBS is computed after adding the corresponding masses in the gas, liquid, and hydrate phases taking into consideration the volume fractions  $S_g$ ,  $S_l$ , and  $S_h$ ; the mass fraction of methane in hydrate  $(1 - \alpha)$ ; and the sediment porosity. The flux of methane in each phase combines the nonadvective and advective terms relative to the porous matrix and the motion of the porous medium with velocity relative to the fixed reference system:

$$\frac{\partial}{\partial t} \left\{ \left[ \theta_{g}^{m} S_{g} + \theta_{\ell}^{m} S_{\ell} + (1-\alpha) \rho_{h} S_{h} \right] \varphi \right\} + \nabla \left[ \mathbf{j}_{g}^{\prime m} + \theta_{g}^{m} S_{g} \varphi \mathbf{v} + \mathbf{j}_{I}^{\prime m} + \theta_{\ell}^{m} S_{\ell} \varphi \mathbf{v} + (1-\alpha) \rho_{h} S_{h} \varphi \mathbf{v} \right] = f_{e}^{m}, \quad (7)$$

where  $\theta_g^{m}$  and  $\theta_l^{m}$  stand for the mass fraction of methane per unit volume of gas and liquid phases, correspondingly;  $f_e^{m}$  (g/[m<sup>3</sup>·s]) is the external supply of methane. This general expression may be used to capture conditions such as methane input along a preexisting fault. The terms  $\mathbf{j'_l}^{m}$  and  $\mathbf{j'_g}^{m}$  are handled as in section 2.2.1. The first term (left-hand side) takes into consideration the mass exchange of



methane during hydrate formation/dissociation between phases (i.e., h and g) when equilibrium is assumed or a pseudo-kinetic law is adopted for modeling the phase transformation (more details in section 2.2.7).

#### 2.2.3. Mass Balance: Mineral

The mineral species is only found in solid particles. The mass balance equation follows:

$$\frac{\partial}{\partial t}[\rho_{s}(1-\varphi)] + \nabla \cdot [\rho_{s}(1-\varphi) \, \textbf{v}] = \textbf{0}, \tag{8}$$

where  $\rho_{\rm s}$  (g/m<sup>3</sup>) is the density of the solid particles.

#### 2.2.4. Energy Balance

The internal energy per unit volume  $(J/m^3)$  is adopted to express the balance of energy presuming thermal equilibrium among the phases. In the absence of fluxes, the total internal energy per unit volume of the medium can be expressed as (Olivella et al., 1994):

$$\frac{E}{V_{total}} = e_s \rho_s (1 - \phi) + \left( e_l \rho_l S_\ell + e_g \rho_g S_g + e_h \rho_h S_h + e_i \rho_i S_i \right) \phi,$$

$$e_l \rho_l = e_l^w \theta_l^w + e_l^m \theta_l^m; e_g \rho_g = e_g^w \theta_g^w + e_a^m \theta_g^m; e_h \rho_h = e_h^w \theta_h^w + e_h^m \theta_h^m,$$
(9)

where  $e_{\alpha}^{i}$  (J/g) represents the specific internal energy per unit mass of each species j in the phase  $\alpha$  and  $e_{\alpha}$  the specific internal energy per unit mass of each phase. These values are computed using the specific heat of the phases c (J/[g·K]) and the local temperature T relative to a reference temperature  $T_{o} = 273$  K (see Table 1). The selected reference temperature does not affect the calculation. The system is presumed to start at equilibrium, and the energy balance is tracked in terms of *energy changes* from the initial condition.

Energy consumption or liberation associated with hydrate formation/dissociation and ice formation/fusion are taken into consideration using the corresponding latent heats or changes in enthalpy *L* (J/g), as summarized in Table 1. Hence, the formulation inherently captures energy changes during endothermic or exothermic processes through specific internal energies and the corresponding changes in volume fractions  $S_{\ell}$ ,  $S_{g}$ ,  $S_{h}$ , and  $S_{i}$ .

The energy flux combines (1) conduction through the HBS  $i_c$  (W/m<sup>2</sup>), (2) transport by fluid mass relative to the mineral skeleton, and (3) transport by the motion of the whole sediment relative to the fixed reference system, as follows:

$$\begin{aligned} \mathbf{j}_{\text{EI}} &= \mathbf{j}''_{l} e_{l}^{w} + \mathbf{j}'_{l}^{m} e_{l}^{m} + e_{l} \rho_{l} S_{l} \boldsymbol{\varphi} \mathbf{v}, \\ \mathbf{j}_{\text{Eg}} &= \mathbf{j}'_{g}^{w} e_{g}^{w} + \mathbf{j}'_{g}^{m} e_{g}^{m} + e_{g} \rho_{g} S_{g} \boldsymbol{\varphi} \mathbf{v}, \\ \mathbf{j}_{\text{Eh}} &= e_{h} \rho_{h} S_{h} \boldsymbol{\varphi} \mathbf{v}, \\ \mathbf{j}_{\text{Ei}} &= e_{i} \rho_{i} S_{i} \boldsymbol{\varphi} \mathbf{v}, \\ \mathbf{j}_{\text{Fs}} &= e_{s} \rho_{s} (1 - \boldsymbol{\varphi}) \mathbf{v}. \end{aligned}$$
(10)

Then, the energy balance equation taking into consideration transport through the phases is

$$\frac{\partial}{\partial t} \Big\{ [\mathbf{e}_{s} \boldsymbol{\rho}_{s} (1 - \boldsymbol{\varphi})] + \Big( \mathbf{e}_{\ell} \boldsymbol{\rho}_{\ell} S_{\ell} + \mathbf{e}_{g} \boldsymbol{\rho}_{g} S_{g} + \mathbf{e}_{h} \boldsymbol{\rho}_{h} S_{h} + \mathbf{e}_{i} \boldsymbol{\rho}_{i} S_{i} \Big) \boldsymbol{\varphi} \Big\} + \nabla . \mathbf{i}_{c} + \nabla . \Big[ \mathbf{j}_{EI} + \mathbf{j}_{Eg} + \mathbf{j}_{Eh} + \mathbf{j}_{Ei} + \mathbf{j}_{Es} \Big] = \mathbf{f}^{E}. \quad (11)$$

The energy supply per unit volume of HBS  $f^{E}$  (W/m<sup>3</sup>) can be used to simulate thermal stimulation of the reservoir.

