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Multiscale Modeling of Coupled Thermo-Hydro-Mechanical-Chemical Behavior in Hydrate-Bearing Sediment

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Abstract

This study presents a hybrid continuum-discrete multiscale computational framework that integrates the material point method (MPM) and the discrete element method (DEM) to model fully coupled thermo-hydro-mechanical-chemical (THMC) behavior of hydrate-bearing sediments (HBS). Key innovation of the framework lies in its direct use of DEM to model microscale mechanisms, such as hydrate bond degradation, particle rearrangement, and pore evolution, thereby bypassing the need for conventional elastoplastic constitutive models to define effective stress. We show that a simple hydrate saturation-dependent contact model within the DEM can effectively reproduce characteristic shear and volumetric responses of HBS under various hydrate saturation and confining stresses. By embedding a DEM-based representative volume element (RVE) at each material point in the MPM grid, microscale mechanical behaviors are seamlessly homogenized to inform large-deformation macroscale multiphysics processes. Numerical simulations of biaxial compression and indenter penetration demonstrate the framework's capability to capture critical phenomena, including shear band formation, shear-induced dilation, and the generation of negative excess pore pressure that drives localized hydrate dissociation. The results further reveal that while higher hydrate saturation enhances shear strength, it also promotes brittle failure and intensified dissociation. Conversely, increased confining stress suppresses volumetric dilation and stabilizes the sediment by mitigating the development of negative pore pressure. This multiscale approach provides a powerful new tool for elucidating complex THMC interactions in HBS, with important implications for assessing hydrate-related geohazards and optimizing gas extraction strategies.

Keywords: Hydrate-bearing sediment, Multiscale modeling, Discrete element method, Material point method, THMC coupling, Large deformation

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1. Introduction

Gas hydrate, an ice-like crystalline compound, is found in extreme environments with high pressure and low temperature, such as oceanic sediments at water depths exceeding 300 meters, where the bottom water temperature is approximately 2°C (Reagan and Moridis, 2007; Ruppel and Kessler, 2017). Changes in pressure and temperature conditions, driven by either natural processes (*e.g.*, sea level fluctuations, sedimentation, and subsurface geothermal flow) or human interventions (*e.g.*, depressurization and thermal stimulation during gas production), can trigger hydrate dissociation (Gatter et al., 2021; Jyothsna and Satyavani, 2024). Hydrates typically function as cementing agents that bind sediment grains and strengthen the soil matrix. Consequently, their dissociation can lead to significant mechanical weakening of the bearing sediments, potentially resulting in geological and geotechnical hazards such as seafloor collapse, submarine landslides, and wellbore instability (Boswell and S. Collett, 2011; Chong et al., 2016; Yin and Linga, 2019). A comprehensive understanding of the mechanical behavior of hydrate-bearing sediments (HBS) is essential for mitigating geohazards and advancing gas hydrate exploitation. However, the complex interactions among coupled heat transfer, multiphase flow, hydrate dissociation kinetics, and geomechanics within the porous HBS system present significant challenges to accurate prediction and analysis.

The mechanical behavior of HBS has been studied through experimental and theoretical investigations for several decades. For cementing-type HBS, it is well-established that its stiffness, peak strength, and dilation angle increase with hydrate saturation (Soga et al., 2006; Waite et al., 2009). It is also found that the contribution of hydrates to the shear behavior arises primarily from their cohesive nature rather than frictional effects, which means the peak strength may vary, but the critical strength at large shear strain is similar regardless of hydrate saturation (Uchida et al., 2012). Furthermore, the formation of hydrate bonds enhances contact stiffness and cohesion at grain contacts, thereby increasing the macroscopic stiffness and shear strength. Additionally, the interlocking of grains also enhances the stiffness and peak strength. However, if the hydrate bonds dissociate or break due to shearing, the soil exhibits mechanical softening behavior. The increased dilation with hydrate saturation can be attributed to a transition from grain-scale to bonded-aggregate-scale particle rearrangements under shearing (Waite et al., 2009). Since HBS exhibit these mechanical properties, they can be effectively modeled as dense or bonded soils. This analogy has been experimentally confirmed through triaxial tests on natural and artificially prepared hydrate-bearing soils (Hyodo et al., 2005; Yun et al., 2007; Hyodo et al., 2013, 2014).

An ideal constitutive model for HBS should incorporate the essential mechanical characteristics of both bonded and dense soils, including enhanced stiffness, strength, and dilatancy, limited compressibility, the degradation of hydrate cementing and grain in-

terlocking due to dissociation and bond breakage, and stress relaxation resulting from hydrate dissociation. Extensions of the Mohr-Coulomb (MC) model have been a popular choice (Freij-Ayoub et al., 2007; Klar et al., 2010). However, these extended MC models can hardly capture all the critical mechanical behaviors of HBS. Recently, a number of critical state models for HBS have been developed to address these limitations by incorporating additional mechanisms (Kimoto et al., 2010; Uchida et al., 2012; Sun et al., 2018). While these models offer improved capabilities, they often require numerous parameters, some of which lack a strong physical basis and are challenging to calibrate, thereby limiting their practical applicability. Despite significant advancements, current constitutive models for HBS still face difficulties in considering the degradation of hydrate cementing and interlocking by hydrate dissociation and plastic deformation, factors that are crucial for addressing hydrate-related engineering challenges and natural geohazards.

Constitutive models for HBS are often empirical and phenomenological, lacking a physical representation of the underlying microscopic mechanisms. In contrast, the discrete element method (DEM) provides a more mechanistic approach for modeling the constitutive behavior (Nguyen et al., 2019; Le et al., 2021). DEM can incorporate various contact models between particles, allowing for the simulation of sediment movement and rearrangement (Gao et al., 2021, 2020), as well as hydrate bond formation, degradation, and breakage (Brugada et al., 2010; Jung et al., 2012; Xu et al., 2016). Moreover, DEM can effectively account for factors such as pore and sediment size distribution, particle stiffness, particle interlocking, and fabric evolution, enabling better predictions of the micromechanical behavior of HBS (Jiang et al., 2014; Xu et al., 2025; Ding et al., 2022). DEM also offers the flexibility to adjust contact models and parameters to accommodate different types of hydrate-bearing soils, which are often challenging to examine through laboratory experiments. As a result of these advantages, DEM has been widely utilized as an alternative to laboratory-scale tests for investigating the mechanical behavior of HBS (Yu et al., 2016; Han et al., 2022; Wang et al., 2024b; Li et al., 2025). Additionally, it has been attempted to model large-scale problems, such as hydrate-related submarine landslides (Jiang et al., 2016). However, the computational demand increases significantly with the number of particles, limiting its applicability in engineering-scale problems.

Another limitation of DEM is its inability to independently simulate the coupled THMC behaviors in an HBS system. DEM should be coupled with other approaches, such as computational fluid dynamics (CFD), to jointly simulate the THMC response (Jiang et al., 2018a,b; Liu et al., 2022; Wang et al., 2024a). For instance, Jiang et al. (2018b) employed the coupled CFD-DEM approach to investigate the undrained shear strength of HBS, observing significant localization in hydrate bond breakage but no such effect in fluid flow or excess pore pressure distribution. Similarly, Wang et al. (2024a) employed a resolved CFD-DEM framework to model solid-fluid interactions, enabling the simulation of particle movements and capturing variations in the hydraulic properties of

granular samples at the particle scale. This approach has also been applied to simulate submarine landslides triggered by seismic loading in hydrate-rich zones (Jiang et al., 2018a). However, incorporating hydrate kinetics into the coupled CFD-DEM framework poses significant challenges, particularly in simulating mass exchange between solid and fluid phases. Additionally, this method remains inefficient for engineering-scale simulations, as the computational cost increases dramatically with the increase in the number of DEM particles.

It is known that DEM is more suitable for simulating the mechanical behavior of hydrate soils at the meso-scale, while the continuum approach, such as the finite element method (FEM) (Ma et al., 2026), material point method (MPM) (Yu et al., 2024d,c), smoothed particle hydrodynamics (SPH) (Feng et al., 2025b,a), and Peridynamics (Yang et al., 2025), is more efficient for capturing the macroscopic multiphysics responses. Therefore, a hierarchical multiscale coupling of both provides a more promising modeling approach (Nitka et al., 2011; Andrade et al., 2011; Han et al., 2020). Such hybrid continuum-discrete coupling schemes, represented by FEM-DEM (Guo and Zhao, 2014) and MPM-DEM (Liang and Zhao, 2019; Liang et al., 2022), have been demonstrated to be effective and powerful in many application scenarios, such as high-porosity sandstone (Wu et al., 2018a, 2019), saturated granular soils (Guo and Zhao, 2016; Liang et al., 2023), and frozen soils (Yu et al., 2024b). Although FEM is extensively applied for THMC modeling of HBS (Sridhara et al., 2018; Queiruga et al., 2019; Sun et al., 2018; Ye et al., 2022), it suffers from mesh distortion during large deformations, leading to inaccuracy or non-convergence, making it less suitable for modeling hydrate dissociation-associated failures and geohazards. By contrast, MPM combines the advantages of Lagrangian particles and Eulerian mesh, and has been well applied to geotechnical failure, large deformation, and multiphysics coupling problems, including landslides, ground collapses, pile driving, and footing penetration, among many other applications (Pinyol et al., 2018; Dunatunga and Kamrin, 2017; Chen et al., 2021; Lei et al., 2021; Baumgarten et al., 2024; Lei et al., 2024; Yu et al., 2024a; Liang et al., 2025).

The aim of this study is therefore twofold: (1) to surpass phenomenological modeling of the mechanical behavior of HBS by conventional constitutive modeling, and (2) to incorporate fully coupled THMC behavior in HBS systems for engineering-scale problems. For this purpose, this study proposes to develop a hierarchical multiscale approach that integrates the THMC-coupled MPM with DEM. The MPM solver is employed to simulate the macroscale THMC responses, while the DEM solver is utilized to capture the path- and history-dependent stress-strain relationships. The multiscale coupling is established by embedding a DEM-based numerical sample of a representative volume element (RVE) at each material point. This framework leverages the strengths of MPM in modeling multiphysics large-deformation and large-scale problems and DEM in reproducing micromechanics-based constitutive behavior of hydrate-bearing soils. Specifically, we will

consider the hydrate cementation effect by incorporating a hydrate saturation-dependent bond contact model into the DEM solver. The yielding framework will be beneficial not only for HBS but also for other cemented soils, such as frozen soils and biocemented sand.

The remaining part of this paper is organized as follows. Section 2 will present the multiscale MPM-DEM approach for THMC-coupled modeling of HBS. Section 3 will detail the preparation of an RVE and its mechanical responses. Section 4 and 5 will present biaxial compression tests and rigid indenter penetration tests to demonstrate the efficacy of the proposed multiscale framework in capturing coupled THMC behavior in HBS. A summary will be given in Section 6.

2. Multiscale computational framework for hydrate-bearing sediment

2.1. Basic assumptions

The HBS is a highly complex multiphase and multi-component system. Before presenting its governing equations, several necessary assumptions are made.

1. Four primary components or phases are considered: sediment (s), hydrate (h), water (w), and gas (g), while the dissolved gas in water and the water vapor in gas are neglected (Klar et al., 2013; Sun et al., 2018; White et al., 2020).
2. For the phase transition process, only the hydrate dissociation is considered, whereas the formation of hydrate is neglected. Additionally, the hydration number is assumed to be 6, meaning that one hydrate molecule decomposes into six water molecules and one gas molecule (Liang et al., 2010; Sloan Jr and Koh, 2007; Ke et al., 2019).
3. While hydrate can be present in various occurrence modes, including pore-filling, contact-cementing, and grain-coating (Waite et al., 2009), this study focuses on the cementing type hydrates. We assume that the hydrates and hosting sediment grains jointly contribute to the soil skeleton of the HBS system, with the hydrate playing the role of cementing agent (Wu et al., 2020; Jiang et al., 2014).
4. The liquid phase is assumed to be weakly compressible, and both liquids and solids exhibit linear thermal expansion. The gas phase is treated as an ideal gas and follows the state equation of ideal gas (Ye et al., 2022).
5. The migration of both fluid and gas is assumed to fulfill Darcy's law, while heat transfer follows Fourier's law (Sun et al., 2018; Ye et al., 2022). Both fluid flow and heat transfer are considered isotropic.

Based on these assumptions, the governing equations, including the mass, momentum, and energy balance equations, are established, alongside the hydrate kinetic reaction model, a soil water retention model, the equations of state for each phase, and a permeability model accounting for changes in porosity and saturation of each phase.

2.2. Continuum theory for THMC modeling of HBS

2.2.1. Preliminaries

According to the mixture theory, all phases in an HBS medium are assumed to be spatially continuous and homogeneously distributed in an averaged sense on the macroscopic scale. Based on this, for an RVE in HBS, as illustrated in Figure 1, the porosity, ϕ , and the saturation of each phase, S_π , can be defined as (Lewis and Schrefler, 1998),

$$\phi := \frac{dV_h + dV_w + dV_g}{dV}, \quad S_\pi := \frac{dV_\pi}{dV_h + dV_w + dV_g}, \quad \pi \in \{h, w, g\}, \quad (1)$$

where dV_h , dV_w , and dV_g are the volumes of the hydrate, water, and gas phases, respectively, in an RVE, and dV is the total volume of the RVE.

In the multiscale framework, the effective stress theory remains the fundamental link between the pore pressure and effective stress responses. Based on the extended Bishop's effective stress theory (Gallipoli et al., 2003; Oka et al., 2006), the total stress can be expressed as,

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}'_{\text{RVE}} - p_f \mathbf{I}, \quad \text{with } p_f = \chi_w p_w + \chi_g p_g, \quad (2)$$

where $\boldsymbol{\sigma}'_{\text{RVE}}$ is the effective stress tensor; p_f is the pore fluid pressure; p_w and p_g are the pore water and gas pressures; and $\chi_w = S_w/(S_w + S_g)$ and $\chi_g = S_g/(S_w + S_g)$ are two Bishop coefficients. Unlike using the conventional constitutive models, the effective stress $\boldsymbol{\sigma}'_{\text{RVE}}$ is now updated by the DEM-based RVE. It should be noted that the DEM is only employed to update the effective stress, while pore pressure variables are still updated by the macroscopic MPM solver.

2.2.2. Mass balance equation

The Mass balance equation for each phase in the Lagrangian description is given as follows,

$$\left\{ \begin{array}{l} \frac{D^s [(1 - \phi)\rho_s]}{Dt} + (1 - \phi)\rho_s \nabla \cdot \mathbf{v}_s = 0, \text{ (Solid)} \end{array} \right. \quad (3)$$

$$\left\{ \begin{array}{l} \frac{D^s (\phi S_h \rho_h)}{Dt} + \phi S_h \rho_h \nabla \cdot \mathbf{v}_s = \dot{m}_h, \text{ (Hydrate)} \end{array} \right. \quad (4)$$

$$\left\{ \begin{array}{l} \frac{D^s (\phi S_w \rho_w)}{Dt} + \phi S_w \rho_w \nabla \cdot \mathbf{v}_s + \nabla \cdot \rho_w \mathbf{J}_w = \dot{m}_w, \text{ (Water)} \end{array} \right. \quad (5)$$

$$\left\{ \begin{array}{l} \frac{D^s (\phi S_g \rho_g)}{Dt} + \phi S_g \rho_g \nabla \cdot \mathbf{v}_s + \nabla \cdot \rho_g \mathbf{J}_g = \dot{m}_g, \text{ (Gas)} \end{array} \right. \quad (6)$$

Here, the operator D^s/Dt denotes the material derivative with respect to the solid phase, defined as $\frac{D^s}{Dt} = \frac{\partial}{\partial t} + \mathbf{v}_s \cdot \nabla$. In addition, ϕ is the porosity. ρ_π is the intrinsic density of phase π , where $\pi \in \{s, h, w, g\}$. $\mathbf{v}_\pi$ is the velocity of phase π , while $\mathbf{J}_\pi = \phi S_\pi (\mathbf{v}_\pi - \mathbf{v}_s)$ is the Darcy velocity, describing the relative flow of the phase with respect to the solid matrix. $\dot{m}_\pi$ is the rate of mass production (or consumption) per unit bulk volume due to hydrate dissociation.

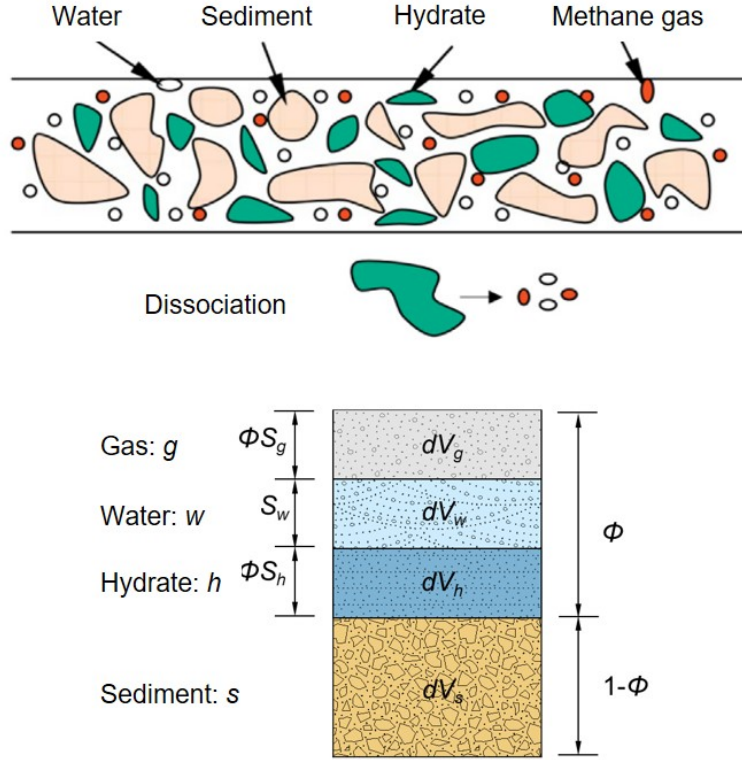


Figure 1: Illustration of the distribution of each phase in an HBS RVE (Chen et al., 2016).

2.2.3. Momentum balance equation

The momentum balance equations for the mixture, water, and gas phases are given as follows,

$$\left\{ \begin{aligned} \rho_{sh} \frac{D^s \mathbf{v}_s}{Dt} + \phi S_w \rho_w \frac{D^s \mathbf{v}_w}{Dt} + \phi S_g \rho_g \frac{D^s \mathbf{v}_g}{Dt} &= \nabla \cdot (\boldsymbol{\sigma}'_{\text{RVE}} - p_f \mathbf{I}) + \rho_m \mathbf{b}, \text{ (Mixture)} \end{aligned} \right. \quad (7)$$

$$\left\{ \begin{aligned} \phi S_w \rho_w \frac{D^s \mathbf{v}_w}{Dt} &= -\phi S_w \nabla p_w + \phi S_w \rho_w \mathbf{b} - (\phi S_w)^2 \frac{\mu_w}{k_a k_{rw}} (\mathbf{v}_w - \mathbf{v}_s), \text{ (Water)} \end{aligned} \right. \quad (8)$$

$$\left\{ \begin{aligned} \phi S_g \rho_g \frac{D^s \mathbf{v}_g}{Dt} &= -\phi S_g \nabla p_g + \phi S_g \rho_g \mathbf{b} - (\phi S_g)^2 \frac{\mu_g}{k_a k_{rg}} (\mathbf{v}_g - \mathbf{v}_s), \text{ (Gas)} \end{aligned} \right. \quad (9)$$

where $\rho_{sh} = (1 - \phi)\rho_s + \phi S_h \rho_h$ is the average density of the hydrate-soil skeleton; $\rho_m = (1 - \phi)\rho_s + \phi S_h \rho_h + \phi S_w \rho_w + \phi S_g \rho_g$ is the average density of the mixture; μ_w and μ_g are the dynamic viscosity of the water and gas phases, respectively; k_a is the absolute permeability; k_{rw} and k_{rg} are the relative permeability of the water and gas phases, respectively; $\mathbf{b}$ is the body force vector; and $\mathbf{I}$ is the identity tensor. Note that the effective stress updated from the RVE should consider the effect of hydrate cementation.

2.2.4. Energy balance equation

The energy balance equation for the mixture is given by,

$$C_m \frac{D^s T}{Dt} + (\rho_w c_w \mathbf{J}_w + \rho_g c_g \mathbf{J}_g) \cdot \nabla T + \nabla \cdot (-\boldsymbol{\kappa}_m \nabla T) - \theta \boldsymbol{\sigma}' : \dot{\boldsymbol{\varepsilon}}^p = q_e, \text{ (Mixture)} \quad (10)$$

where T is the temperature; $C_m = (1 - \phi)\rho_s c_s + \phi S_h \rho_h c_h + \phi S_w \rho_w c_w + \phi S_g \rho_g c_g$ and $\kappa_m = (1 - \phi)\kappa_s + \phi S_h \kappa_h + \phi S_w \kappa_w + \phi S_g \kappa_g$ are respectively the heat capacity and the thermal conductivity of the mixture; c_π and κ_π are respectively the specific heat capacity and the thermal conductivity of phase π ; $\theta \boldsymbol{\sigma}':\boldsymbol{\varepsilon}^p$ represents the heat generation due to plastic deformation (Vishnu et al., 2022); and q_e is the heat source due to hydrate dissociation, calculated by (Ye et al., 2022),

$$q_e = \Delta H \dot{m}_h = (C_0 + C_1 T) \dot{m}_h, \quad (11)$$

where ΔH is the enthalpy change, and C_0 and C_1 are coefficients characterizing the latent heat of hydrate dissociation, taken as 446,120 J/kg and 132.638 J/(kg·°C), respectively.

Remark 1. It is important to note that thermal conductivity depends on the skeleton and pore structures, which can be updated based on the evolving RVE fabric. The same applies to hydraulic conductivity. Additionally, macroscopic plastic heat generation can also be derived from the RVE scale (Zhao et al., 2020). However, due to limited scope, these aspects are reserved for future investigation. This work focuses exclusively on the effective stress updates derived from the RVEs.

2.2.5. Hydrate reaction model

The mass source term $\dot{m}_\pi$ in the mass balance equations (Eqs. (4-6)) is determined based on the kinetic reaction rate of hydrate (R_r) in a given temperature and pressure condition as follows (Liang et al., 2010; Ruan et al., 2012),

$$\dot{m}_h = -M_h R_r, \quad \dot{m}_g = M_g R_r, \quad \dot{m}_w = N_h M_w R_r, \quad (12)$$

where M_h , M_g , and M_w represent the molar masses of hydrate, gas, and water, respectively, while N_h denotes the hydration number. The hydrate kinetic reaction rate R_r is calculated using the Kim-Bishnoi model (Kim et al., 1987; Clarke and Bishnoi, 2001b,a; Sloan, 1987),

$$R_r = K_0 \exp\left(-\frac{\Delta E}{RT}\right) \phi S_h (p_e - p_f), \quad (13)$$

$$p_e = A_1 \exp\left(A_2 - \frac{A_3}{T + 273.15}\right), \quad (14)$$

where K_0 is the kinetic dissociation constant; ΔE is the activation energy, taken as 78,151 J/mol; R is the gas constant; A_{geo} is the surface area to volume ratio of hydrate particles, taken as 7.5×10^5 /m; and p_e is the hydrate stability pressure; and A_1 , A_2 , and A_3 are regression coefficients, given as follows: $A_1 = 1.15$ Pa, $A_2 = 49.3185$, and $A_3 = 9,459$ °C⁻¹. This model takes into account the combined effects of temperature, pore pressure, hydrate content, and pore topology characteristics.

2.2.6. Soil water retention model

In HBS, gas and water can be trapped within the voids as "residual gas" and "residual water", with their magnitudes influenced by hydrate saturation. To account for this, an effective water saturation S_e is defined as (Lewis and Schrefler, 1998; Sun et al., 2018),

$$S_e := \frac{S_w / (1 - S_h) - S_{wr}}{1 - S_{wr} - S_{gr}}, \quad (15)$$

where $S_{wr} := dV_{wr}/(dV_w + dV_g)$ and $S_{gr} := dV_{gr}/(dV_w + dV_g)$ are the residual water saturation and residual gas saturation, respectively; and V_{wr} and V_{gr} are the volumes of residual water and residual gas, respectively.

The effective saturation can be determined using the soil-water retention model. The well-established Van Genuchten model is employed in this work (Van Genuchten, 1980; Sun et al., 2018; White et al., 2020; Zhang et al., 2024), expressed as,

$$S_e = \left(1 + (p_c/p_0)^{1/(1-m)}\right)^{-m}, \quad (16)$$

where $p_c = p_g - p_w$ is the capillary suction, with p_g and p_w the pore gas pressure and pore water pressure, respectively; p_0 is the reference pressure; and m is a constant model parameter.

2.2.7. Absolute and relative permeability model

The absolute permeability k_a is influenced by both porosity and hydrate saturation. The following equation is adopted to evaluate k_a (Masuda, 1999; Liang et al., 2010; Ruan et al., 2012; Ye et al., 2022),

$$k_a = k_0 \left(\frac{\phi}{\phi_0}\right)^{1.5} \left(\frac{1 - \phi}{1 - \phi_0}\right)^3 (1 - S_h)^{m_h}, \quad (17)$$

where k_0 is the hydrate-free permeability at the porosity of ϕ_0 and m_h is a permeability reduction parameter related to the pore structure

The relative permeabilities for the water and gas phases, k_{rw} and k_{rg} , are calculated using a modified Corey's model (Corey, 1954; Liang et al., 2010; Ruan et al., 2012),

$$k_{rw} = \left(\frac{S_w/(1 - S_h) - S_{rw}}{1 - S_{rw} - S_{rg}}\right)^{n_w}, \quad k_{rg} = \left(\frac{S_g/(1 - S_h) - S_{rg}}{1 - S_{rw} - S_{rg}}\right)^{n_g}, \quad (18)$$

where n_w and n_g are two material constants.

2.3. Discrete element model for HBS considering hydrate bond

As aforementioned, DEM has been widely used to investigate the cross-scale mechanical behavior of HBS (Ding et al., 2022; Wang et al., 2024b; Li et al., 2025; Xu et al., 2025). In different work, the hydrate may be treated as a pore-filling particle or cementing

agent, corresponding to the pore-filling and cementing types of HBS, respectively. Both types of models can be implemented within the current multiscale framework seamlessly. In this study, we focus mainly on the cementing-type hydrate. For simplicity but without loss of generality, we adopt a simple bond contact model to capture the cementation effects when hydrate is present, together with a frictional contact model to represent basic grain-to-grain interactions in the absence of hydrate bonds (Liang and Zhao, 2019; Liang et al., 2023; Zhao et al., 2022).

This approach naturally accounts for the following effects: (1) the cementation effect of hydrate, (2) the influence of hydrate saturation on the bond strength and sediment stiffness, (3) hydrate bond breakage when the grain contact force exceeds the bond strength, (4) bond degradation during hydrate dissociation, (5) the dependence of sediment strength and stiffness on hydrate saturation, confining stress, and packing density, (6) path- and history-dependent stress-strain relationships during mechanical loading and hydrate dissociation, and (7) other microscopic properties of HBS.

2.3.1. Basic frictional contact model

The contact forces between any two contacting particles, such as particle A and particle B (as illustrated in Figure 2), are linearly related to their relative displacements. The tangential contact force is further constrained by the Coulomb friction condition. These relationships are described as follows,

$$\begin{cases} f_n = -k_n u_n, \\ \Delta f_t = -k_t \Delta u_t, \quad |f_t| \leq \mu |f_n|, \end{cases} \quad (19)$$

where f_n and f_t are the normal and tangential components of the contact force (positive for tensile forces); k_n and k_t are the normal and tangential stiffnesses; u_n and u_t are the normal and tangential displacements; and μ is the friction coefficient at the contact. The stiffness parameters k_n and k_t are linked with the grains' Young's modulus (E_c) and Poisson's ratio (ν_c) through $k_n = E_c \bar{r}$ and $k_t = \nu_c k_n$, where $\bar{r} = 2r_A r_B / (r_A + r_B)$ is the harmonic mean radius of the two contacting particles with radii r_A and r_B (Smilauer et al., 2023).

2.3.2. Hydrate saturation-dependent bond contact model

In the presence of hydrate, a bond contact model is employed. Rather than simulating hydrate and sediment grains as distinct entities, each DEM grain is conceptually treated as a composite of hydrate and sediment, where the grain size and elastic properties are defined as functions of hydrate saturation. The intergranular cementation is then modeled using a point-bond model, where the bond strength is also a function of hydrate saturation. The equivalent size of the sediment-hydrate mixed particle is given by,

$$r_{eq} = r_0 \left(\frac{V_s + V_h}{V_{s0}} \right)^{1/D} = r_0 \left(\frac{1 - \phi_0 + (\phi_0 + \varepsilon_v) S_h}{1 - \phi_0} \right)^{1/D}, \quad (21)$$

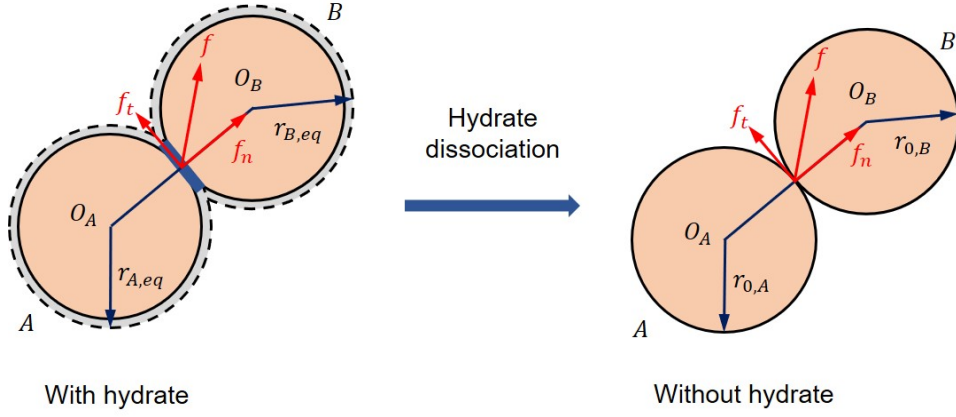


Figure 2: Illustration of contact model in DEM solver

where r_0 is the initial grain size; V_{s0} is the initial volume of the solid phase; V_s and V_h are the current volumes of the solid phase and the hydrate phase, respectively; ϕ_0 is the initial porosity; ε_v is the volumetric strain; S_h is the hydrate saturation degree; and D is the dimension.

The maximum normal and tangential contact forces, f_n^{max} and f_t^{max} , are defined as (Wu et al., 2018b, 2023),

$$\begin{cases} f_n^{max} = C_n \min \{r_A^2, r_B^2\}, \\ f_t^{max} = \mu f_n + C_t \min \{r_A^2, r_B^2\}, \end{cases} \quad (22)$$

where C_n and C_t represent the normal and tangential cohesion strength of the bond. If either the normal or tangential force exceeds its corresponding maximum threshold, the bond will break. In the case of a tensile normal force, the contact is entirely lost. Otherwise, the contact transitions to a purely frictional contact.

The bond strength and the particle stiffness (Young's modulus) are dependent on the hydrate saturation as follows (Yu et al., 2024b),

$$\begin{cases} C_i = C_{i0} + \Delta C_i^{max} \Phi(S_h), & i = n, t, \\ E_c = E_{c0} + \Delta E_c^{max} \Phi(S_h). \end{cases} \quad (24)$$

Here, C_{i0} and E_{c0} are the cohesion strength without hydrate bond and the Young's modulus of pure soil grains, respectively. ΔC_i^{max} and ΔE_c^{max} are the maximum additional cohesion and modulus due to the hydrate bond, respectively. Additionally, Φ is a function related to the hydrate saturation S_h .

Since the bonding effect might not be significant when hydrate saturation is low, an exponential function Φ is adopted for Φ_{ci} and Φ_{ki} ,

$$\Phi = \exp[-\eta_h(1 - S_h/S_{h,max})], \quad (26)$$

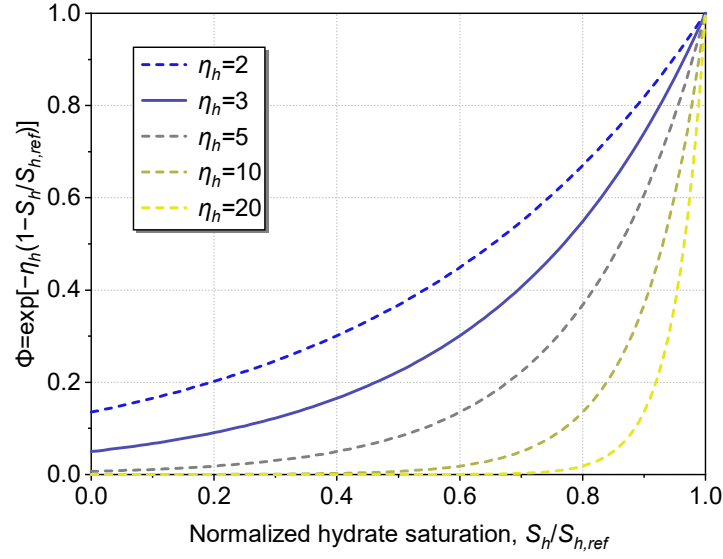


Figure 3: Φ function with different shape parameter η_h .

where $S_{h,max}$ is the (reference) maximum saturation of hydrate, η_h is a shape parameter. Figure 3 shows the Φ as a function of η_h . As can be seen, Φ decreases with hydrate saturation.

Remark 2. The bond properties can also be correlated with pressure and temperature, as adopted by some existing DEM simulations for hydrate-bearing soils (Jiang et al., 2016, 2017). In our model, hydrate saturation is directly dependent on pressure and temperature, inherently capturing these effects. Additionally, the multiscale approach enables the dynamic simulation of pressure and temperature changes, which, in turn, allows for the real-time updating of hydrate saturation. This is traditionally challenging to achieve with purely DEM-based modeling.

2.3.3. Boundary imposition and stress homogenization

To reduce the boundary effect from rigid boundaries (*e.g.*, rigid confining walls), periodic boundary conditions are employed in the DEM simulations (Liang et al., 2023). At each MPM time step, the incremental displacement gradient $\nabla \mathbf{u}$ is received from the macroscale MPM material point and prescribed as the boundary condition for the RVE. It is important to note that the RVE used here corresponds to the updated configuration from the previous step, rather than the initial RVE. Therefore, in the current step, only the incremental displacement gradient is required to update the RVE. This update strategy naturally accounts for path- and history-dependent granular mechanics. Under non-isothermal conditions, the incremental displacement gradient in the MPM solver is calculated as,

$$\nabla \mathbf{u} = \Delta t_{\text{MPM}} \nabla \mathbf{v}_s - \frac{\beta_{sh}}{3} \Delta T \mathbf{I}, \quad (27)$$

where Δt_{MPM} is the MPM time step size. The second term on the right-hand side represents the volumetric expansion or contraction due to thermal effects. It is important to note that this incremental displacement gradient represents the total deformation within a single MPM time step. For each DEM time step, the applied deformation should be $\nabla \mathbf{v}_{\text{DEM}} = \nabla \mathbf{u} / \Delta t_{\text{DEM}}$, in which Δt_{DEM} is the DEM time step size.

Remark 3. Note that the time step size of the MPM solver, Δt_{MPM} , and that of the DEM solver, Δt_{DEM} , need not be identical. Δt_{MPM} is governed by the CFL condition derived from the macroscopic governing equations, whereas Δt_{DEM} is determined by particle-scale properties such as density and stiffness. These two time steps are mutually independent and do not influence one another.

After applying the boundary condition, the homogenized Cauchy stress of the RVE is computed based on the well-established Love-Weber formula (Nicot et al., 2013),

$$\boldsymbol{\sigma}'_{\text{RVE}} = \frac{1}{V_{\text{RVE}}} \sum_{N_c} \mathbf{d} \otimes \mathbf{f}, \quad (28)$$

where “ $\otimes$ ” denotes the dyadic product between two vectors; V_{RVE} is the volume of the RVE; N_c is the total number of all contacts inside the RVE; $\mathbf{d}$ is the branch vector joining the centers of contacting particles; and $\mathbf{f}$ is the contact force.

2.4. Multiscale coupling strategy and solution procedure

The multiscale coupling is implemented by attaching an RVE to each material point. The one-point multiphase MPM serves as the upscale solver for modeling macroscopic multiphysics, while the DEM serves as the downscale solver for updating hydrate-saturation-dependent mechanical responses. A schematic of the overall strategy of the coupled MPM-DEM approach is shown in Figure 4. The detailed coupling strategy with the update-stress-first (USF) scheme is given as follows.