#### 2.2.5. Momentum Balance (Equilibrium)

In the absence of inertial forces (i.e., quasi-static problems) the sediment momentum balance reduces to the equilibrium equation:

$$\nabla . \boldsymbol{\sigma}_t + \boldsymbol{b} = \boldsymbol{0},\tag{12}$$

where  $\sigma_t$  (N/m<sup>2</sup>) is the total stress tensor and **b** (N/m<sup>3</sup>) the body forces vector. The constitutive equation for the HBS permits rewriting the equilibrium equation as a function of sediment velocity, temperature, gas, and liquid pressures.



#### 2.2.6. Constitutive Equations

The constitutive equations capture the coupling among the various phenomena considered in the formulation. Given the complexity of the problem, simple yet robust constitutive laws are selected for this framework.

*Conductive heat flow.* The Fourier's law governs the heat flow  $\mathbf{i}_{c}$  (W/m<sup>2</sup>), for three-dimensional flow conditions and isotropic thermal conductivity,

$$\mathbf{i}_{c} = -\lambda_{hbs} \nabla T,$$
 (13)

where  $\lambda_{hbs}$  (W/[m·K]) is the thermal conductivity of the HBS. A nonlinear volume average model is selected to track the evolution of  $\lambda_{hbs}$  during the simulation,

$$\lambda_{hbs} = \left[ (1 - \phi) \lambda_{s}^{\beta} + \phi \left( S_{h} \lambda_{h}^{\beta} + S_{i} \lambda_{i}^{\beta} + S_{g} \lambda_{g}^{\beta} + S_{\ell} \lambda_{\ell}^{\beta} \right) \right]^{\beta}.$$
(14)

This law reduces to the parallel and series models when  $\beta = 1$  and  $\beta = -1$ , respectively. Experimental data gathered for dry, water-saturated, and hydrate-filled kaolin and sand plot closer to the series model in all cases (Cortes et al., 2009; Yun et al., 2007). An adequate prediction for all values and conditions is obtained with  $\beta \approx -0.2$ . Table 1 lists the thermal conductivities for the different phases.

Advective Fluid Flow. The generalized Darcy's law governs the advective fluxes (m/s) in the liquid and the gas phases:

$$\mathbf{q}_{\alpha} = -\mathbf{K}_{\alpha} (\nabla \mathsf{P}_{\alpha} - \rho_{\alpha} \mathbf{g}); \qquad \alpha = \ell, \mathbf{g}, \tag{15}$$

where  $P_{\alpha}$  (N/m<sup>2</sup>) is the pressure of the phase and **g** is the gravity vector (i.e., the scalar  $g = 9.8 \text{ m/s}^2$  times the vector [0,0,1]<sup>T</sup>). The second term in parentheses captures the change in elevation in the vertical direction; the negative sign results from assuming that the vertical axis increases upward.

The tensor  $\mathbf{K}_{\alpha}$  (m<sup>4</sup>/[N·s]) captures the medium permeability for the  $\alpha$  phase in three-dimensional flow; if the medium is isotropic,  $\mathbf{K}_{\alpha}$  is the scalar permeability  $K_{\alpha}$  times the identity matrix. The permeability  $\mathbf{K}_{\alpha}$  depends on the sediment intrinsic permeability  $\mathbf{k}$  (m<sup>2</sup>),  $\alpha$ -phase  $\mu_{\alpha}$  dynamic viscosity (N·s/m<sup>2</sup>), and relative permeability  $\mathbf{k}_{\alpha}$  []:

$$\mathbf{K}_{\alpha} = \mathbf{k} \frac{\mathbf{k}_{\mathbf{r}\alpha}}{\mu_{\alpha}}; \qquad \qquad \alpha = \ell, \mathbf{g}. \tag{16}$$

The viscosity of the liquid  $\mu_{\ell}$  phase varies with temperature *T* (K):

$$\mu_{\ell}[\text{Pa.s}] = 2.1 \cdot 10^{-6} \exp\left(\frac{1808.5 \text{ K}}{\text{T}}\right). \tag{17}$$

While the viscosity of gases is often assumed independent of pressure, experimental data in a wide-range pressure of interest show a dependence. Published data in Younglove and Ely (1987) are fitted to develop a pressure and temperature dependent expression for the viscosity of methane gas (fitted range: 270 K < T < 290 K and 0.1 MPa <  $P_q$  < 40 MPa).

$$\mu_{g}[Pa.s] = 10.3 \cdot 10^{-6} \left[ 1 + 0.053 \frac{P_{g}}{MPa} \left( \frac{280 \, \text{K}}{\text{T}} \right)^{3} \right]. \tag{18}$$

The intrinsic permeability of the hydrate-bearing medium k with hydrate saturation  $S_h$  and porosity  $\phi$  is estimated from the intrinsic permeability in the medium without hydrates  $k_o$  determined at porosity  $\phi_o$  (Minagawa et al., 2008):

$$k = k_0 \frac{\Phi^3}{(1-\Phi)^2} \frac{(1-\Phi_0)^2}{\Phi_0^3} (1-S_h - S_i)^N.$$
(19)



where N is a parameter that accounts for the effect of hydrates and ice presence on the permeability law. The relative permeabilities for liquid  $k_{r\ell}$  and gas  $k_{rg}$  increase as the degree of saturation of each phase increases with respect to the mobile phase saturation  $S_{\ell} + S_{g}$ . A single parameter power function properly reproduces experimental data

$$k_{r\ell} = \left(\frac{S_\ell}{S_\ell + S_g}\right)^a = \left(S_\ell^*\right)^a, \tag{20}$$

$$k_{rg} = \left(1 - \frac{S_{\ell}}{S_{\ell} + S_g}\right)^b = \left(1 - S_{\ell}^*\right)^b, \tag{21}$$

where  $S_{\ell}^* = S_{\ell}/(S_{\ell} + S_g)$  is the effective liquid saturation in the HBS. Exponents a and b are typically 3–4 (see Gupta et al., 2006; Minagawa et al., 2008). The relative permeability of a phase vanishes when the phase stops percolating (in the absence of other coupling phenomena); percolation thresholds vary around  $S_g \sim 0.3$  and  $S_{\ell} \sim 0.3$  for gas and liquid flow. While the power function does not stop flow at percolation thresholds, relative permeabilities become very small and do not contribute to transport phenomena relevant to production processes. Alternative relative permeability functions have been proposed (Teymouri, 2018).