2.4.1. Step 1: MPM Solver - Map Particles to Nodes & Update Particle Properties First

(1.1) Map material point information (e.g., mass, momentum, heat capacity, and heat) to nodes, calculate nodal velocities, $\mathbf{v}_{sI}^k$, and temperature, $\mathbf{v}_{\pi I}^k$:

$$M_{sh}^k = \sum_p^{n_p} (m_{sp}^k + m_{hp}^k) S_{Ip}, \quad \mathbf{v}_{sI}^k = (M_{sh}^k)^{-1} \sum_p^{n_p} (m_{sp}^k + m_{hp}^k) \mathbf{v}_{sp}^k S_{Ip}, \quad (29)$$

$$M_{\pi}^k = \sum_p^{n_p} m_{\pi p}^k S_{Ip}, \quad \mathbf{v}_{\pi I}^k = (M_{\pi}^k)^{-1} \sum_p^{n_p} m_{\pi p}^k \mathbf{v}_{\pi p}^k S_{Ip}, \quad \pi \in \{w, g\}, \quad (30)$$

$$C_m^k = \sum_p^{n_p} V_p^k C_{mp}^k S_{Ip}, \quad T_I^k = (C_m^k)^{-1} \sum_p^{n_p} V_p^k C_{mp}^k T_p^k S_{Ip}, \quad (31)$$

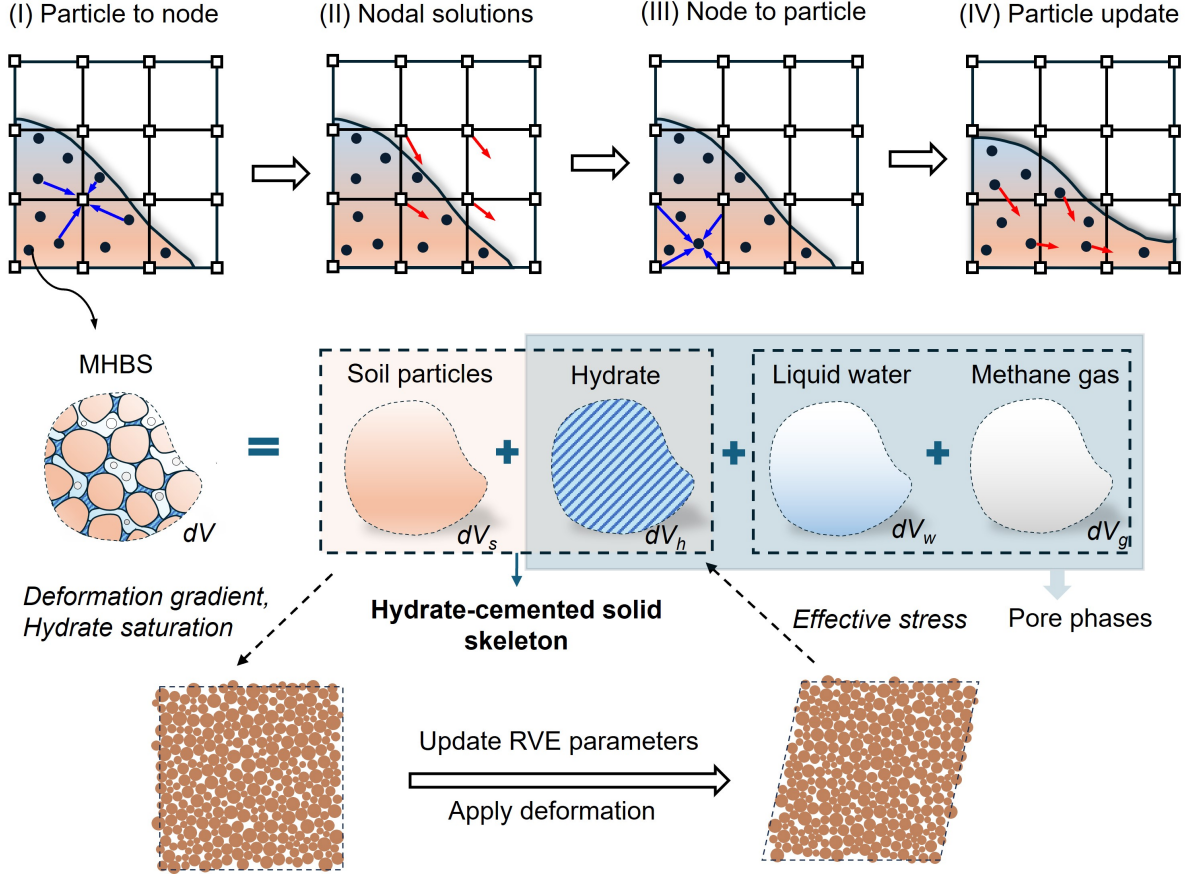


Figure 4: Illustration of the multiscale modeling strategy for HBS.

where the subscripts p and I denote material point and node indices, respectively; the superscript k and $k + 1$ denote the current and next time steps, respectively; S_{Ip} is the MPM interpolation function regarding material point p and node I ; and n_p is the number of particles.

(1.2) Compute particle strain, $\dot{\epsilon}_p^{k+1}$, and incremental displacement gradient, $\nabla \mathbf{u}_p^{k+1}$:

$$\dot{\epsilon}_p^{k+1} = \frac{1}{2} \left(\nabla \mathbf{v}_{sp}^k + (\nabla \mathbf{v}_{sp}^k)^T \right) - \frac{\beta_{sh}}{3} \dot{T}_p^k \mathbf{I}, \quad (32)$$

$$\nabla \mathbf{u}_p^{k+1} = \Delta t \left(\nabla \mathbf{v}_{sp}^k - \frac{\beta_{sh}}{3} \dot{T}_p^k \mathbf{I} \right), \quad (33)$$

where the particle velocity gradient is compute as $\nabla \mathbf{v}_{sp}^k = \sum_I \mathbf{v}_{\pi I}^k \nabla S_{Ip}$; Δt is the time step size of the MPM solver; and β_{sh} is the volumetric thermal expansivity of the hydrate-soil skeleton. Then, the volumetric strain and porosity can be updated using the strain rate.

(1.3) Update the rate of hydrate saturation, $\dot{S}_{hp}^{k+1}$,

$$\dot{S}_{hp}^{k+1} = (\phi_p^{k+1})^{-1} \left(\frac{\dot{m}_h}{\rho_h} + \beta_{sh} \dot{T}_p^k - S_{hp}^{k+1} \dot{\epsilon}_{sp}^{k+1} \right), \quad (34)$$

where $\dot{\varepsilon}_{sp}$ is the rate of volumetric strain of the solid phase.

(1.4) Update the rate of pore gas and liquid pressures, $\dot{p}_{wp}^{k+1}$ and $\dot{p}_{gp}^{k+1}$,

$$\begin{bmatrix} \tilde{K}_{ww} & \tilde{K}_{wg} \\ \tilde{K}_{gw} & \tilde{K}_{gg} \end{bmatrix}_p \begin{Bmatrix} \dot{p}_w^{k+1} \\ \dot{p}_g^{k+1} \end{Bmatrix}_p = \begin{Bmatrix} \tilde{f}_w \\ \tilde{f}_g \end{Bmatrix}_p, \quad (35)$$

where the components of the LHS matrix and the RHS vector, $\tilde{K}_{ww}$, $\tilde{K}_{wg}$, $\tilde{K}_{gw}$, $\tilde{K}_{gg}$, $\tilde{f}_w$ and $\tilde{f}_g$, are derived from the mass balance equations and their detailed expression of can be found in [Appendix B](#) and [Yu et al. \(2026\)](#).

(1.5) Update other properties, including densities of each phase, absolute and relative permeability, and source terms.

2.4.2. Step 2: MPM/DEM Message Passing & Run DEM Solver to Shear RVE

(2.1) Transfer the updated incremental displacement gradient $\nabla \mathbf{u}_p^{k+1}$ and the hydrate saturation S_{hp}^{k+1} from material points to the corresponding DEM RVEs:

$$\nabla \mathbf{u}_p^{k+1} \rightarrow \nabla \mathbf{u}_{\text{RVE}}^{k+1}, \quad S_{hp}^{k+1} \rightarrow S_{h,\text{RVE}}^{k+1}. \quad (36)$$

(2.2) Update the RVE parameters (*e.g.*, grain elastic modulus, bond strength, and particle size) based on hydrate saturation according to Eq. (21) and Eqs. (24 - 26);

(2.3) Shear RVE by enforcing the velocity gradient:

$$\nabla \mathbf{v}_{\text{RVE}}^{k+1} = \nabla \mathbf{u}_{\text{RVE}}^{k+1} / \Delta t_{\text{DEM}}, \quad (37)$$

where Δt_{DEM} is the time step size of the DEM solver. Then, calculate the homogenized stress based on Eq. (28).

(2.4) Transfer the updated RVE stress tensor and other microscopic information (*e.g.*, bond state and fabric distribution), if necessary, to the corresponding material points.

2.4.3. Step 3: MPM Solver - Update Nodal Solutions, Map Nodes to Particles, & Update Particles

(3.1) Compute nodal forces and calculate nodal acceleration $\dot{\mathbf{v}}_{\pi I}^{k+1}$ using a node-based implicit scheme:

$$\begin{bmatrix} M_{sh} & M_w & M_g \\ \Delta t Q_w^d & M_w - \Delta t Q_w^d & 0 \\ \Delta t Q_g^d & 0 & M_g - \Delta t Q_g^d \end{bmatrix}_I \begin{Bmatrix} \dot{\mathbf{v}}_s^{k+1} \\ \dot{\mathbf{v}}_w^{k+1} \\ \dot{\mathbf{v}}_g^{k+1} \end{Bmatrix}_I = \begin{Bmatrix} \mathbf{f}_m^{\text{ext}} + \mathbf{f}_m^{\text{int}} \\ \mathbf{f}_w^{\text{ext}} + \mathbf{f}_w^{\text{int}} + Q_w^d \cdot (\mathbf{v}_w^k - \mathbf{v}_s^k) \\ \mathbf{f}_g^{\text{ext}} + \mathbf{f}_g^{\text{int}} + Q_g^d \cdot (\mathbf{v}_g^k - \mathbf{v}_s^k) \end{Bmatrix}_I. \quad (38)$$

where Q_w^d and Q_g^d are the nodal drag force coefficients. $\mathbf{f}_{(*)}^{\text{ext}}$ are $\mathbf{f}_{(*)}^{\text{int}}$ are the nodal internal and external forces.

(3.2) Compute nodal heats from particles and calculate temperature rate $\dot{T}_I^{k+1}$ using an explicit scheme:

$$\dot{T}_I^{k+1} = (\mathcal{E}_{TI}^{\text{source}} + \mathcal{E}_{TI}^{\text{ext}} + \mathcal{E}_{TI}^{\text{int}} + \mathbf{Q}_{wI}^{\text{conv}} \cdot (\mathbf{v}_{wI}^k - \mathbf{v}_{sI}^k) + \mathbf{Q}_{gI}^{\text{conv}} \cdot (\mathbf{v}_{gI}^k - \mathbf{v}_{sI}^k)) / \tilde{C}_{mI}, \quad (39)$$

where $\mathcal{E}_{TI}^{source}$, $\mathcal{E}_{TI}^{ext}$, and $\mathcal{E}_{TI}^{int}$ are the nodal heat sources, internal and external heat; $\mathbf{Q}_{wI}^{conv}$ and $\mathbf{Q}_{gI}^{conv}$ are nodal coefficients related to heat convection; and $\tilde{C}_{mI}$ is the modified nodal heat capacity.

(3.3) Map updated nodal temperature and velocity variables to particles and update particle temperature and velocities:

$$\mathcal{V}_p^{k+1} = \mathcal{V}_p^k + \Delta t \sum_I^{n_I} \dot{\mathcal{V}}_I^{k+1} S_{Ip}, \quad \mathcal{V} = \mathbf{v}_s, \mathbf{v}_w, \mathbf{v}_g, T. \quad (40)$$

(3.4) Update particle displacements $\mathbf{u}_p$ and positions $\mathbf{x}_p$:

$$\Delta \mathbf{x}_p^{k+1} = \Delta \mathbf{u}_p^{k+1} = \mathbf{v}_{sp}^k \Delta t + \frac{1}{2} \dot{\mathbf{v}}_{sp}^{k+1} \Delta t^2. \quad (41)$$

For the details of the MPM discretizations and the solution algorithm, readers may refer to our previous work (Yu et al., 2026).

3. RVE preparation

In this study, 2D examples are employed to demonstrate the efficacy of the proposed multiscale framework for modeling HBS. While 3D simulations remain computationally expensive at present, the framework is equally applicable to 3D cases.

3.1. RVE generation

The RVE is generated using the bond contact model by setting a zero bond strength, which is equivalent to a pure frictional contact model. The microparameters used for the RVE preparation are listed in Table 1. A dense RVE packing with 500 grains and an initial porosity of approximately 0.18 is prepared under an isotropic confining stress of 100 kPa, as illustrated in Figure 5b. The distribution of contact normal orientations is shown in Figure 5a, indicating that the RVE exhibits relatively isotropic packing.

Remark 4. The use of 500 grains per RVE is a compromise between computational accuracy and efficiency. The RVE must be sufficiently large to capture the characteristic mechanical behavior of the meso-scale sample. However, an excessively large RVE leads to a significant, often exponential, increase in computational cost. Previous studies have established that for a 2D RVE, approximately 400 grains (Guo and Zhao, 2014; Wu et al., 2018a; Liang et al., 2023) strike a reasonable balance. Accordingly, we selected a slightly larger value of 500 grains to enhance representativeness while maintaining tractable computational demands.

Remark 5. Notice that the RVE is prepared under a relatively low confining stress (100 kPa) to achieve a stable initial packing. However, it is crucial to note that the subsequent mechanical response is governed by the current state transmitted from the

MPM material point. During the simulation of macroscopic boundary value problems, the embedded RVEs routinely experience effective stresses in the MPa range. The path- and history-dependent nature of our DEM model ensures that the RVE's response evolves appropriately to these high-stress conditions.

Remark 6. It is also important to note that the porosity of a DEM RVE characterizes the space occupied by fluid phases (*i.e.*, water and gas), which differs from the hydrate-free porosity defined in the MPM framework. However, it should be acknowledged that, in the current model, using the RVE porosity to update the macroscopic porosity can be tricky, as this study employs a highly simplified DEM model for hydrates. This limitation can be addressed in future work by adopting a more sophisticated 3D DEM model for hydrate-soil interactions.

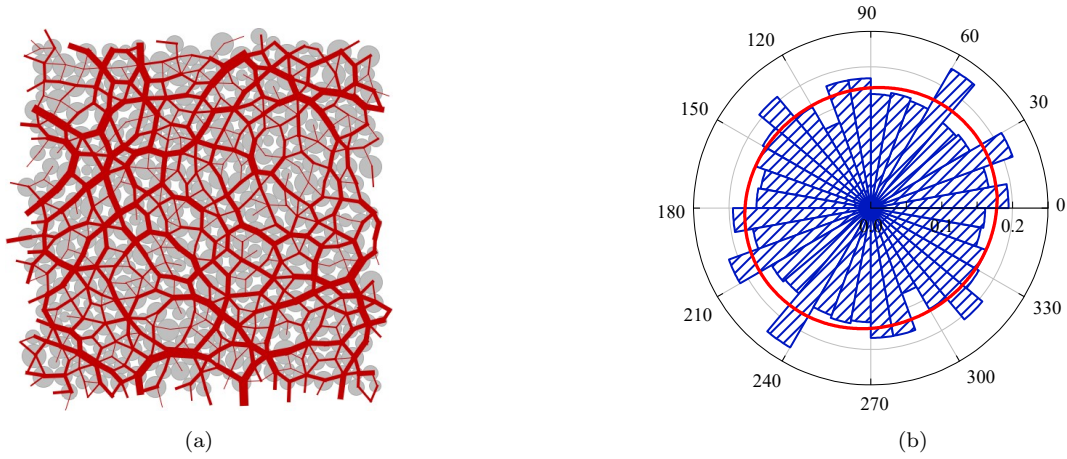


Figure 5: (a) RVE force chain and (b) contact normal orientation distribution.

Table 1: Microscopic parameters used for RVE preparation.

DEM parameters	Value
Grain density, ρ_{grain} : kg/m ³	2650
Grain size, r_{grain} : mm	3~7
Young's modulus, E_c : MPa	600
Poisson's ratio, ν_c	0.8
frictional coefficient, μ	0.5
Number of grains in an RVE, N_{grain}	500

Once the RVE packing is prepared, the bond parameters are assigned based on the hydrate saturation condition. For a condition without hydrate ($S_h = 0$), the soil is modeled as a low-cohesion material with a bond strength of 20 MPa. At a hydrate

saturation of 0.5, the additional cohesion is set to 200 MPa, while the additional modulus is defined as 20 GPa. The shape parameter, η_h , which is a critical factor governing the global mechanical response of the HBS RVE, is carefully chosen as 3 in this study. A summary of the parameters for the saturation-dependent bond model is provided in Table 2.

Table 2: Hydrate saturation-dependent RVE parameters.

DEM parameters	Value
Hydrate-free Young's modulus, E_{c0} : GPa	5
Additional Young's modulus at $S_h = 0.5$, ΔE_c^{max} : GPa	20
Cohesion without hydrate, C_{i0} : MPa	20
Maximum additional cohesion, ΔC_{imax} : MPa	200
Shape factor, η	3

3.2. RVE responses

To validate whether the RVE with the selected parameters can effectively capture the key mechanical characteristics of HBS, a series of biaxial compression tests is performed on RVE samples under varying hydrate saturation levels and confining stresses. Five saturation conditions are tested, specifically 0.5, 0.35, 0.23, 0.12, and 0, with corresponding Φ values of 1.0, 0.4, 0.2, 0.1, and 0.05, respectively. Each sample is tested under four confining stress conditions, *i.e.*, 0.8, 1.6, 3.2, and 6.4 MPa. The test conditions, including the corresponding grain Young's modulus and cohesion values, are summarized in Table 3.

Table 3: Biaxial test on RVE with different hydrate saturation.

Test ID	S_h	S_h/S_{hmax}	Φ	E_c : GPa	C_i : MPa	σ_c : MPa
RVE-Test-1	0	0	0.05	6	30	0.8, 1.6, 3.2, 6.4
RVE-Test-2	0.12	0.24	0.1	7	40	0.8, 1.6, 3.2, 6.4
RVE-Test-3	0.23	0.46	0.2	9	60	0.8, 1.6, 3.2, 6.4
RVE-Test-4	0.35	0.7	0.4	13	100	0.8, 1.6, 3.2, 6.4
RVE-Test-5	0.5	1.0	1.0	25	220	0.8, 1.6, 3.2, 6.4

Figure 6(a) and (b) present the axial stress (σ_{yy})-axial strain (ε_{yy}) relationships for samples with different hydrate saturation under confining stress of 0.8 MPa and 1.6 MPa. The results reveal that (1) The Young's modulus increases with hydrate saturation; (2) the peak strength increases with hydrate saturation, while the critical strength is relatively similar for all hydrate saturation conditions; (3) high saturation samples exhibit more

obvious strength softening at large strains. The severe fluctuations in the curves for higher saturation samples are likely caused by frequent bond breakage. Another potential factor is the limited number of particles used in the simulation. It is important to note, however, that this limitation does not compromise the model's ability to faithfully reflect the overall mechanical trends of hydrate soils. Figure 6(c) and d show the evolution of volumetric strain with axial strain. All samples present a slight volumetric contraction first and then dilation. The degree of volumetric dilation grows with the hydrate saturation. These are consistent with the reported mechanical characteristics of HBS samples (Waite et al., 2009; Jung et al., 2012).