The interfacial tension between liquid and gas sustains the difference between the liquid and gas pressures  $P_{\ell}$  and  $P_{g}$ . Let us define the capillary pressure  $P_{c} = P_{g} - P_{\ell}$ . In a porous network, the capillary pressure and the effective liquid saturation  $S_{\ell}^{*}$  are related. Different models have been implemented in the code for the capillary pressure including equation (22), which is based on Van Genuchten (1978). The code is also capable to consider the effect of variation in porosity on the retention curve (Rodriguez et al., 2007).

$$S_{\ell}^{*} = \frac{S_{\ell}}{S_{\ell} + S_{g}} = \left[1 + \left(\frac{P_{c}}{P_{o}}\right)^{\frac{1}{1-m}}\right]^{-m}$$
(22)

The model parameters  $P_o$  (can be taken as the air entry value) and m (typically 0.05 < m < 0.4) relate to the porosity structure of the HBS: Finer grains and denser sediments imply higher  $P_o$  and lower m values. A modification of the Brooks and Corey (1964) water retention model incorporating scaling parameters (Civan, 2000; Clement et al., 1996; Rockhold et al., 2002) to account for the presence of hydrates in the pore space, as suggested by Gupta et al. (2015) is also available:

$$S_{\ell}^{*} = \frac{S_{\ell}}{S_{\ell} + S_{g}} = \left[\frac{P_{c}}{P_{0}f_{Sh}f_{\varphi}}\right]^{-m_{bc}}$$
(23)

in which  $P_c$  and  $P_0$  are the capillary pressure and air entry value, respectively;  $S_l^*$  represents the effective liquid saturation;  $m_{bc}$  is a sediment parameter;  $f_{Sh}$  and  $f_{\phi}$  are the scaling parameters depending on hydrate saturation (Clement et al., 1996; Rockhold et al., 2002) and porosity (Civan, 2000), respectively, as follows:

$$F_{Sh} = (1 - S_h)^{-\frac{C_1 m_{bc} - 1}{C_1 m_{bc}}},$$
 (24)

$$f_{\phi} = \frac{\phi_0}{\phi} \left(\frac{1-\phi}{1-\phi_0}\right)^{C_2},\tag{25}$$

where  $C_1$  and  $C_2$  are model parameters.

Nonadvective flux. The Fick's law governs the nonadvective flux of species in phases:

$$\mathbf{i}_{\alpha}^{j} = -\mathbf{D}_{\alpha}^{j} \nabla \theta_{\alpha}^{j},$$
 (26)

where  $\mathbf{D}_{\alpha}^{j}$  represent the dispersion tensor accounting for mechanical dispersion and molecular diffusion (Olivella et al., 1994, 1996),  $\alpha$  stands for the phases (l,g), and *j* for the species (m,w).



The mass of dissolved methane per unit volume of liquid phase  $\theta_l^m$  is evaluated by means of the Henry's law as follows:

$$\theta_l^m = \frac{P_m}{H_H} \frac{M_m}{M_{\dot{w}}} \rho_l \tag{27}$$

in which  $M_{\rm m}$  and  $M_{\rm w}$  are the molecular mass of methane and water, respectively;  $P_{\rm m}$  represents the partial pressure of methane; and H<sub>H</sub> stands for the Henry's constant.

The mass of vapor water per unit volume of gas  $\theta_q^w$  is calculated using the Psychometric law:

$$\theta_g^w = \left(\theta_g^w\right)^0 \exp\left(\frac{P_C M_w}{\mathsf{RT}[K]\rho_l}\right) \ , \ \left(\theta_g^w\right)^0 = \frac{M_w P_{v(T)}}{\mathsf{RT}[K]} \ , \ P_{v(T)} = 136075 \exp\left(\frac{-5239.7}{T[K]}\right), \tag{28}$$

where  $P_{v(T)}$  is the vapor pressure at the corresponding temperature T.

*Mechanical constitutive model.* Geomechanical behavior of HBS depends on stress level, hydrate saturation, load history, hydrate morphology, and sediment type. Experimental evidences indicate that hydrates impact on different aspects of sediment behavior: stiffness, peak stress, post-peak softening, and dilation during shearing (Dai et al., 2011; Ghiassian & Grozic, 2013; Grozic & Ghiassian, 2010; Hyodo et al., 2014; Masui et al., 2005; Miyazaki et al., 2011; Yoneda et al., 2015). Several models have been proposed to describe the mechanical behavior of HBS (e.g., Gai & Sánchez, 2017; Kimoto et al., 2007, 2010; Klar et al., 2010; Lin et al., 2015, 2017; Pinkert & Grozic, 2014; Shen et al., 2016; Sultan & Garziglia, 2011; Sun et al., 2015; Uchida et al., 2012; Zhang et al., 2018).

An elastic model that includes the dependence of Young's modulus on  $S_h$ , as suggested by Santamarina and Ruppel (2010), is available in the proposed framework:

$$E_{\rm Sh} = [E_{\rm Sed} + dE_{\rm Sed}(\phi_0 - \phi)] \left( {}^{\sigma_{\zeta}}\!\!\!\!/_{\sigma_{C0}} \right)^{b_E} + c_E E_{\rm Hyd}(S_{\rm h})^{d_E}$$
(29)

in which  $E_{Sh}$ ,  $E_{Sed}$ , and  $E_{Hyd}$  are the Young's modulus of HBS, hydrate-free sediments (at the reference porosity  $\phi_0$  and confining stress of  $\sigma_{C0} = 1$  KPa), and pure hydrate, respectively;  $dE_{Sed}$  accounts for the dependence of  $E_{Sed}$  on  $\phi_0$ ;  $b_E$ ,  $c_E$ , and  $d_E$  control the sensitivity of  $E_{Sed}$  on the confining stress  $\sigma_C$ .

A more advanced elastoplastic model for HBS based on the strain-partition method (Pinyol et al., 2007) was proposed by Sánchez et al. (2017). This model explicitly contemplates the two basic HBS constituents: the sediment skeleton and hydrates. This approach allows distinguishing between the mechanical contributions of the different solid phases present in the sediment. A strain-partition variable that evolves during loading link hydrates and soil skeleton strains. An isotropic scalar damage model describes the mechanical response of the hydrate, and a critical state soil mechanics model represents the sediment skeleton behavior. The principle of virtual work is advocated to obtain the expressions relating the external effective stress with the two stress components. Sánchez et al. (2017) presents the mathematical formulation alongside a thorough assessment of the model, including not only tests at constant  $S_h$  (as it was done in most of the previous studies) but also experiments involving hydrate dissociation. Table 2 lists the main model components together with the parameters adopted in section 3.1.