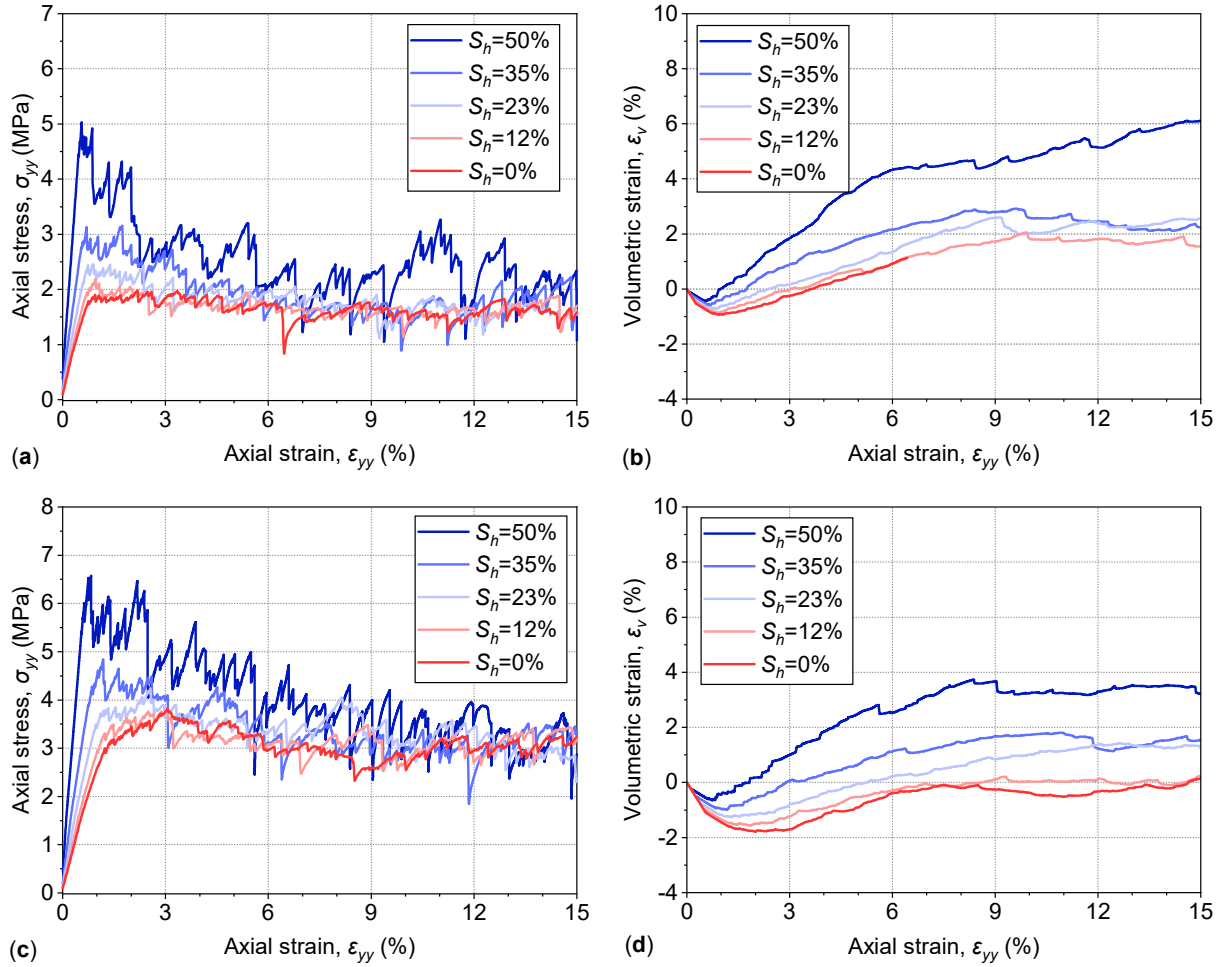


Figure 6: RVE responses in biaxial compression test: (a) $\Phi = 1.0$, (b) $\Phi = 0.4$, and (c) $\Phi = 0.2$.

Figure 7 further compares key strength parameters of the RVE samples and the experimental data (Soga et al., 2006; Masui et al., 2005, 2006; Waite et al., 2009). The Young's modulus E_{50} is calculated at 50% of the stress at failure. The cohesion and friction angle are determined based on the Mohr circles. The dilation angle, ψ , is determined by (Waite et al., 2009),

$$\frac{\Delta \varepsilon_v}{\Delta \varepsilon_{yy}} = \frac{-2 \sin \psi}{1 - \sin \psi}, \quad (42)$$

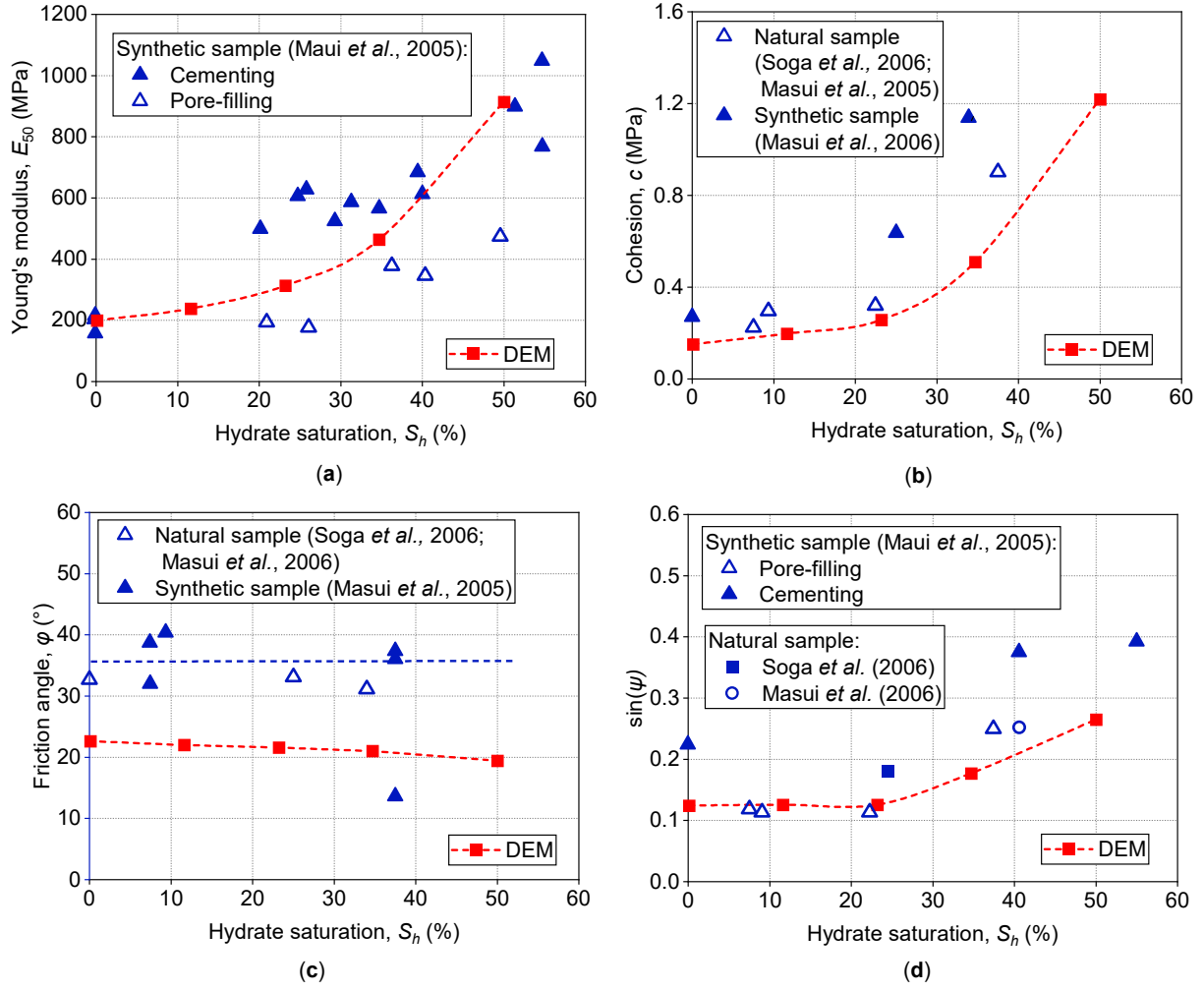


Figure 7: (a) Young's modulus E_{50} , (b) cohesion c , (c) friction angle φ , and (d) dilation angle $\sin \psi$ versus hydrate saturation obtained from RVE biaxial tests. The red square markers with dashed lines represent the DEM-based RVE results, while the blue markers show the laboratory-tested data on either synthetic or natural HBS samples (Masui *et al.*, 2005, 2006; Soga *et al.*, 2006; Waite *et al.*, 2009).

where $\Delta \varepsilon_v$ is the change in volumetric strain and $\Delta \varepsilon_{yy}$ is the change in axial strain. Figure 7(a) and (b) show that the Young's modulus ranges from 200 MPa to 1000 MPa, while the cohesion varies between 100 kPa and 1200 kPa. These values are closely aligned with those reported for laboratory-formed cementing hydrate samples (Masui *et al.*, 2005).

Furthermore, it can be observed that the variations in stiffness, cohesion, and dilation angle are less pronounced under low hydrate saturation conditions, which is consistent with laboratory tests. However, the friction angle, as shown in Figure 7(c), exhibits no significant dependence on hydrate saturation, aligning with experimental findings as well. However, the magnitude shows some discrepancy, which is about 20° for the DEM RVE. This is probably because the rolling resistance is not considered in the DEM model. Nonetheless, this value remains within the physically reasonable range for HBS samples. Figure 7(d) indicates that the dilation angle tends to increase with hydrate saturation, a

trend that becomes more pronounced at higher saturation levels. The results of the RVE biaxial tests demonstrate that the DEM RVE with saturation-dependent bond properties successfully captures the key mechanical characteristics of HBS samples under varying saturation conditions.

With the RVE prepared, two classical benchmarks, including the biaxial compression test and the rigid indenter penetration test, are conducted to evaluate the efficacy of the proposed multiscale framework in capturing coupled THMC behaviors of HBS in meso- and large-scale problems. The effect of confining stress and hydrate saturation will be further investigated.

4. Numerical example I: Undrained biaxial compression test

4.1. Model setups

The multiscale framework is first applied to simulate undrained biaxial compression tests on HBS, with a particular focus on shear localization (Liang and Zhao, 2019). Figure 8 illustrates the model setup for the test, in which an HBS sample with dimensions of 2 m by 4 m is considered. Both lateral boundaries of the sample are subjected to a constant confining pressure σ_c . Rough, rigid plates are attached to the top and bottom boundaries, with their movements constrained in the x directions. The top plate moves monotonically downward with a constant vertical velocity $v_y = 0.1$ m/s, while the bottom plate is fully fixed. The loading velocity of the top plate is increased linearly from zero to the prescribed magnitude in the first 0.1 s to reduce stress oscillation. Quadrilateral cells with a cell size of 0.1 m and four material points per cell are employed for the background mesh. The macroscopic material parameters for the MPM solver are given in Table 4. A series of cases with varying confining stress (*i.e.*, 0.8, 1.6, and 3.2 MPa) and hydrate saturation (*i.e.*, 50%, 35%, and 23%) are simulated. The case with hydrate saturation $S_h = 50\%$ and confining stress $\sigma_c = 0.8$ MPa (denoted as 'BCT-50-0.8') serves as the reference case for comparative analysis. Plastic heat generation is considered in all cases, except for the last case denoted by 'BCT-50-0.8-NPH'. A complete list of the test cases is provided in Table 5.

4.2. Global and local THMC responses

This section takes the case of 'BCT-50-0.8' as an example for discussion while leaving the comparison with other cases to the subsequent subsections.

4.2.1. Stress-strain responses

Global stress-strain responses. The global stress-strain relationship for the 'BCT-50-0.8' case is presented in Figure 9. The vertical stress σ_{yy} and the shear stress σ_{yx} are computed from the vertical and horizontal reaction forces acting on the loading plate, normalized by the plate area. As can be seen, σ_{yy} reaches its first peak at $\varepsilon_{yy} \approx 0.5\%$,

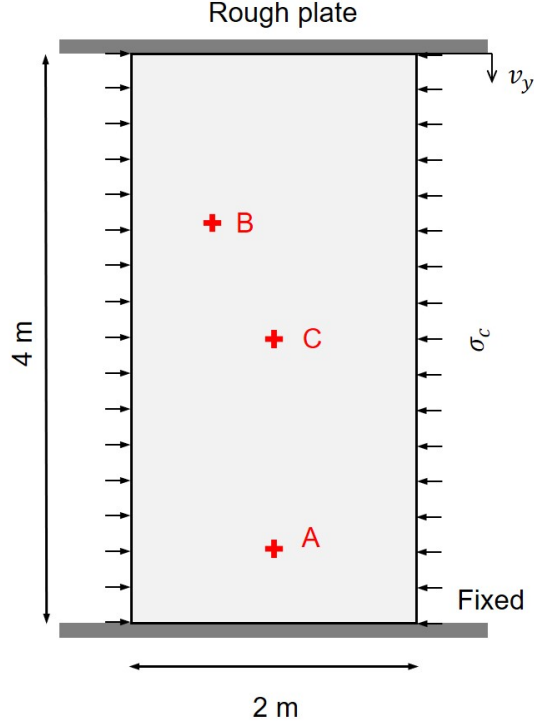


Figure 8: Model setup of biaxial compression test of HBS.

Table 4: Material parameters adopted for MPM solver.

Parameters	Solid, s	Hydrate, h	Water, w	Gas, g
Initial density, ρ_π : kg/m ³	2,650	900	1,000	-
Specific heat capacity, c_π : J/(kg·°C)	800	2,010	4,200	2,100
Thermal conductivity, κ_π : W/(m·°C)	0.836	0.393	0.556	0.0335
Viscosity, μ_π : Pa·s	-	-	1×10^{-3}	7×10^{-6}
Molar mass, M_π : kg/mol	-	0.124	0.018	0.016
Gas constant, R	-	-	-	8.314
Kinetic hydrate dissociation rate, R_r	$K_0 = 3.6 \times 10^{-5}$ mol/(m ² · Pa · s),			
Effective saturation, S_e	$p_0 = 1 \times 10^4$ Pa, $m = 0.5$, $S_{wr} = 0.2$, $S_{gr} = 0.3$			
Heat source, $\Delta H = C_0 + C_1 T$: J/kg	$C_0 = 446,120$ J/kg, $C_1 = 132.638$ J/(kg·K)			
Absolute permeability k_a : m ²	$k_0 = 1 \times 10^{-14}$ m ² , $m_h = 10$			
Relative permeability, $k_{r\pi}$	$n_w = 4$, $n_g = 2$			

Note: The parameters adopted in this study are based on Refs. [Chen et al. \(2016\)](#), [Hardwick and Mathias \(2018\)](#), [Sun et al. \(2018\)](#), and [Ye et al. \(2022\)](#).

followed by slight fluctuations. Afterward, it gradually decreases until reaching a relatively stable state with $\sigma_{yy} \approx 3$ MPa. In contrast, the magnitude of σ_{yx} , ranging between 0.1 MPa and -0.2 MPa, is much smaller than that of σ_{yy} . Despite significant fluctuations

Table 5: A summary of test conditions of the biaxial compression tests.

Test ID	S_h [%]	S_w [%]	S_g [%]	σ_c [MPa]	Plastic heat
BCT-50-0.8	50	40	10	0.8	Yes
BCT-50-1.6	50	40	10	1.6	Yes
BCT-50-3.2	50	40	10	3.2	Yes
BCT-35-0.8	35	52	13	0.8	Yes
BCT-23-0.8	23	61.6	15.4	0.8	Yes
BCT-50-0.8-NPH	50	40	10	0.8	No

Note: The test ID, for example, ‘BCT-50-1.6’, indicates a biaxial compression test (BCT) with hydrate saturation $S_h = 50\%$ and confining stress $\sigma_c = 1.6$ MPa. In addition, ‘NPH’ in the last test indicates that no plastic heat was considered.

being observed in σ_{yx} , a distinct peak is observed at $\varepsilon_{yy} = 5\%$, after which σ_{yx} gradually decreases to nearly zero. The fluctuations in σ_{yx} are closely associated with the formation and development of shear bands within the soil sample.

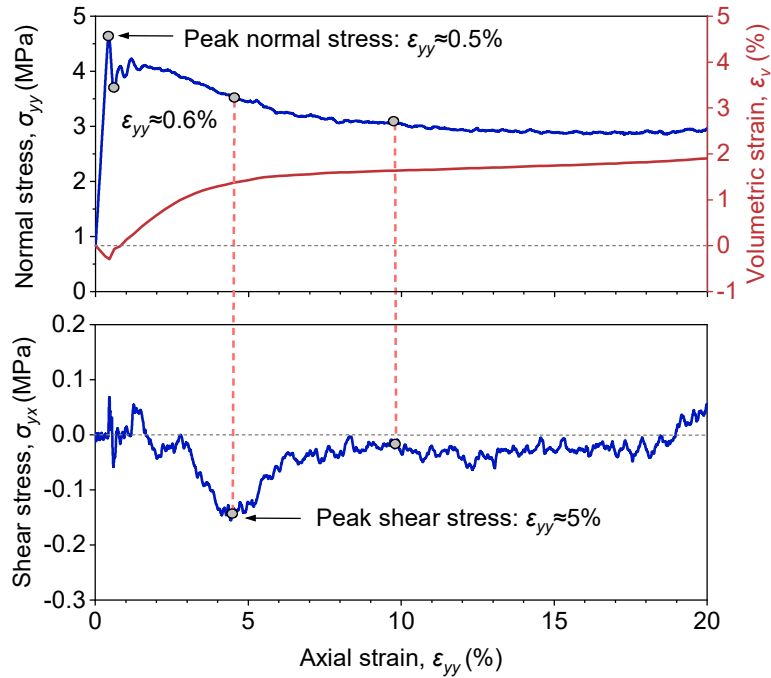


Figure 9: Global stress-strain relation for case ‘BCT-50-0.8’ in biaxial compression test.

Figure 10(a) illustrates the distributions of equivalent deviatoric strain (ε_d) at four critical loading states: a) $\varepsilon_{yy} = 0.6\%$ - the state immediately after the peak normal stress, b) $\varepsilon_{yy} = 5\%$ - the peak shear stress state, c) $\varepsilon_{yy} = 10\%$ - the critical state, and d) $\varepsilon_{yy} = 20\%$ - the final state. At $\varepsilon_{yy} = 0.6\%$, two X-shaped shear bands are initiated, indicating the beginning of the plastic yielding in response to the sharp decrease in normal stress.

The generation of two, rather than one, X-shaped shear bands is potentially due to the constraint of the top and bottom boundary plates. By $\varepsilon_{yy} = 5\%$, the two X-shaped bands merge into one, with the leftward-tilting shear band more dominant. Meanwhile, the resisting shear stress due to constraint by the rough top plate points to the left (negative in value), as observed in Figure 9. The constraint of the rough top plate restricts the further deformation of the sample to the right side and enhances the development of the rightward-tilting shear band. At $\varepsilon_{yy} = 10\%$, both normal and shear stresses gradually drop, while both shear bands continue to develop. When the loading approaches the final state at about $\varepsilon_{yy} = 20\%$, the cross-shape shear bands develop in full.