#### 2.2.7. Phase Boundaries—Reaction Kinetics

The phase boundaries for methane hydrate and ice are expressed in terms of pressure and temperature. We adopted a methane-hydrate phase boundary expression that follows the format in Sloan and Koh (2008), but it is adjusted to satisfy values computed using the HWHYD software (2001):

$$P_{eq-mh}[kPa] = e^{\left(\frac{40.234 - \frac{8860}{t_{eq}[k]}}{t_{eq}[k]}\right)} \qquad \text{methane hydrate.} \tag{30}$$

Water salinity also affects the phase boundary of the gas hydrate mixture. Based on Kamath and Godbole (1987) studies, we assumed a linear relationship between the temperature of disassociation and the salinity weight concentration for a given pressure. We account for the effect of salinity on the hydrate phase boundary correcting (30) as follows:

$$\mathsf{P}_{\mathsf{eq}-\mathsf{mh}}[\mathsf{kPa}] = \mathsf{e}^{\left(40.234 - \frac{880}{\mathsf{f}_{\mathsf{eq}} - \mathfrak{a}_{\mathsf{S}}\mathsf{I}_{\mathsf{S}}}\right)}, \tag{31}$$

where  $\alpha_s$  is the slope of the temperature-salinity curve (assumed as 0.55) and  $I_s$  is the salinity weight concentration.



<b>Table 2</b> Geomechanical Model <sup>a</sup>					
Sediment skeleton (ss)Critical state soil mechanics model					
Elastic	$K_{ss}^{'}=\frac{v}{\kappa}p_{ss}^{'};\qquad\qquad \epsilon_{ss}^{q}=\frac{q_{ss}}{G_{ss}}$	p <sub>ss</sub> ': mean effective stresses K <sub>ss</sub> : elastic bulk modulus G <sub>ss</sub> : shear modulus v: specific volume			
Hardening	$\label{eq:pc} \frac{dp_c}{p_c} = \frac{v}{\lambda - \kappa} d\epsilon^{vp} \qquad p_d = c \mu C_h$	κ: elastic vol. parameter = 0.002 $p_c$ : apparent preconsolidation pressure $p_c = 11.5$ (MPa) $ε^{VP}$ : plastic vol. strain λ: plastic vol. parameter = 0.12 $p_d$ : hardening variable (hydrate)			
Subloading	$dR = -\eta \ln R  d\varepsilon^{P} $	c: parameter accounting $S_h$ effect; $c = 16$ $ de^{P} $ : plastic strain vector norm <i>R</i> : subloading ratio			
Yield surface	$F_{s} = \frac{q_{ss}^{2}}{M^{2}} + p_{ss}^{'}2 - Rp_{ss}^{'}(p_{c} + p_{d})$	<i>M</i> : critical line slope = 1.17 $q_{ss}$ : deviatoric stresses $\gamma_F$ : yield surface constant			
Hydrate (h)Damage Mo Elastic	del $\epsilon_h^v = \tfrac{p_h}{K_h}; \ \tfrac{q_h}{G_{hs}}$	K <sub>h</sub> hydrate bulk modulus: 9,600 (MPa) G <sub>h</sub> : hydrate shear modulus: 4,300 (MPa)			
Stress-strain	$\boldsymbol{\sigma}_{h} = e^{-L} \boldsymbol{D}_{h0} \boldsymbol{\varepsilon}_{h} = \boldsymbol{D}_{h} \boldsymbol{\varepsilon}_{h}$	<ul> <li>v, q, and h stand for volumetric, deviatoric and hydrate</li> <li>σ: stress; ε: strain</li> <li>D<sub>h0</sub>: elastic hydrate stiffness matrix</li> <li>D<sub>k</sub>: hydrate stiffness matrix</li> </ul>			
Damage evolution	$r_{(L)}=r_0e^{r_1L}$	$r_{0:}$ threshold damage variable = 1e-6 $r_1$ damage rate constant = 2.9			
Partition variable	$\mu=\mu_0e^{-\frac{L}{2}}$	$\mu$ : partition variable; $\mu_0$ : initial $\mu$ ; $\mu_0 = 1$ <i>L</i> : isotropic damage variable			
Coupling Sediment Ske Coupling equations	eleton $\leftrightarrow$ HydrateStrain Partition Conce $\epsilon_{h}^{v} = \frac{\mu}{1+C_{h}\mu} \epsilon^{v} \epsilon_{h}^{q} = \frac{\mu}{1+C_{h}\mu} \epsilon^{q}$	ept $C_h$ : hydrate vol. concentration = 0.195 $\varepsilon$ indicates strain			

<sup>a</sup>Model described in detail in Sánchez et al. (2017).

The phase boundary for the ice-water transition exhibits low sensitivity to pressure. For the most common  $l_h$  ice phase, the linear fit for the pressure range between 0 and 20 MPa is (based on Wagner & Kretzschmar, 2008):



**Figure 2.** Phase boundaries for water-gas mixtures in the pressure-temperature space. The phases in each quadrant depend on the availability of water and gas and the *PT* trajectory.

$$P_{eq-ice}[MPa] = 13.0(273.16 - T[K]) \qquad Ice (0 \le P \le 20 \text{ MPa}).$$
(32)

Figure 2 presents the four zones associated with the methane-water system resulting from superimposing the hydrate and ice phase boundaries on the pressure-temperature domain. Note that the ice + gas condition I + G in the *c* quadrant is assumed to remain I + G upon pressurization into the *d* quadrant because of limited solid-gas interaction in the absence of beneficial energy conditions: The enthalpy for ice-to-hydrate transformation is H = -48.49 kJ/mol (i.e., an endothermic process).