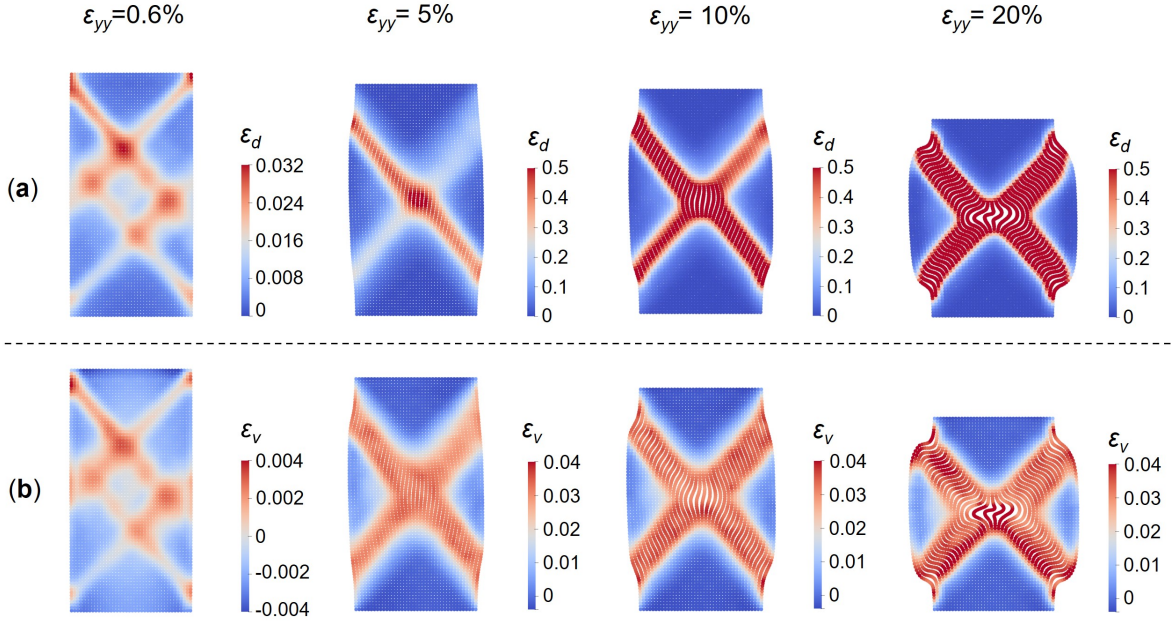


Figure 10: Distributions of (a) equivalent deviatoric strain ε_d and (b) volumetric strain ε_v at the axial strain of 0.6%, 5%, 10%, and 20%.

Figure 10(b) further present the distributions of volumetric strain ε_v . The shear deformation results in volumetric dilation within the soil sample, with an incremental volumetric strain of approximately 4% observed at the final state. Consequently, the porosity increases from its initial value of 0.4 to over 0.42 within the shear band. The cross-shaped shear band divides the sample into four distinct regions: the top and bottom pentagonal zones and the left and right triangular zones. Slight volumetric contraction is observed in the pentagonal regions due to compression. The global volumetric strain of the sample is further plotted in Figure 9. The total volume of the sample at any given time is calculated by summing the volumes of all material points. Initially, the sample undergoes volumetric contraction, reaching its maximum contraction at the peak normal strain. Beyond this point, continuous volumetric dilation is observed. By the final state, the global volumetric change of the sample approaches 2%. Shear-induced

dilation is a characteristic mechanical behavior of hydrate-bearing soils, and it has been effectively captured by the proposed multiscale method. The dilation within the shear band is primarily caused by the particle rearrangements at the grain scale to accommodate shear deformation. The bonding aggregates the soil grains and thus creates larger-sized grains with more kinematic constraints, which further enhances the dilation, as can be observed in Figure 11 where large voids are generated in the RVE due to aggregate-scale dilation. This behavior is important for accurately modeling the mechanical response of HBS, which is inherently considered in the presented multiscale modeling approach.

Local stress-strain responses. Figure 12 presents the local stress-strain relationships at three representative material points.

- **Point A.** Located in the bottom pentagonal region outside the shear band, Point A exhibits a linear increase in shear stress (q) to a peak value of approximately 1.75 MPa at a small deviatoric strain (ε_d) of 0.5%, followed by a gradual decrease to around 0.75 MPa. The effective stress path in Figure 12(c) confirms that Point A undergoes an almost perfect loading-unloading process. Being outside the shear band, the volumetric strain at this point is minimal and dominated by contraction.
- **Point B.** Located inside the rightward-tilting shear band in the upper right region of the sample, Point B shows a rapid increase in stress to a peak at $\varepsilon_d = 0.5\%$, followed by a decrease as the shear band continues to develop. Figure 13 shows that the RVE at this point undergoes severe deformation and bond breakage. The volumetric strain at Point B initially exhibits slight contraction, then transitions to dilation, and stabilizes at approximately 3%.
- **Point C.** Positioned at the center of the X-shaped shear band, Point C is influenced by the development of both intersecting shear bands. As a result, Point C undergoes

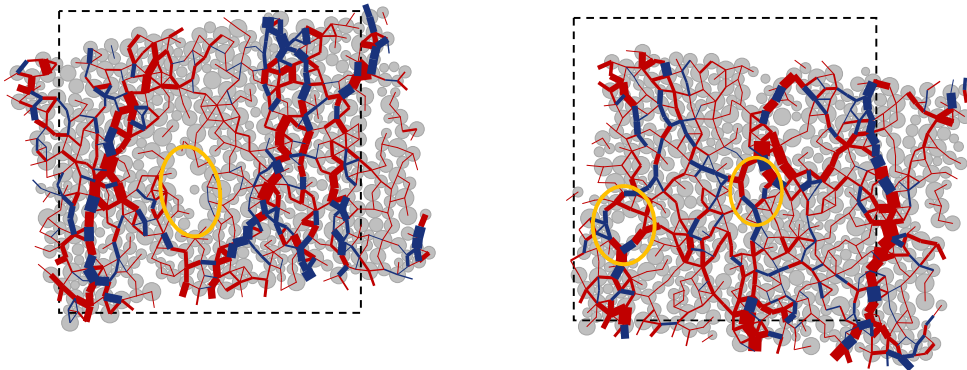


Figure 11: Two typical RVEs with obviously enlarged voids observed after shearing, as highlighted by the yellow ellipses. These large void spaces are generated due to aggregate-scale deformation. The red lines represent active bond contacts, while the black lines indicate either broken bonds or pure frictional contacts. The dashed rectangular frame indicates the initial shape of the RVE.

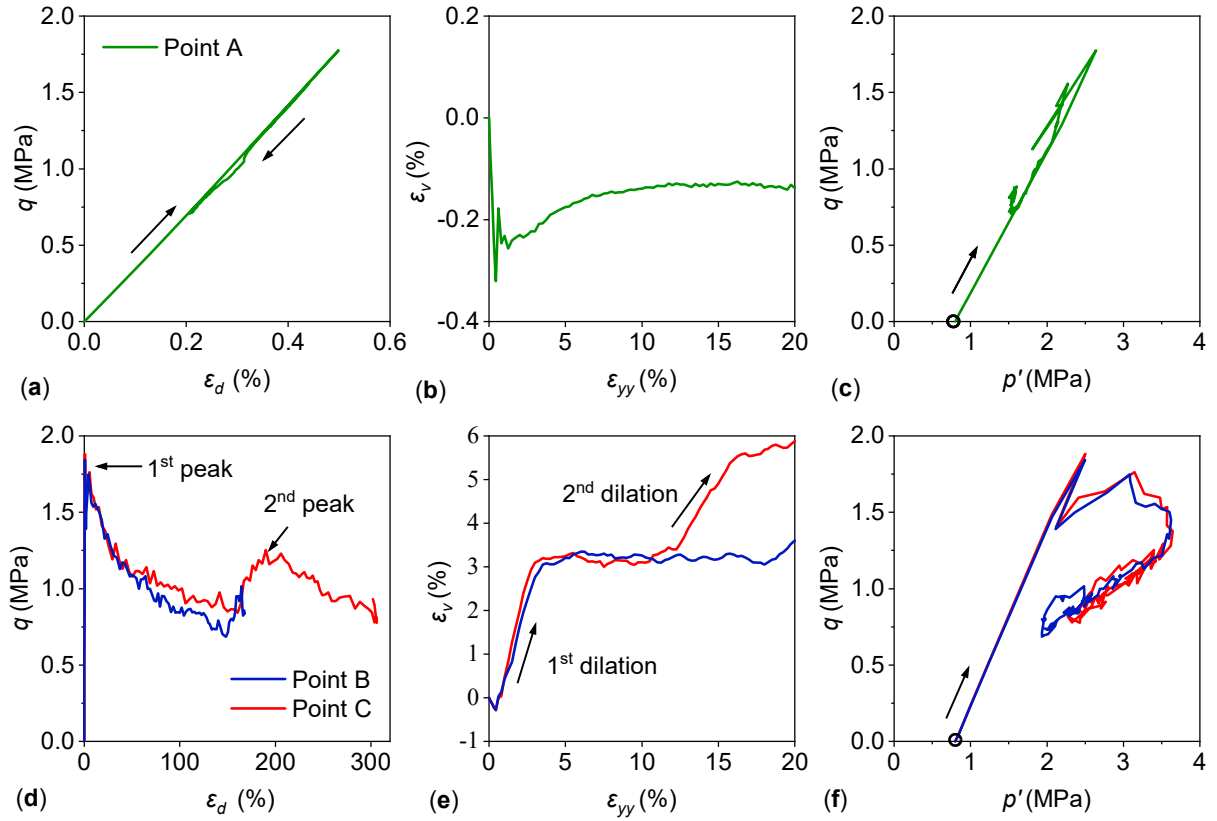


Figure 12: Local stress-strain responses for selected material points in biaxial compression test: (a-c) Point A, (d-f) Points B and C. The initial coordinates of Points A, B, and C are (0 m, 0.5 m), (−0.5 m, 2.7 m), and (0 m, 2 m), respectively. In (a), the arrow indicates that the material at Point A experiences a linear loading–unloading response. In (d) and (e), the arrows denote the presence of dual peaks in the q – ε_d curve and the associated two-stage dilation behavior in the ε_v – ε_{yy} curve at Point C. This behavior is attributed to the asynchronous initiation and evolution of the leftward- and rightward-tilting shear bands. In (c) and (f), the arrows indicate the direction of stress-path evolution.

a secondary increase in both shear stress and volumetric strain, as clearly depicted in Figure 12(d) and 12(e).

Additionally, the effective stress paths for Points B and C indicate that the effective mean stress continues to rise as the shear stress reaches its peak, before both stresses eventually decline. This behavior is attributed to the development of negative excess pore pressure within the shear band, which will be discussed in detail in the following section. In addition to the stress-strain and volumetric responses, other important mesoscale properties, such as the rotation and fabric anisotropy of the RVE during shear deformation, can also be analyzed using this framework. However, these aspects are beyond the scope of this discussion. Interested readers may refer to Liang and Zhao (2019) for further details.

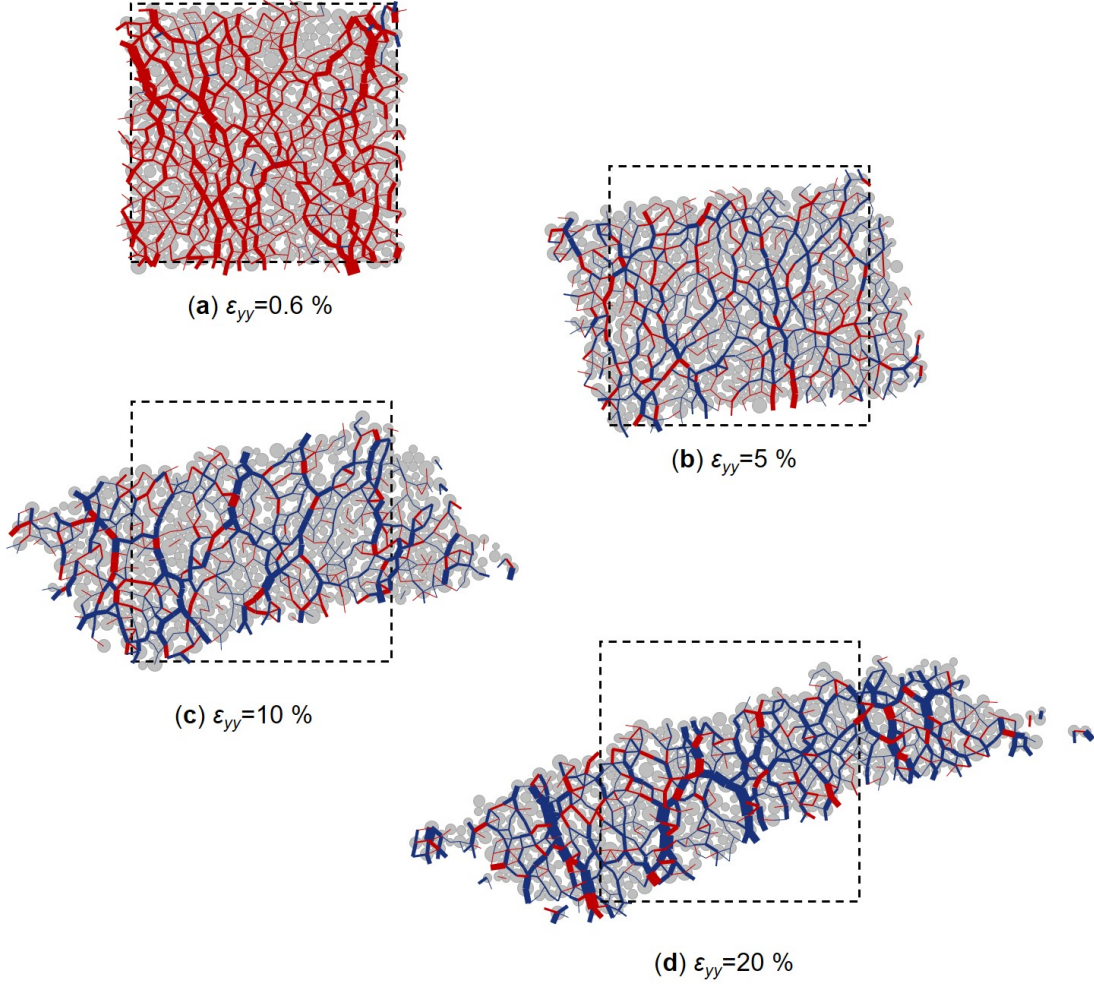


Figure 13: Deformed RVE and force chains at Point B. The red and black lines represent active bond contacts and broken bonds (or pure frictional contacts), respectively.

4.2.2. Pore pressure characteristics

The dilative deformation associated with shear band formation can lead to a reduction in pore pressure within the shear band region. Figure 14 illustrates the spatial distributions of excess pore gas pressure (p_g) and excess pore water pressure (p_w) at various loading stages. At $\varepsilon_{yy} = 0.6\%$, negative excess pressures (p_g and p_w) are observed within the shear bands as a result of volumetric dilation, while regions outside the shear bands exhibit positive excess pore pressures due to volumetric contraction. As the loading progresses to $\varepsilon_{yy} = 5\%$, the reduction in pore gas and liquid pressures becomes more pronounced, with a maximum negative value of approximately -1.6 MPa. This substantial pressure drop underscores the significant effect of localized deformation on pore pressure redistribution. With continued loading, the magnitude of the pore pressure within the shear bands gradually increases. Similar phenomena of negative excess pore pressure induced by shear dilatancy have been observed in laboratory triaxial tests on hydrate-bearing sediments, as reported by Yan et al. (2023). The consistency between these experimental observations

and the numerical results highlights the critical role of dilatancy in driving pore pressure evolution within shear bands under undrained or low-permeability conditions.

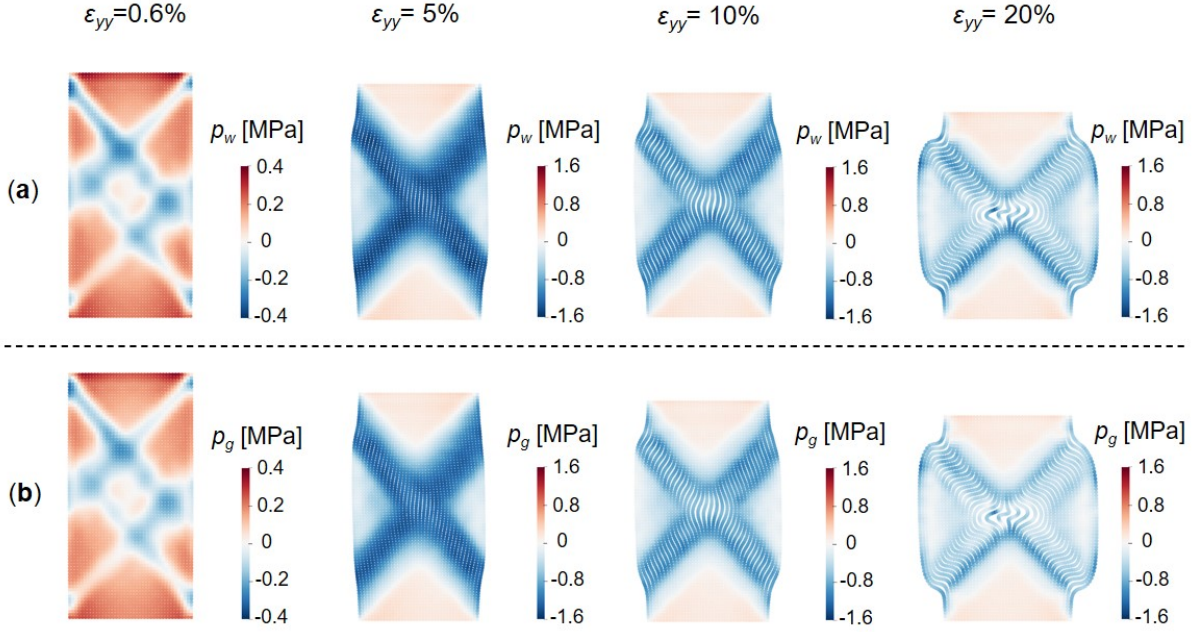


Figure 14: Distributions of (a) excess pore water pressure p_w and (b) excess pore gas pressure p_g at the axial strain of 0.6%, 5%, 10%, and 20%. Note that p_w and p_g all denote excess pore pressure hereafter.

Figure 15(a) and d show the evolution of p_g (solid lines) and p_w (dashed lines) at Points A, B, and C. At Point A, the excess pore pressure initially increases and then decreases, but remains positive (positive value means compression), consistent with the volumetric contraction trend observed at this point. At Points B and C, the excess pore pressures similarly show an initial rise to a magnitude comparable to that of Point A but subsequently drop dramatically into negative values due to shear dilation. When ε_{yy} reaches approximately 3%, both p_g and p_w reach their lowest values for Points B and C. After this point, although the volumetric strain becomes constant (as shown in Figure 12e), the pressures gradually increase due to gas dissolution. Notably, at Point C, the pressure exhibits a significant second drop followed by a secondary peak. This behavior corresponds to the second dilation stage, which is dominated by the development of the rightward-inclined shear band. The negative excess pore pressures generated in the shear bands enhance the effective mean stress (p'), as shown in Figure 12f. Such phenomena cannot be captured in dry granular samples, as reported by Liang and Zhao (2019), underscoring the importance of performing coupled hydromechanical simulations for hydrate-bearing soils.