At any given location, the hydrates could be in contact with either water or free gas. Therefore, the model compares the equilibrium pressure  $P_{eq-mh}$  or  $P_{eq-1}$  against a volume average pressure  $P^*$ 

$$P^{*} = \frac{S_{g}}{S_{g} + S_{w}}P_{g} + \frac{S_{\ell}}{S_{g} + S_{\ell}}P_{\ell} = \left(1 - S_{\ell}^{*}\right)P_{g} + S_{\ell}^{*}P_{\ell}. \tag{33}$$



At any given location, the hydrate or ice mass could be in contact with either water or free gas. While stability will depend on gas fugacity (hydrate) and water activity (ice), we adopt a formulation based on pressure. Therefore, the model compares the equilibrium pressure  $P_{eq-mh}$  or  $P_{eq-ice}$  against a volume average pressure  $P^*$ . Gas hydrate dissociation/formation is generally modeled including specific surface, as in models based on results by Kim et al. (1987). We propose a totally different approach, inspired by saturation index based models to simulate precipitation/dissolution phenomena in porous media (e.g., Lasaga, 1998). It is assumed that the rate of formation or dissociation is driven by the distance  $\delta$  to the corresponding equilibrium phase boundary:

$$\delta = \sqrt{\left[\delta_{T}(T - T_{eq})\right]^{2} + \left[\delta_{P}(P_{fI} - P_{eq})\right]^{2}}$$
(34)

where  $\delta_T$  (K<sup>-1</sup>) and  $\delta_P$  (MPa<sup>-1</sup>) are scaling parameters; default values are  $\delta_T = 1/K$  and  $\delta_P = 0.1/MPa$ . Hydrate formation/dissociation (or ice formation/thawing) processes induce changes in the phase saturations (i.e.,  $S_{ji}$ , j = l, g, h, i). Any phase that is not stable for the current *P*-*T* conditions (i.e., according to the phase boundaries, Figure 2) will transit to the pertinent stable phase. We assume that rate of change for a given time step is a fraction  $\zeta$  of the potential change (i.e., the unstable phase). The factor  $\zeta$  is a function of the distance to the corresponding phase boundary:

$$\xi = 1 - \Psi^{\delta}. \tag{35}$$

The preselected parameter  $\psi$  establishes the rate of change of the unstable phase, which can be calibrated from experimental results. For example, the updated hydrate (or ice) volume fraction at time interval k + 1 outside the stability zone is

$$S^{k+1} = S^k \left( 1 - \frac{\xi}{S^k} \varDelta t \right) = S^k \left( 1 - \xi' \right)$$
 for either ice melting or hydrate dissociation, (36)

where  $0 \le \xi' \le 1.0$ . This equation approximates the hydrate/ice phase mass balance equation.

The equations below compute the increment in hydrate saturation ( $\Delta S_h$ ) related to the hydrate formation (from free gas) for the two possible cases shown in Figure 2 (Zone *b*):

gas limited(excess water)
$$\frac{\rho_{\ell} S_{\ell}}{\rho_{g} S_{g}} \ge \frac{\alpha}{1-\alpha} \rightarrow \Delta S_{h} = \frac{1}{1-\alpha} \frac{\rho_{g}}{\rho_{h}} \Delta S_{g},$$
 (37)

water limited(excess gas) 
$$\frac{\rho_{\ell} S_{\ell}}{\rho_{g} S_{g}} \le \frac{\alpha}{1-\alpha} \rightarrow \Delta S_{h} = \frac{1}{\alpha} \frac{\rho_{\ell}}{\rho_{h}} \Delta S_{\ell},$$
 (38)

where the changes in saturations are obtained from the kinetics outlined in equations (35) and (36). Other phase transformations are similarly approached (Teymouri, 2018). This flexible formulation allows us to capture different rates of reaction, relative to mass flux and drainage conditions.

## 3. Numerical Analysis

We have implemented the numerical framework for HBS discussed in the previous sections in the fully THM coupled FE software CODE\_BRIGHT (Olivella et al., 1996). We have adapted and expanded this program to represent all species and phases encountered in HBS. One main unknown (state variable) is related to each balance equation (e.g.,  $\mathbf{u}$ , T,  $P_{h}$ ,  $P_{g}$ , and  $\phi$  are associated with the momentum, energy, water mass, methane mass, and mineral balance equations). Constitutive equations relate the main unknowns to the dependent variables (e.g., gas and liquid fluxes depend on phase pressure; partial saturations on capillary pressure; and stresses on strains). A mass conservative approach has been adopted by discretizing directly the accumulation terms, as proposed by Celia et al. (1990). All the governing equations are solved simultaneously (in a monolithic manner) and the Newton-Raphson method is adopted to tackle the nonlinearities of the problem. In the following sections we applied the proposed approach to analyze three application cases.



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Figure 3. Effect of confinement on shear behavior and hydrate dilatancy. Reservoirs at (a) ~50 m, (b) ~100 m, and (c) ~300 m deep.

### 3.1. Effect of Dilation and Confinement on HBS Behavior

The dilatant behavior of sediments upon shearing strongly depends on hydrate saturation and confinement. Sediment stiffness peak strength, post-peak softening, and dilation tend to increase with hydrate saturation (Yoneda et al., 2015). Strength in soils increases with confinement, while post-peak softening and dilation generally decrease. It has been argued that the large dilations upon shearing typically exhibited in HBS may induce a tensile failure in the hydrate (Jung & Santamarina, 2011), which could also impact on sediment global strength (Pinkert & Grozic, 2014).

We have adopted Sánchez et al. (2017) geomechanical model to investigate this feature of soil behavior considering three potential hydrate reservoirs located at different depths to study the impact of confinement on sediment dilation. We have selected typical model parameters (Table 2) from the comprehensive study conducted in Sánchez et al. (2017). The selected geomechanical model tracks the stress changes in both constituents (i.e., hydrates and pure sediment) during shearing, enabling analyzing the development of possible tensile stresses in the hydrates. Figure 3 presents the mechanical response the three possible reservoirs at depths: 50 m (Figure 3a), 100 m (Figure 3b), and 300 m (Figure 3c). As expected, sediment strength increases with confinement, while dilation decreases. The plots show the evolution of the global stresses together with the contributions of the soil skeleton and hydrate to the mechanical response of the HBS. The stress paths in the p-q plane are also presented. At the beginning of shearing, the mean stress in the hydrate (p<sub>h</sub>) increases in the three tests but then decreases, as the sediment starts to dilate. The shallower reservoir develops the largest tensile stresses (around -150 kPa), while the deeper one is always under compression.



**Figure 4.** (a) Schematic view of a hydrate-bearing sediment subsample specimen (21C to 02E), indicating the position of the ball valve and thermocouple (after Yun et al., 2010). (b) Image selected for developing the 3-D heterogeneous model. (c) S<sub>h</sub> distribution heterogeneous model. (d) Schematic view of the adopted boundary conditions.

These results suggest that hydrates in sediments subjected to large volumetric expansions may develop tensile stress during shearing, as hypothesized in Jung and Santamarina (2011). The proposed model allows coupling this feature of HBS mechanical behavior with the sediment thermo-hydro-chemical conditions, allowing a comprehensive evaluation of the hydrate stability. This aspect can be relevant in analysis involving significant sediment shearing at low confinement, as when drilling through shallow hydrate reservoirs or producing methane from them.

### 3.2. Modeling a Gas Production Laboratory Test

Yun et al. (2010) characterized a natural HBS recovered from the Krishna-Godavari Basin in offshore India during the first Indian National Gas Hydrate Program expedition in 2006. The instrumented pressure testing chamber was used to gather good quality specimens and maintain them at 4 °C and 13 MPa. A core 380 mm long and 50 mm in diameter was subsampled under pressure to simulate depressurization induced gas production. Figure 4a presents the X-ray image of the sample prior to testing. The controlled depressurization of the pressure core began with a slow pressure decrease (i.e., an average rate of 0.18 MPa/min), down until reaching the hydrate stability phase boundary. The depressurization rate was reduced afterward, to about 0.025 MPa/min, until achieving the atmospheric pressure. The temperature was continuously monitored during the controlled depressurization with a thermocouple located 54 mm away from the valve (Figure 4a).

To represent the cylindrical sample we adopted a 2-D axisymmetric model with a uniform mesh discretization consisting of 750 elements. In a first analysis we assumed a homogeneous hydrate distribution  $S_h = 0.298$  (Yun et al., 2010). The initial conditions correspond to the experimental ones: P = 13 MPa,





**Figure 5.** Experimental results versus numerical analysis based on homogeneous hydrate distribution. (a) *PT* paths and phase boundaries. (b) Time evolution of pressure. (c) Gas produced in terms of pressure evolution. (d) Temperature evolution during the experiment.

T = 4 °C, and  $\phi_0 = 0.61$ . Figure 4d presents a schematic representation of the adopted boundary conditions. We assumed an impermeable flow boundary around the shell, but at the ball-valve position where we imposed the depressurization rates discussed above. We considered a heat radiation condition around the shell for the thermal problem to maintain the temperature at the boundary at 4 °C. We adopted equation (14) for the thermal conductivity with  $\beta = -0.2$ ; equation (19) for the intrinsic (isotropic) permeability with  $k_{\text{HBS}} = 5.2 \times 10^{-13} \text{ m}^2$  (at  $\phi_0$ ). We also assumed a = b = 3 in equations (20) and (21), respectively. We adopted  $\psi = 0.99$ . We assumed the hydrate phase boundary described by equation (31) for a salt concentration of around 4% and the ice-liquid water phase boundary as in equation (32).

For the capillary pressure curve, equation (23) is adopted with parameters:  $P_0 = 0.1$  MPa,  $m_{bc} = 1.2$ ,  $C_1 = 3$  and  $C_2 = 2$ .

An elastic behavior of the sediment is assumed. We consider that the effect of hydrate saturation on the Poisson ratio v is negligible (v = 0.3). The model parameters in equation (29) are assigned according to previous studies (Gupta et al., 2015):  $E_{Hyd} = 1.35$ GPa,  $b_E = 0$ ,  $c_E = 1$ , and  $d_E = 1$ . The formation consisted of fine-grained clayey sediments of high specific surface and high plasticity (Yun et al., 2010); Based on Waite et al. (2009) a Young's modulus of the hydrate-free sediment  $E_{Sed} = 0.03$  GPa was adopted.

Figure 5a shows the evolution of the experimental and modeled *PT* trajectories. The endothermic character of the hydrate dissociation is well captured by the model, predicting a sharp change of the *PT*-path



**Figure 6.** (a) Schematic view of a hydrate-bearing sediment subsample specimen (21C to 02E) after depressurization, indicating the heterogeneity in the porosity field (after Yun et al., 2010). (b) Image selected for developing the 3-D heterogeneous model. (c) Distribution of porosity in the heterogeneous model at the end of the simulation.

direction (i.e., toward the left, in the *PT* plane), once the hydrate phase boundary is touched. The heat consumed during hydrate dissociation induced a significant cooling of the sample, reaching subzero temperatures. Once the hydrate dissociation was completed, the *PT* path left the phase boundary and the temperature increased because of the ambient heat. The simulated *PT* trajectory satisfactorily reassembles the experimental one. Figure 5b shows the experimental and simulated pressure evolutions versus time, where the two depressurization rates discussed above are clearly observed. Figure 5c presents the comparison between experimental and simulated gas productions. The model well predicts the maximum amount of produced gas but at a faster rate (particularly at advanced stages of the experiment). The main trends in terms of temperature evolution are qualitatively well simulated (Figure 5d), but the minimum temperature is underpredicted by the model (i.e., model ~-5 °C, test ~-2.5 °C). The thermocouple was located (Figure 5a) in a zone with hydrate saturation lower than the average, it is then possible that the local temperature at that position may be higher than the ones developed in other sections, where the cooling induced by the hydrate dissociation was more intense because of the higher *S*<sub>h</sub>. A simulation based on a homogenous *S*<sub>h</sub> distribution cannot capture this type of trend. We developed a model considering a heterogeneous hydrate distribution to achieve a better description of the test conditions.

We adopted one of the core X-ray images (Figure 4b) to develop a 3-D model considering a 2-D axisymmetric geometry (Figure 4c). We use MATLAB to generate a nonuniform  $S_h$  distribution based on the specimenimage grayscale color. This model perhaps does not capture the full complexity of the natural specimen with the actual  $S_h$  variability but does represent an improvement respect to the initial homogenous model. We conducted the new simulation considering the same boundary conditions adopted in the homogeneous model. Figure 6a presents the X-ray image at the end of depressurization, together with Figure 6b that shows the section adopted for developing the nonhomogenous porosity distribution field (obtained following a similar approach to the one explained for  $S_h$ ) and also the computed porosity field at the end of the test (Figure 6c). Figure 7 presents the main results associated with this modeling. The main difference with respect to the previous analysis is that now the minimum temperature recorded during the test is



**Figure 7.** Experimental results versus numerical analysis based on the heterogonous hydrate distribution. (a) *PT* paths and phase boundaries. (b) Time evolution of pressure. (c) Gas produced in terms of pressure evolution. (d) Temperature evolution during the experiment.

perfectly captured by the heterogonous model. We have also included in the *PT* plane the changes in  $S_h$  and  $S_i$  during the experiment (Figure 7a). Hydrate saturation starts to decrease when the hydrate boundary is reached by the *PT* path (point 1) and continues reducing until point 3, when all the hydrates dissociate. Ice starts to form when the *PT* trajectory reaches the ice-liquid water transition (point 2) and continues forming until the phase transition is reached again (point 4). The ambient heat and the exothermic character of the ice formation reaction trigger the temperature increases between points 3 and 4.  $S_i$  starts to decrease beyond this point because of thawing.