4.2.3. Hydrate/gas saturation changes

With the pore pressure within the shear band decreasing by up to 1.6 MPa (from an initial pressure of 3.75 MPa), the hydrate phase equilibrium shifts outside its stability

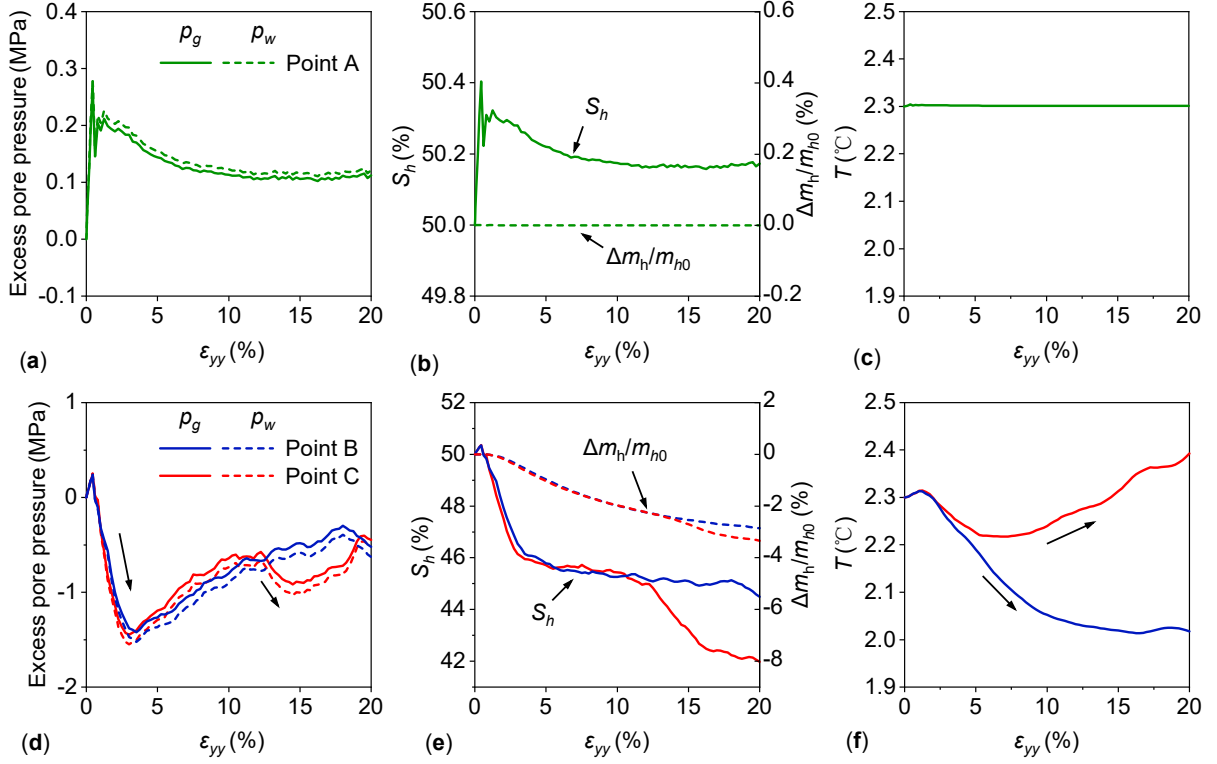


Figure 15: Local responses of excess pore water/gas pressure (p_w and p_g), hydrate saturation (S_h), and temperature (T) at (a-c) Point A and (d-f) Points B and C. In (d), the arrows highlight the two decreasing stages in excess pore pressure at Point C. In (f), the arrows highlight the opposite temperature evolution path with and without consideration of shear heating.

zone, resulting in hydrate dissociation and subsequent gas production. Figure 16 shows the spatial distribution of hydrate saturation S_h and gas saturation S_g . The results indicate that the pore pressure drop at $\varepsilon_{yy} = 0.6\%$ leads to immediate reduction of hydrate saturation in the shear band, possibly caused by hydrate dissociation. As shear band development progresses, the degree of hydrate saturation inside the band continues to decline. Notably, a slight increase in hydrate saturation is observed outside the shear band. This phenomenon arises because the void volume (V_v) decreases in these regions, while the hydrate volume (V_h) remains unchanged (no hydrate formation considered in the simulation). Consequently, since the hydrate saturation $S_h = V_h/V_v$, the reduction in V_v results in a relative increase in S_h .

There are two primary mechanisms that govern the evolution of hydrate saturation: (1) hydrate dissociation/formation and (2) porosity change due to skeleton deformation, as clearly expressed by the hydrate phase mass balance equation:

$$\phi \frac{D^s S_h}{Dt} = \underbrace{\frac{\dot{m}_h}{\rho_h}}_{\text{hydrate reaction}} + \underbrace{[(1-\phi)S_h\beta_s + \phi S_h\beta_h]}_{\text{volumetric change}} \frac{D^s T}{Dt} - S_h \nabla \cdot \mathbf{v}_s. \quad (43)$$

Therefore, the reduction of hydrate saturation in the shear band is caused not only by

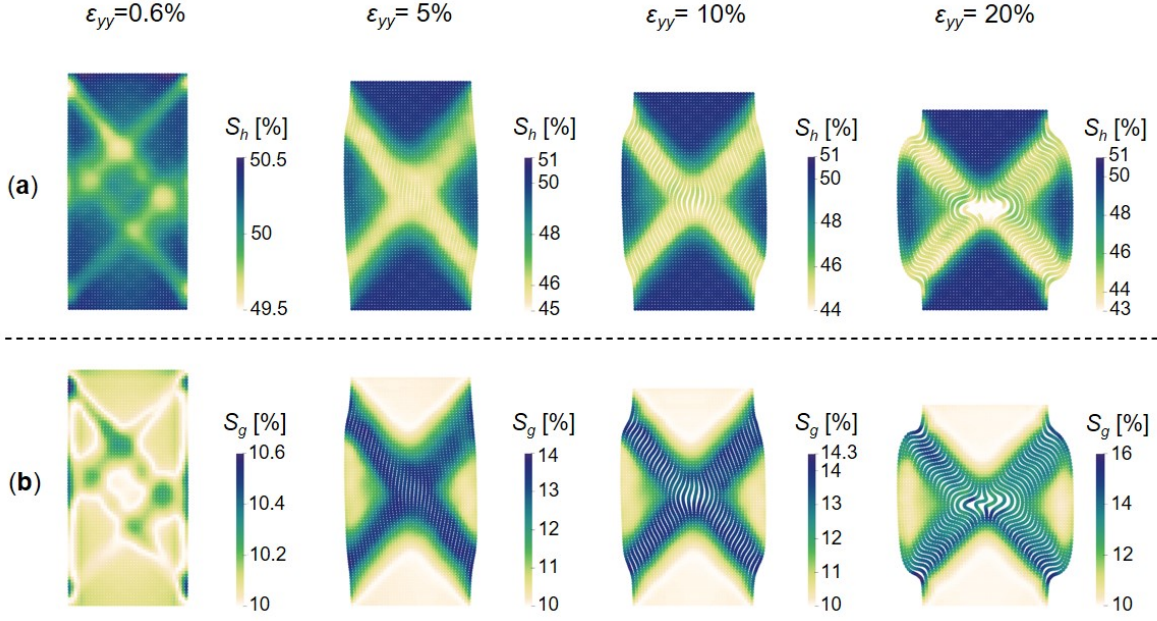


Figure 16: Distributions of (a) hydrate saturation S_h and (b) gas saturation S_g at the axial strain of 0.6%, 5%, 10%, and 20%. The water saturation S_w can be obtained by $1 - S_h - S_g$.

hydrate dissociation but also by volumetric dilation. It is more apparent to characterize the degree of hydrate dissociation by the ratio of hydrate mass (or volume) change: $\Delta m_h/m_{h0}$, in which Δm_h is the hydrate mass change and m_{h0} is the initial hydrate mass. It is easy to link the ratio with porosity ϕ , volumetric strain ε_v , and hydrate saturation as follows:

$$\frac{\Delta m_h}{m_{h0}} \approx \frac{\Delta V_h}{V_{h0}} = \frac{V_h}{V_{h0}} - 1 = \frac{V_h}{V_v} \frac{V_v}{V} \frac{V}{V_0} \frac{V_0}{V_{v0}} \frac{V_{v0}}{V_{h0}} - 1 = \frac{\phi S_h (1 + \varepsilon_v)}{\phi_0 S_{h0}} - 1, \quad (44)$$

where ϕ_0 , S_{h0} , V_0 , V_{v0} , V_{h0} are the initial porosity, initial hydrate saturation, initial volume, initial void volume, and initial hydrate volume, respectively.

Figure 12(b) and e plot the evolution of hydrate saturation and the hydrate mass change ratio ($\Delta m_h/m_{h0}$) at three selected points. As can be seen, the hydrate saturation at Point A is slightly increased compared to the initial state (increases first and then decreases to a positive constant value), while the mass of hydrate remains unchanged, indicating that the saturation change is solely a result of porosity change. At Points B and C, S_h undergoes significant declines and sharp changes in decreasing rate. However, the evolution of the hydrate mass change ratio shows that the dissociation of hydrate progresses at a relatively constant rate (with slight variations in response to pressure and temperature changes). This suggests that one should reconsider whether it is accurate enough to use hydrate saturation as the only state variable to characterize the effect of hydrate dissociation on HBS property changes.

4.2.4. Temperature evolutions

Hydrate dissociation is an endothermic process, and thus, its occurrence within the shear bands is expected to be accompanied by a temperature decrease. On the other hand, shear-induced irreversible deformation generates plastic work dissipation, resulting in a temperature rise within the shear band (Vishnu et al., 2022). These two competing effects jointly govern the evolution of the temperature field. Figure 17(a) shows the temperature distribution at different loading stages. At $\varepsilon_{yy} = 0.6\%$, when the shear band is just forming, a slight temperature increase is observed in the shear band region. As hydrate dissociation intensifies, significant temperature reductions can be observed. Apparently, the initial temperature rise is caused by plastic heat generation, and the following temperature drop is caused by dissociation-related heat absorption. Notably, a localized temperature increase is observed along the central axis of the shear band, where plastic deformation (and plastic heat generation) is more pronounced. At the final state ($\varepsilon_{yy} = 20\%$), a considerable temperature rise is observed at the center of the X-shaped shear band. The competing effect can be more clearly visualized from the temperature evolution at Points B and C, as shown in Figure 12f. The temperature at Point B continuously decreases after a minor initial increase, indicating a heat absorption-dominated process. In contrast, Point C experiences a second rise in temperature after a period of drop, showing a transition from a heat absorption-dominated process to a heat generation-dominated one.

However, if the plastic heating effect is not considered, the temperature decreases only, and more pronounced decrease magnitudes are recorded, as shown in Figure 17(b). Plastic heating, often overlooked in many HBS simulation studies, plays a crucial role in the THMC coupling behavior of an HBS system. This effect becomes particularly significant in large shear deformation scenarios, as it can accelerate hydrate dissociation and contribute to the destabilization of the sediment system.

4.2.5. Mechanism of dilation-induced hydrate dissociation

The shear dilation-induced hydrate dissociation and the associated THMC chain responses are identified through the biaxial compression test using the proposed multiscale method. The chain process and underlying mechanism are illustrated in Figure 18. As hydrate-bearing sediment is typically a dense, bonded soil, shear localization often occurs upon loading, accompanied by volumetric dilation. This shear-induced dilation generates negative excess pore pressures within the shear bands, destabilizing the hydrate-gas phase equilibrium and triggering hydrate dissociation. However, the negative pore pressure increases the effective mean stress, which acts to suppress further dilation. At the same time, the gas/water produced by hydrate dissociation raises the pore pressure, counteracting the pressure drop caused by volumetric dilation. The hydrate dissociation process absorbs heat, resulting in a decrease in temperature. However, plastic heat generation

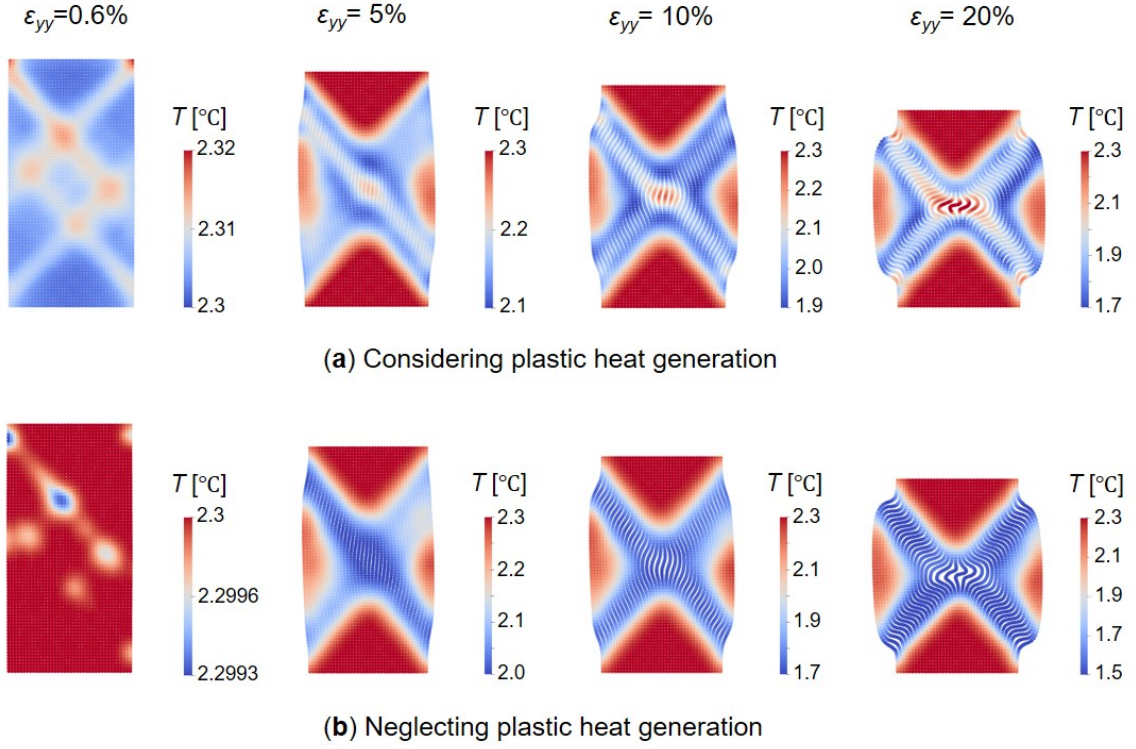


Figure 17: Distributions of temperature T (a) considering plastic generation and (b) neglecting plastic heat generation at the axial strain of 0.6%, 5%, 10%, and 20%. Note that the initial temperature is 2.3 °C.

from shear deformation delays this temperature drop, creating conditions favorable for further hydrate dissociation. In addition, the loss of hydrate leads to a reduction in soil stiffness and strength, which promotes further shear deformation. As a result, several competing processes collectively contribute to the mechanical deformation, hydraulic response, hydrate reaction, and heat transfer in an HBS system.

Remark 7. A key implication of shear dilation-induced hydrate dissociation is that rapid shear deformation, such as earthquake-induced plate movement in submarine hydrate-bearing sediment, can trigger fast dissociation of hydrate. Moreover, the formation of shear bands may act as effective seepage paths, facilitating methane gas leakage and further accelerating dissociation. This mechanism could be one of the triggers of submarine landslides associated with submarine earthquakes and earthquake-induced hydrate dissociation. A thorough validation of this hypothesis will be reserved for future work.

4.3. Effects of hydrate saturation and confining stress

Having established the chain of THMC mechanisms in the previous section, we now systematically investigate how these processes are influenced by two key factors: initial hydrate saturation and confining stress. It is expected that samples with low hydrate saturation and high confining stress conditions present less dilatancy and less hydrate

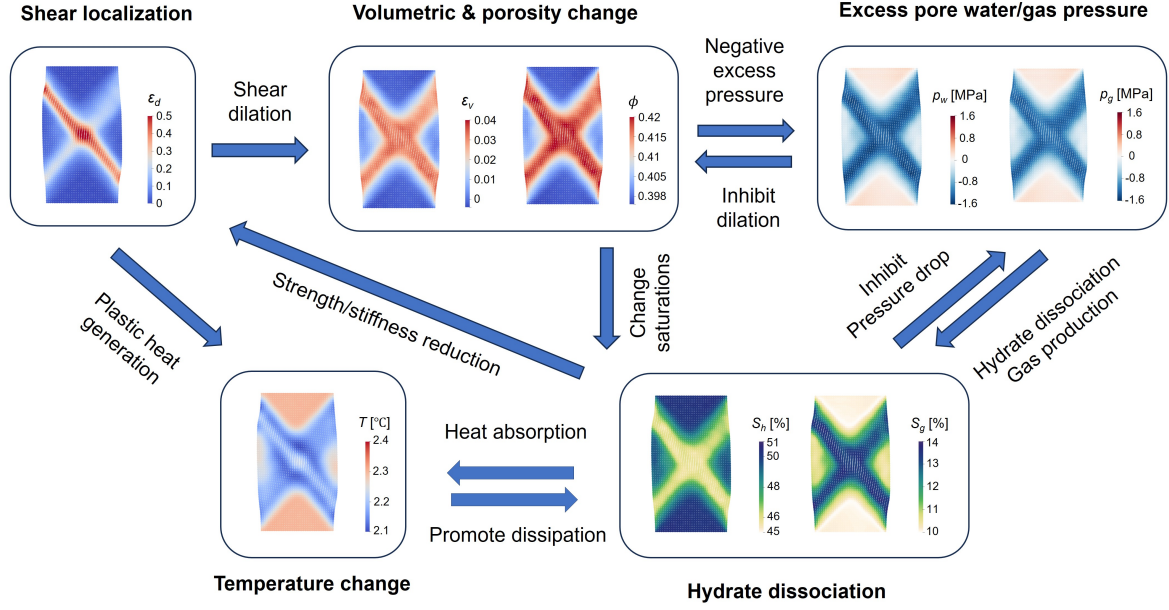


Figure 18: Mechanisms of shear dilation-induced hydrate dissociation.

dissociation. This section investigates in detail these effects on the THMC responses in HBS. Figure 19 compares the global stress-strain relations, Figure 20 compares the distribution of ε_d , ε_v , p (*i.e.*, excess pore pressure), and S_h at the axial strain of 5%, and Figure 21 and Figure 22 compare the local responses at the central Point C.