Figure 8 presents the contours of  $S_h$  distribution during depressurization at different times for both samples, homogenous (left images) and nonuniform (right images). The homogenous modeling shows that the dissociation front initially propagates from the bottom of the sample (where the depressurization is induced) and stabilizes at a distance of around 6.5 cm from the bottom. After 110' (approximately) a radial front also develops, which progresses toward the center of the sample until the end of the experiment. These two clear dissociation fronts observed in the homogenous analysis are also apparent in the heterogeneous modeling, but they are much less marked in this case, because the local changes in temperature (and the corresponding temperature recuperation times) are not uniform in the dissociation front (i.e., because of the nonuniform  $S_h$  distribution) leading to a diffuse and nonuniform progression of the dissociation front.

The model has contributed to a comprehensive analysis of the different physics involved in this experiment. The underprediction of the minimum temperature obtained in the initial analysis was not related to a possible deficiency of the proposed formulation to properly capture the cooling during the endothermic hydrate dissociation, but it was associated with the no-uniform  $S_h$  distribution observed in this specimen.



**Figure 8.** Evolution of  $S_h$  contours at different times for analyses assuming uniform (left) and heterogeneous (right)  $S_h$  distributions.

#### 3.3. Axisymmetric Cylindrical Flow in a Confined Reservoir

A cylindrical reservoir confined between two impermeable layers with radial flow toward a vertical production well is a geometry typically adopted to model gas production from HBS. In this section we explore the response of such a reservoir at steady state conditions when two permeability regions exist (i.e., dissociated sediment and intact HBS reservoir). The limitations of this type analysis is discussed, together with the influence of the main properties and variables of this problem (e.g., sediment permeability, pressure, and temperature) on the extent of the dissociated area based on possible initial and boundary conditions. An analytical solution involving two permeability fields was proposed by Terzariol et al. (2017) for a spherical geometry. We propose here a simple equation based on a cylindrical domain (which is more representative of the reservoir conditions) to study limits for gas production from HBS via depressurization for given boundary conditions. We then use the analytical solution to study some typical reservoir conditions, and we apply these results to verify our FE program for the particular conditions of this problem.

### 3.3.1. Analytical Solution

At steady state, the pressure distribution in a radial flow through a reservoir confined by impermeable overburden and underburden layers is inversely proportional to the logarithm of the radial distance to the vertical wellbore. Considering radial flow conditions governed by Darcy's law in a thin and confined reservoir with impermeable layers (Figure 9):

$$v = k \frac{dh}{dr},$$
 (39)

$$r = \frac{q_{\rm l}}{2\pi r \rm H},$$
(40)

where v is the flow velocity, k is the coefficient of permeability of the medium, h is the pressure head (in a thin reservoir, the variation of pressure head with elevation is negligible), r is the radius (from the wellbore center),  $q_l$  is the flow rate, and H is the sediment thickness. By combining these two equations and solving them in cylindrical coordinates, the flow equation is obtained:

ν

$$\int_{r_1}^{r_2} \frac{q_1 dr}{r} = -\int_{h_1}^{h_2} (2\pi H k) dh$$
(41)

being the flow between two given points:

$$q_{I} = -\frac{2\pi H k(h_{2} - h_{1})}{ln \left(\frac{r_{2}}{r_{1}}\right)}. \tag{42}$$





**Figure 9.** Two zones can be identified under the steady state condition when the pressure drop is kept constant and hydrate stops dissociating: an inner zone where hydrate has been depleted and an outer zone where hydrate remains stable.

Two zones can be identified under steady state conditions (when well and far pressures are kept constant and hydrates stop dissociating): the inner zone, where hydrates were depleted, and the outer zone, where hydrates remains stable (Figure 9). Let us define the size of the produced zone as  $r^*$  and the head pressure at a distant boundary as  $h_{\text{far}}$ . The inner zone is characterized by the permeability of the free hydrate soil  $k_{\text{Sed}}$  and the outer zone by the HBS permeability  $k_{\text{HBS}}$ . Gas is released from the inner zone  $r \leq r^*$ . Therefore, at steady state conditions:

$$\frac{2\pi H k_{\text{Sed}}(h^* - h_w)}{\ln\left(\frac{r^*}{r_w}\right)} = \frac{2\pi H k_{\text{HBS}}(h_{\text{far}} - h^*)}{\ln\left(\frac{r_{\text{far}}}{r^*}\right)},$$
(43)

where  $h^*$  and  $h_w$  are the pressure heads at the dissociation front and at the wellbore area, respectively, and  $r_w$  is the well radius. Therefore, the ultimate radius  $r^*$  can be obtained from:

$$\mathbf{r}^{*} = \left( \mathbf{r}_{w} \mathbf{r}_{far}^{\left(\frac{k_{sad}}{k_{HBS}}\right) \left(\frac{h^{*} - h_{w}}{h_{far} - h^{*}}\right)} \right)^{\left(1 + \left(\frac{k_{sed}}{k_{HBS}}\right) \left(\frac{h^{*} - h_{w}}{h_{far} - h^{*}}\right)\right)^{-1}}.$$
(44)

The length of the reservoir  $r_{far}$  is such that (under steady state conditions) the incoming flow into the reservoir keeps the pressure head equal to its initial value. The ultimate dissociation front radius in a thin and confined hydrate deposit is a function of: (1) the radius of the wellbore area and the imposed pressure head at this radius; (2) the pressure head at the dissociation front (which in turn depends on the reservoir temperature through the methane hydrate phase boundary); (3) the pressure head at a distant boundary (equal to the reservoir initial pressure); and (4) the ratio between the hydraulic conductivity of the already dissociated hydrate sediments and that of the HBS (Figure 9).