4.3.1. Effect of initial hydrate saturation

Three samples, respectively with initial hydrate saturation of 23%, 35%, and 50%, are tested under the confining stress of 0.8 MPa. The simulation results for $S_h = 23\%$ and $S_h = 35\%$ cases exhibit similar trends to the $S_h = 50\%$ case, such as the volumetric dilation, negative excess pore pressure, and the dual peak in stress and excess pore pressure. However, the magnitude of primary fields shows evident divergences, indicating the critical influence of hydrate saturation on the THMC behavior in the sediment. The key findings are summarized as follows:

(1) **Peak strength and dilative behaviors of HBS.** As depicted in the global stress-strain relations (Figure 19(a) and b), the peak normal stress increases proportionally with S_h , confirming that higher hydrate saturation enhances shear strength. The $S_h = 50\%$ sample exhibits pronounced strain softening post-peak, whereas the $S_h = 23\%$ sample shows negligible softening or hardening (Figure 19(a)). This divergence arises because hydrates primarily contribute to sediment strength through cohesive bonding rather than frictional resistance, as evidenced by the convergence of residual stresses at large strains across all cases. Global volumetric strain analysis (Figure 19(b)) further reveals that low S_h samples (*e.g.*, 23%) display limited dilation due to weaker hydrate-cemented structures.

(2) **Shear localization dynamics.** Shear band development is highly sensitive to

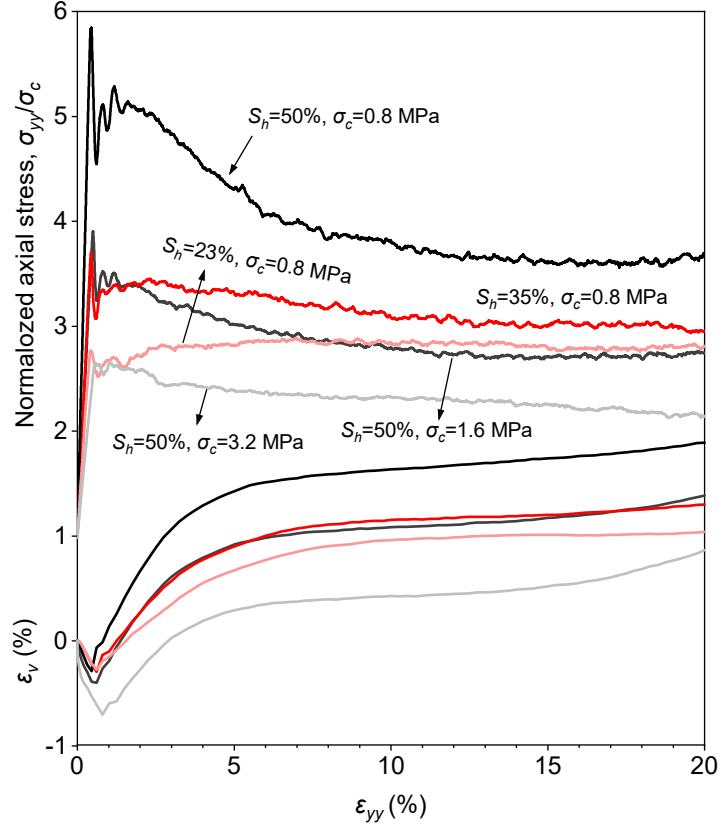


Figure 19: Comparison of global stress-strain responses for cases with varied initial situations and confining stress. Note that the axial stress σ_{yy} is normalized by the confining stress σ_c .

hydrate saturation. At 5% axial strain, the $S_h = 50\%$ sample exhibits rapid shear band formation, whereas low S_h samples (23% and 35%) show delayed localization (20(a)). This phenomenon is attributed to the cohesive nature of hydrate bonds: higher S_h enhances sediment stiffness and brittleness, enabling localized failure once the cohesive strength is exceeded. In contrast, low S_h samples retain greater ductility due to weaker cementation, resulting in distributed deformation rather than discrete shear bands (Zeng et al., 2023).

(3) **Negative excess pore pressure.** High S_h samples (50%) exhibit more significant reduction in pore pressure (Figure 7.17c), driven by pronounced volumetric dilation within well-developed shear bands (Figure 20(b) and c, and Figure 21(b) and (d)). Dilation increases soil volume, reducing pore pressure and elevating effective stress (Figure 21(c)), thereby enhancing shear resistance. Conversely, low S_h samples (23%) generate minimal excess pore pressure due to restricted dilation and underdeveloped shear bands. Additionally, hydrate dissociation is less concentrated and less pronounced in low S_h samples, as evidenced by reduced ratio of hydrate mass loss and higher residual temperatures compared to the 50% case (Figure 21(e) and (f)).

In summary, hydrate saturation critically controls the transition from ductile to brittle failure, pore pressure dynamics, and strain localization patterns. These insights highlight

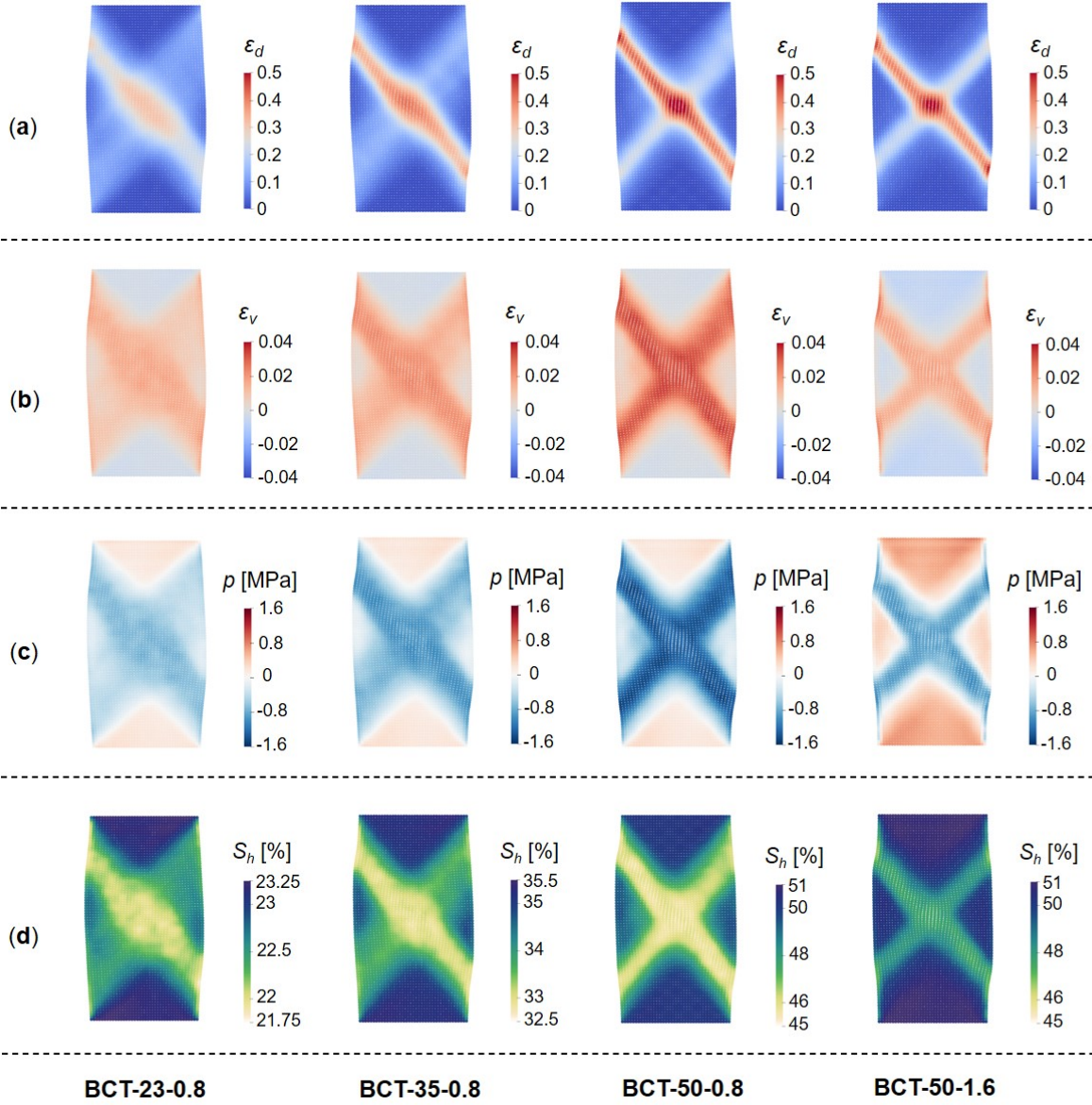


Figure 20: Comparison of (a) deviatoric strain ϵ_d , (b) volumetric strain ϵ_v , (c) excess pore pressure ϵ_p , and (d) hydrate saturation S_h for case BCT-23-0.8, BCT-35-0.8, 'BCT-50-0.8', and BCT-50-3.2 at the axial strain of 5%.

the cohesive role of hydrates in sediment strengthening and their implications for geomechanical stability in hydrate-bearing formations.

4.3.2. Effect of confining stress

Many studies have investigated the effect of confining stress on the mechanical responses of HBS, but few have discussed its effect on the coupled THMC responses. Three tests with confining stress of 0.8, 1.6, and 3.2 MPa are performed. The main findings are summarized as follows.

(1) **Global stress-strain responses and volumetric behavior.** The global stress-

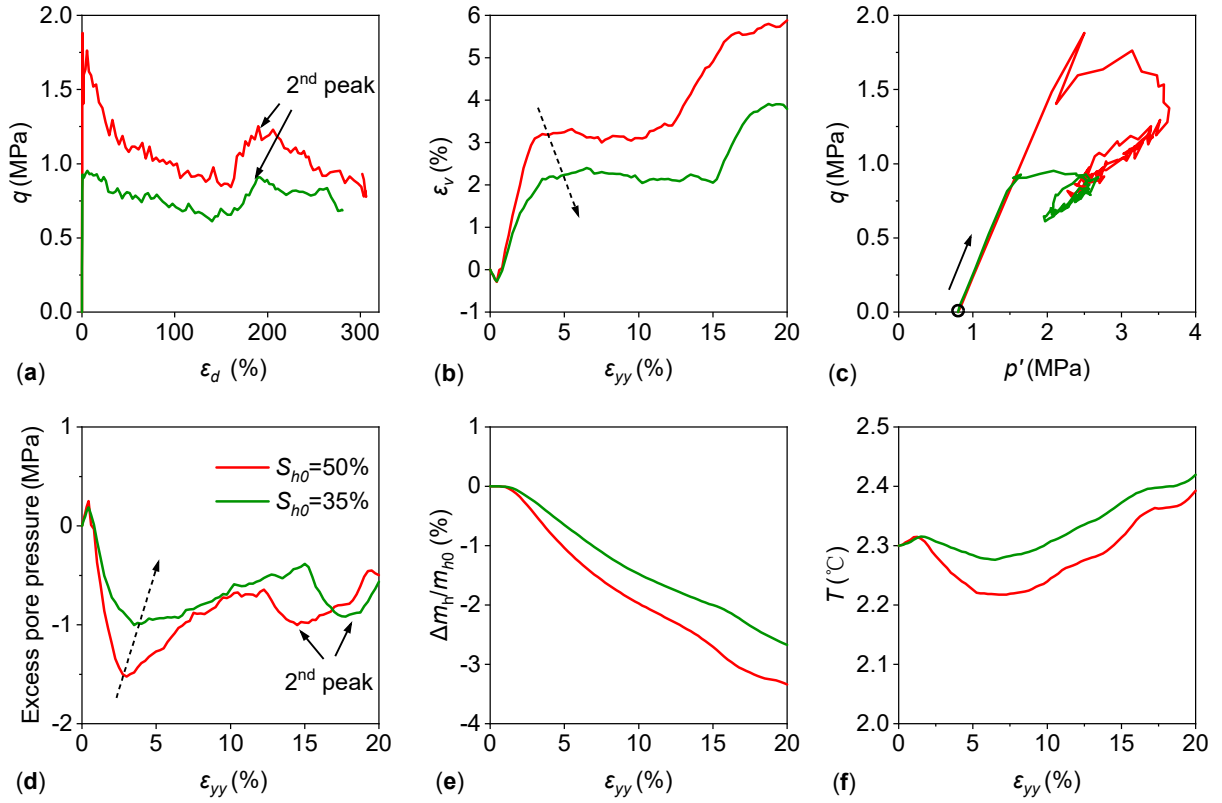


Figure 21: Comparison of local responses at the center of the sample with initial hydrate saturation of 50% and 35%: (a) shear stress q , (b) volumetric strain ε_v , (c) stress path, (d) excess pore pressure, (e) hydrate mass change, and (f) temperature T . In (b) and (e), the dashed arrows highlight that with the decrease in initial hydrate saturation, the volumetric dilation within the shear band decreases and the resulting excess pore pressure becomes less negative.

strain relations (Figure 19) demonstrate that confining stress significantly influences both peak strength and volumetric strain. At higher confining stress (3.2 MPa), the peak shear stress (q) increases compared to the 0.8 MPa case, reflecting enhanced soil strength due to greater lateral constraint. However, the axial strain at peak stress increases, suggesting a transition toward more ductile failure under elevated confinement (Miyazaki et al., 2011). Volumetric strain (ε_v) trends reveal suppressed dilation at 3.2 MPa, with the sample exhibiting nearly neutral volumetric behavior (Figure 19d). This contrasts with the 0.8 MPa case, where pronounced dilation occurs due to lower confinement, allowing particle rearrangement. The inhibition of dilation under high confining stress aligns with reduced void space compression and restricted particle movement, thereby diminishing the material's capacity to expand during shearing.

(2) **Shear localization and inclined angle reduction.** Shear band geometry evolves with confining stress, as evidenced by the decreasing inclined angle of localization under higher confinement (Figure 19(a) and b). At 0.8 MPa, shear bands form at steeper angles, consistent with dilation-driven failure typical of brittle materials. In contrast, the

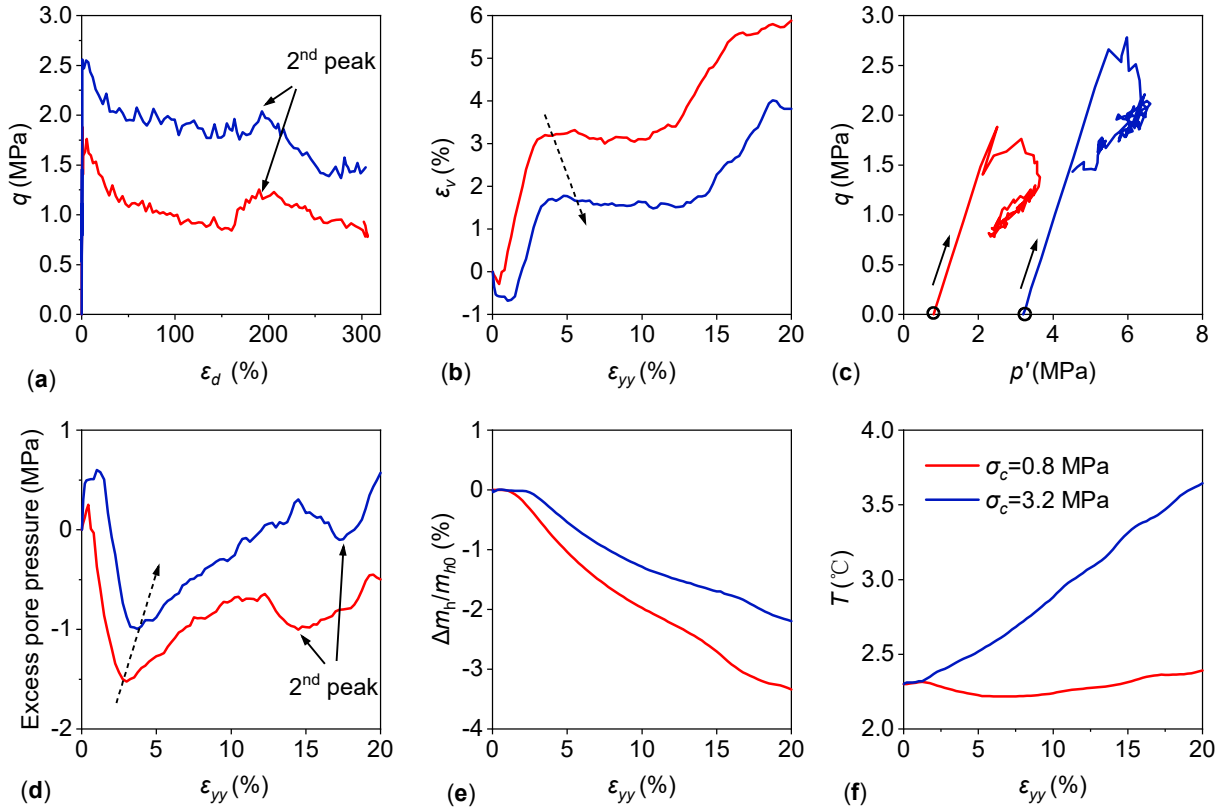


Figure 22: Comparison of local responses at the center of the sample with confining stress of 0.8 MPa and 3.2 MPa: (a) shear stress q , (b) volumetric strain ε_v , (c) stress path, (d) excess pore pressure, (e) hydrate mass change, and (f) temperature T . In (b) and (e), the dashed arrows highlight that with the increase in confined stress, the volumetric dilation and the negative excess pore pressure within the shear band becomes less significant.

3.2 MPa case shows a lower-angle shear band attributed to the suppression of dilation and a shift toward ductile deformation. Elevated confining stress increases mean effective stress, reducing the critical state stress ratio (q/p') required for failure. This lowers the theoretical shear band angle, which correlates with the internal friction angle. Additionally, restricted dilation under high confinement limits strain localization to narrower zones, promoting shear band propagation at reduced angles. The transition underscores the interplay between confinement, dilation, and failure mode in hydrate-bearing sediments.

(3) **Suppression of negative excess pore pressure.** Negative excess pore pressure diminishes with increasing confining stress (Figure 20(c) and Figure 22d), a consequence of inhibited volumetric dilation (Figure 20(b) and Figure 22(b)). At 0.8 MPa, significant dilation generates negative pore pressure by expanding the soil skeleton. Under 3.2 MPa, however, confinement restricts dilation, leading to less pronounced pore pressure reduction or even slight positive excess pressure due to contractive tendencies. This suppression of negative pore pressure diminishes the effective stress enhancement. Furthermore, reduced

hydrate dissociation (Figure 20(d) and Figure 22e) under high confinement—owing to limited volumetric strain—may stabilize pore pressure evolution, as less hydrate breakdown occurs to release water or gas. These mechanisms collectively highlight how confining stress governs pore pressure dynamics by modulating volumetric strain and hydrate stability.

In summary, elevated confining stress enhances peak strength but suppresses dilation, alters shear band geometry through ductility transitions, and mitigates negative pore pressure generation. These effects mirror, to some extent, the role of high hydrate saturation in promoting brittleness, yet they arise from distinct mechanical constraints imposed by lateral stress rather than hydrate bonding.