This equation shows that the extent of the dissociated area at steady state condition for this particular problem (i.e., radial flow in a confined reservoir) depends on the selected  $r_{far}$ , so it is not unique. Therefore, the results obtained with models based on this geometry will depend on the length of the domain, where the (fix) pressure at the far boundary (generally equal to the initial reservoir pressure) is imposed. The proposed equation is in any case very useful to explore the influence of different factors and conditions that will impact on the amount of gas produced for a given initial and boundary conditions. It is also an excellent tool to verify numerical tools.





**Figure 10.** Analytical solution and numerical model results related to the HBS reservoir with impermeable confining layers for the different cases.

Transient changes in temperature that can take place during gas production (e.g., heat associated with hydrate dissociation) can affect the rate of gas production but do not impact on the position of the final dissociation front, because the steady state condition does not dependent on this type of transient effect. Therefore, isothermal analyses are valid when studying HBS reservoirs at steady state conditions.

#### 3.3.2. Cases Involving Cylindrical Flow

Several cases were prepared based on various initial and boundary conditions, and different production strategies, by imposing a variety of pressures at the wellbore. The same  $k_{\text{HBS}} = 1 \times 10^{-12} \text{ m}^2$ , initial  $S_h = 0.5$ ,  $r_w = 0.1 \text{ m}$ , and reservoir length (1,200 m) were adopted in all the analyses. The different ratios between  $k_{\text{Sed}}$  and  $k_{\text{HBS}}$  were obtained by selecting different values of the coefficient *N* (equation (19)). The relative pressure dissociation  $h_{rp}$  is defined as  $(h^* - h_w)/(h_{\text{far}} - h^*)$ . The cases analyzed are:

•	Case A h <sub>far</sub> (m) : 1020	h <sub>w</sub> (m) : 306	T ( <sup>°</sup> C) : 12	h <sub>rp</sub> : 7.14,
•	Case B h <sub>far</sub> (m) : 1224	h <sub>w</sub> (m) : 306	T ( <sup>°</sup> C) : 12	h <sub>rp</sub> : 2.14,
•	Case C h <sub>far</sub> (m) : 1224	h <sub>w</sub> (m) : 510	T ( <sup>°</sup> C) : 12	h <sub>rp</sub> : 1.44,
•	Case D h <sub>far</sub> (m) : 1224	h <sub>w</sub> (m) : 306	T ( <sup>°</sup> C) : 10	h <sub>rp</sub> : 0.91,
•	Case E h <sub>far</sub> (m) : 1224	h <sub>w</sub> (m) : 306	T ( <sup>°</sup> C) : 8	h <sub>rp</sub> : 0.47.

Figure 10 presents the results from the analytical solution (lines), showing the interplay between the relative sediment permeability  $k_{Sed}/k_{HBS}$  and the relative pressure dissociation. For example, when the permeability contrast between already dissociated and hydrate sediments is the highest, the dissociation front is the farthest. This implies that the permeability enhancement during dissociation plays an essential role in the depressurization propagation in hydrate reservoirs. For a fixed  $k_{Sed}/k_{HBS}$ , Cases B, D, and E assist to study the effect of the reservoir initial temperature (i.e., all the other factors are identical), showing that warmer reservoirs release larger amounts of gas. Cases A and C have the same hydraulic gradient, and the same initial temperature, but different initial pressures. Under these conditions, the lower the initial reservoir pressure, the larger the amount of gas produced. Similar meaningful discussions can be conducted involving other variables and factors, showing the usefulness of this type of solution.

We developed a 2-D axisymmetric model including a single vertical producing well that replicates the analytical solution geometry and allows us verifying our code under these particular conditions. We adopted a thin and long (L = 1,200 m) reservoir confined by impermeable layers. The final discretization consists of 2,503 elements. We conducted a mesh sensitivity analysis to confirm that the adopted domain discretization was appropriate. We selected equation (22) for the capillary pressure model with  $P_o = 100$  kPa and m = 0.5. We also assumed a = b = 3 in equations (20) and (21), respectively.

Each FE steady state simulation corresponds to one point in Figure 10, we conducted 30 analyses in total (indicated by symbols). To reach the steady state condition we considered long-term depressurization in the simulations. Therefore, the cases ran until practically no changes in the variables were observed. A very satisfactory agreement between numerical and analytical results was obtained, indicating that the suggested solution is capable of capturing the most relevant features of HBS behavior associated with these particular flow conditions and could then be extended to other scenarios.

# 4. Conclusions

We have analyzed a variety of problems associated with HBS (from laboratory tests to field scale simulations) involving hydrate dissociation and ice formation/thawing. We have combined numerical simulations together with analytical solutions and constitutive modeling with the goal of gaining a better understanding on HBS behavior. The main component of this research is a coupled THM formulation for HBS that allows integrating in a unique and consistent framework all the physics and interactions that control the behavior of this type of soil. It is a truly coupled mathematical framework that solves all the governing equations simultaneously in a monolithic manner. We have implemented this formulation in CODE\_BRIGHT, an existing and validated computer program to tackle multiphysics problems in geological media.



We have shown that the typical dilatant behavior upon shearing observed in HBS, particularly at low confinements and high *S*<sub>h</sub>, may induce tensile stresses in hydrates. We investigated this feature of soil behavior by using an advanced geomechanical model capable of distinguishing between the mechanical contributions of the soil skeleton and hydrates. Furthermore, previous studies have suggested that this type of phenomenon can move the hydrates outside the stability zone (Jung & Santamarina, 2011). Shallow HBS reservoirs subjected to shearing are more susceptible to this type of behavior.

We have also analyzed a laboratory scale gas production test conducted on a natural highly heterogeneous HBS sample in the lab under controlled conditions. The main tendencies observed in the experiment, in terms of pressure evolution, gas produced, and temperature, were qualitatively well reproduced by the model. The simulations also assisted to understand the propagation of the dissociation fronts inside the sample and the patterns of ice formation/thawing during the experiment.

To verify further the proposed formulation, we developed an analytical solution for predicting the maximum amount of gas that can be produced via depressurization from HBS from a cylindrical reservoir (of a given length) confined by two layers after achieving steady state conditions. This solution is useful because it allows investigating the effect of key reservoir properties on its response. The comparisons between the numerical model and analytical solution confirmed that the proposed numerical code is well suited to estimate the limits of gas production from HBS reservoirs.

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