5. Numerical example II: Vertical penetration of a rigid indenter

The vertical penetration of a rigid indenter is simulated as a classical geomechanical test to assess the bearing capacity and failure mechanisms of a material under different stress paths and boundary conditions than those of the biaxial test. This serves to demonstrate the robustness and versatility of our framework in handling complex, engineering-scale boundary value problems involving large deformations and failure.

Again, the effects of hydrate saturation and the confining stress are explored. The model setup of the problem is depicted in Figure 23. A rectangular HBS foundation with dimensions of 18 m $\times$ 6 m is simulated. A rectangular rigid indenter with a width of 1.6

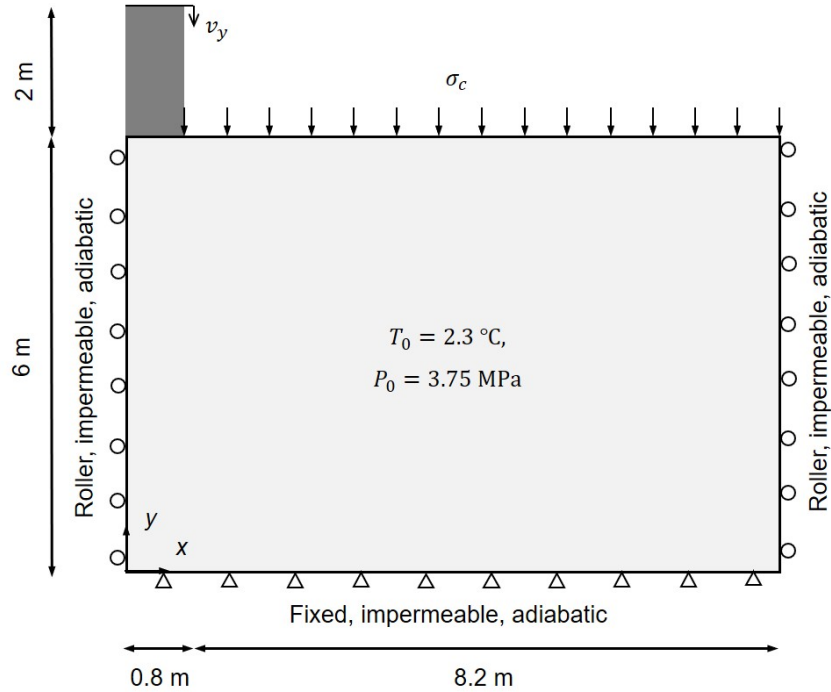


Figure 23: Model setup of indenter penetration test on HBS.

m and a height of 1.8 m is placed exactly at the center of the foundation surface. Given the symmetry of the problem geometry, only half of the domain is simulated. Note that although the RVE anisotropy may influence the global responses (Liang et al., 2021), it is minimal for this problem since a rather isotropic RVE is employed, as indicated by the nearly symmetric cross-shaped shear bands in the biaxial tests. For the half domain, the right and left are two roller boundaries, with lateral movements constrained, while the bottom is a fully fixed boundary. All three boundaries are impermeable and adiabatic. The top surface, except for the region where the indenter is placed, is free to drain and deform and is subject to a confining stress of σ_c . The rigid indenter moves monotonically downward with a vertical velocity v_y , which is increased linearly from zero to 1 m/s before being maintained at this constant value. The initial temperature and pressure conditions and the material properties are the same as the biaxial test.

Four cases are conducted:

- Case 1: $S_{h0} = 0.23$, $\sigma_c = 0.8$ MPa - Low saturation case.
- Case 2: $S_{h0} = 0.35$, $\sigma_c = 0.8$ MPa - Midium saturation case.
- Case 3: $S_{h0} = 0.5$, $\sigma_c = 0.8$ MPa - High saturation case.
- Case 4: $S_{h0} = 0.5$, $\sigma_c = 1.6$ MPa - High confining stress case.

5.1. Bearing capacity and failure patterns

The resistance force q_R on the rigid indenter versus normalized settlement (d/B) is plotted in Figure 24, in which d is the settlement, and B is the width of the indenter ($B = 1.6$ m). Figure 25 shows the distribution of deviatoric strain (ε_d) at $d/B = 0.5$, which represents a rather large penetration depth.

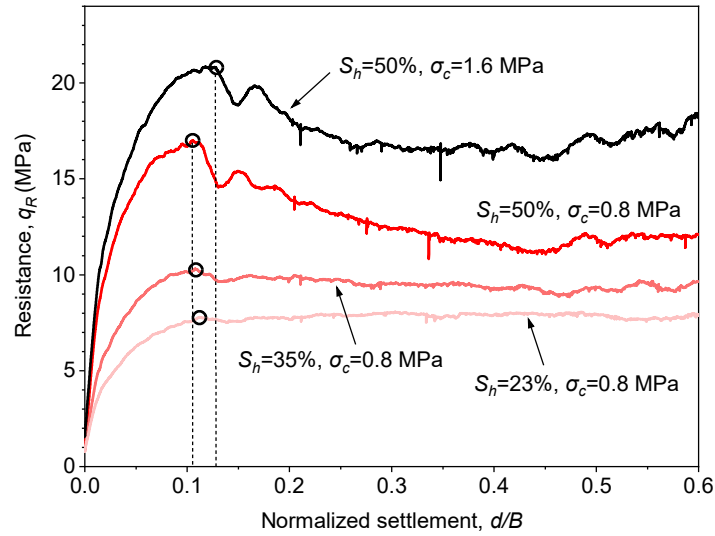


Figure 24: Normalized resistance (σ_{yy}/σ_c) versus normalized settlement (d/B) of the rigid indenter.

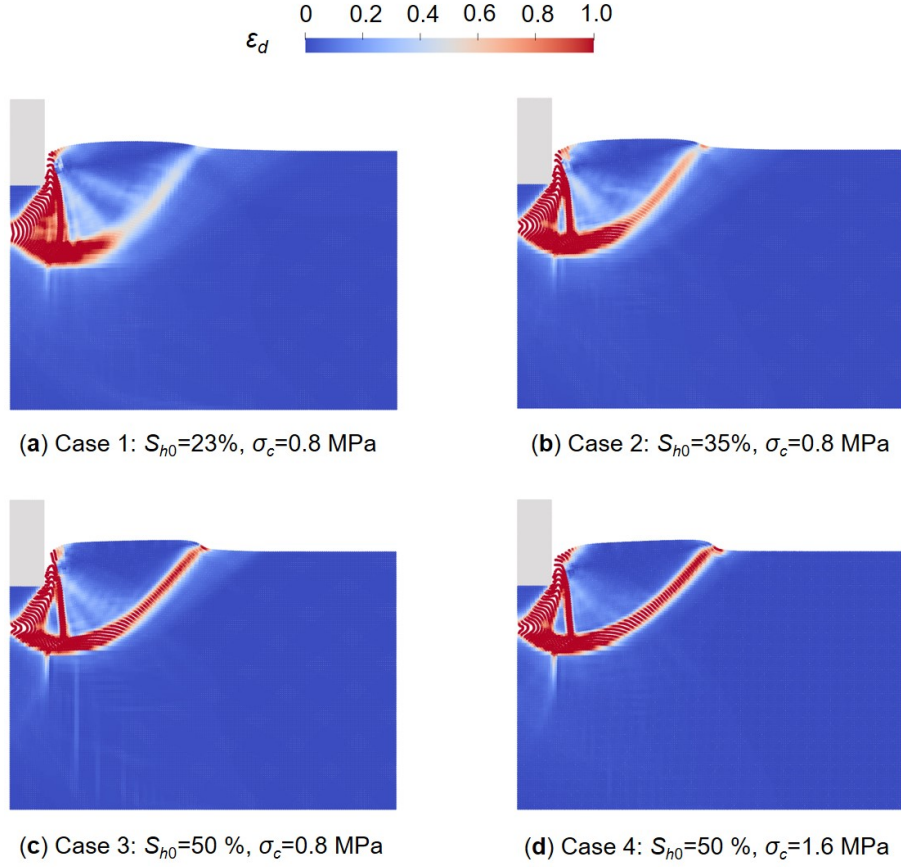


Figure 25: Simulation results of the rigid indenter penetration test: distribution of the deviatoric strain (ε_d) at $d/B = 0.5$.

Case 3 is taken as an example case for discussion before the comparative analysis with other cases. Apparently, Case 3 displays a typical general shear failure pattern, consistent with the dense and highly bonded nature of a high-saturation HBS foundation. The development of the shear bands in this case can be described as follows: (a) under applied load, stress concentrates at the edges/corners of the indenter, exceeding the soil's elastic limit, and localized yielding begins beneath the indenter edges; (b) strain localization occurs as plastic deformation becomes confined to narrow zones, forming incipient shear bands; (c) the shear bands extend diagonally toward the ground surface, connecting the active wedge (beneath indenter), the radial shear zone, and the passive wedge (near surface); (d) the passive wedge uplift occurs as the shear band reach the surface, forming visible bulges; (e) the shear bands merge into a complete failure plane, separating the rigid blocks outside bands from highly deformed material within bands. The bearing capacity q , *i.e.*, resistance on the rigid indenter, shows a sharp decrease after reaching the peak at the normalized settlement of approximately 10%. After a softening stage, the residual bearing capacity remains at a relatively constant value.

With the decrease in the initial hydrate saturation S_{h0} (Case 1 and Case 2), the

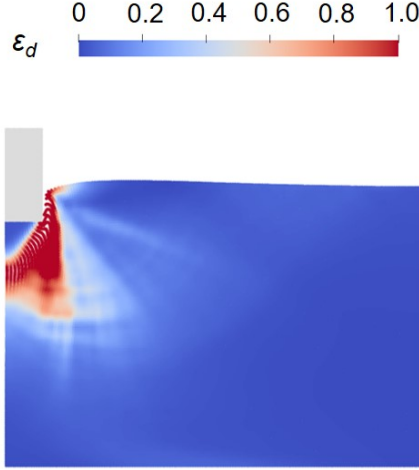


Figure 26: Simulation results of the rigid indenter penetration test: distribution of deviatoric strain (ε_d) at $d/B = 0.5$ for the case without hydrate, *e.g.*, $S_h = 0$.

failure modes tend to transition from a general shear failure pattern to a local shear failure pattern, as the soil becomes less dense and less bonded. This is evident by the following phenomena at low S_{h0} cases: (a) the strain localization comes less pronounced, with shear bands failing to fully propagate to the ground surface; (b) the passive wedge uplift diminishes significantly, resulting in only minor surface distortions rather than distinct bulges; (c) the bearing capacity curve exhibits a more gradual post-peak softening behavior, lacking the sharp drop observed in general shear failure. However, with the increase in confining stress (Case 4), the general failure pattern is enhanced, as evidenced by the increased bearing capacity and the critical settlement where the peak load is reached. If the initial hydrate saturation drops to zero, a clear punching shear failure pattern is observed, as shown in Figure 26. The successful capture of the transition of the failure mode demonstrates the efficacy of the proposed multiscale method for modeling the mechanical responses of HBS.

5.2. Pre- and post-failure THMC responses

The distributions of volumetric strain, excess pore pressure, relative hydrate mass change ($\Delta m_h/m_{h0}$), and temperature at $d/B = 0.5$ are shown in Figure 27 - Figure 30, respectively. As the initial hydrate saturation is not the same for Cases 1 to 3, a comparison of the evolution of hydrate saturation between them is not so straightforward. Alternatively, the relative hydrate mass change, which is more fair to compare, is shown instead of the hydrate saturation. At the initial loading stage, the region below the rigid indenter behaves in a compressive state with volumetric contraction and positive excess pore pressure. However, as the load increases and shear bands begin to develop, the mechanical response transitions to shear-induced dilation, triggering a chain of THMC coupling responses, similar to the biaxial compression examples.

885 Within the shear bands, the densely packed HBS structure undergoes dilation (positive
 886 volumetric strain, as shown in Figure 27) due to particle rearrangement and hydrate
 887 cracking, particularly in high-saturation and low-confining-stress specimens. Dilation
 888 reduces pore pressure (Figure 28), creating a transient suction effect that temporarily
 889 enhances shear strength (effective stress increase). More importantly, as discussed in the
 890 biaxial compression examples, the pore pressure drop shifts the hydrate phase equilibrium,
 891 causing significant hydrate dissociation (Figure 29). The dissociation occurs mainly within
 892 the shear bands, whereas the regions outside the shear band, including the triangular
 893 wedge beneath the rigid indenter, show no hydrate dissociation. The dissociation of
 894 hydrates further causes the following chain responses: (1) the liberated gas and water
 895 further increase the pore pressure, and absorbing heat, inhibiting the hydrate dissociation;
 896 (2) the loss of hydrate cementation decreases soil stiffness and strength, while reduction
 897 of hydrate fraction together with the expansion of pore space increase the permeability,
 898 accelerating the pore pressure dissipation. Additionally, the plastic heat generation due
 899 to plastic deformation also plays a significant role in promoting hydrate dissociation. In
 900 short, the indenter penetration tests display basically the same THMC responses as those

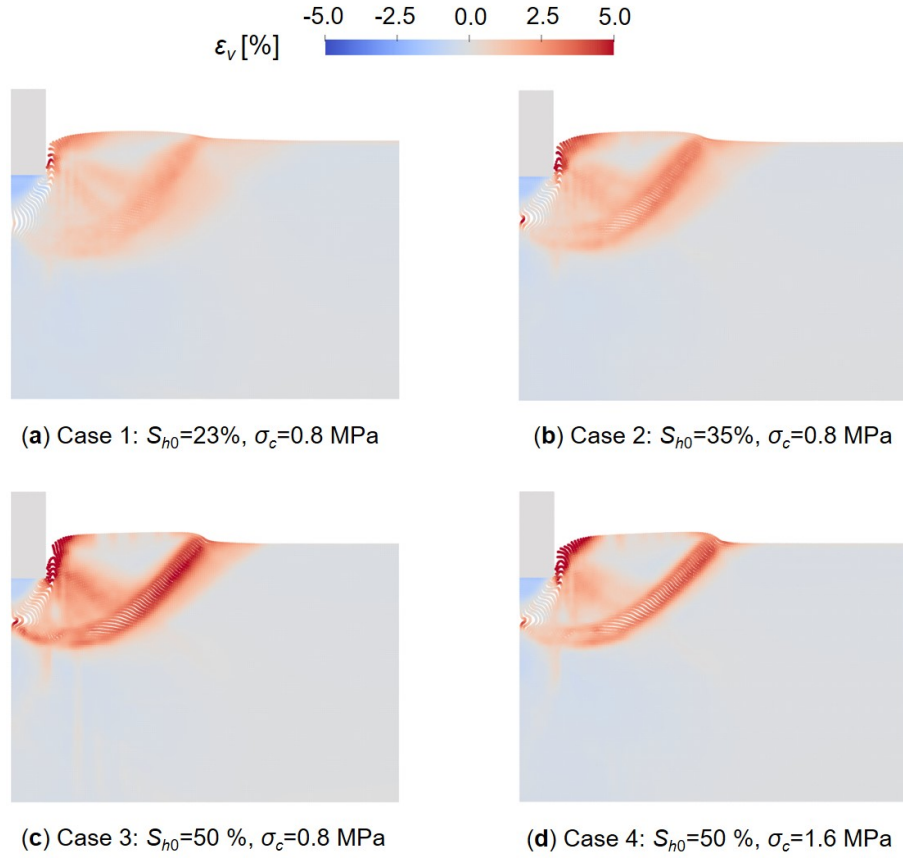


Figure 27: Simulation results of the rigid indenter penetration test: distribution of volumetric strain (ε_v) at $d/B = 0.5$.

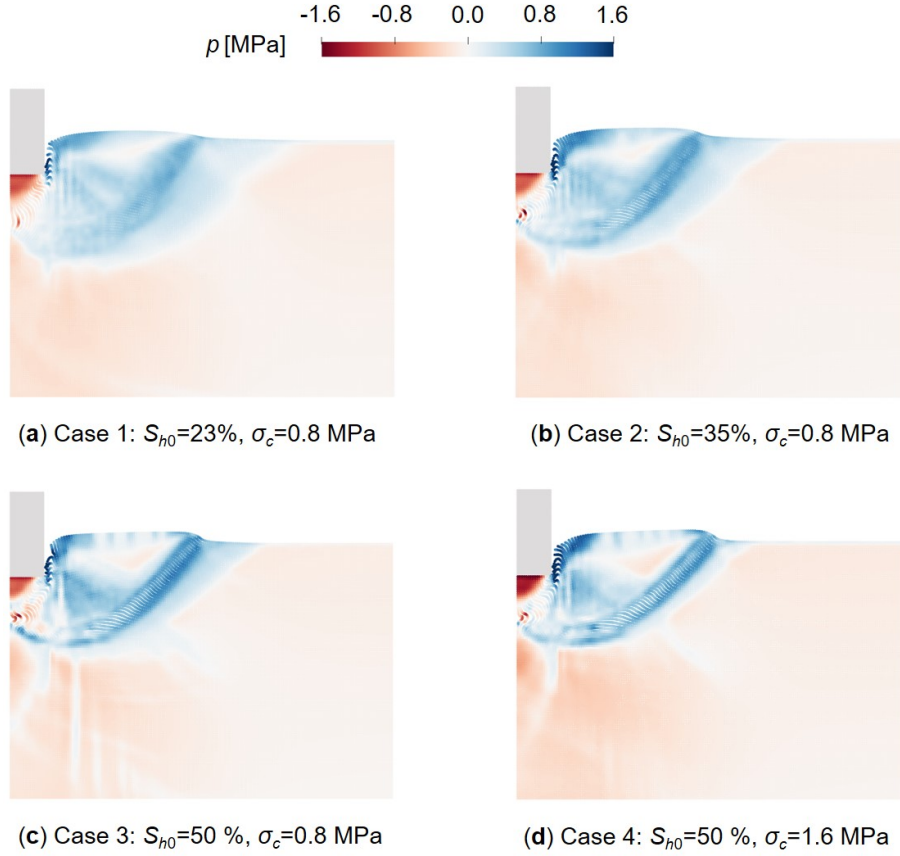


Figure 28: Simulation results of the rigid indenter penetration test: distribution of excess pore pressure at $d/B = 0.5$.

of the biaxial compression test, including the effect of hydrate saturation and confining stress, showing the robustness of the multiscale method in capturing both sample scale and field scale problems. Due to the similar evolution mechanism, the detailed local response analyses will not be conducted further.

6. Concluding remarks

This study presents a novel hybrid continuum-discrete multiscale computational framework to address the persistent challenges in modeling THMC-coupled phase transitions, large deformations, and constitutive behavior in hydrate-bearing sediments (HBS). Key contributions and findings are summarized as follows:

1. Within this framework, a fully coupled THMC-MPM is adopted to update key macroscale field variables in HBS, including sediment deformation, pore water/gas pressure, temperature, and hydrate/gas/water saturation, and a hydrate-saturation-dependent bonded-based DEM model is employed to simulate the micro- and mesoscale mechanical responses of hydrate-bearing sediment. The multiscale coupling is achieved

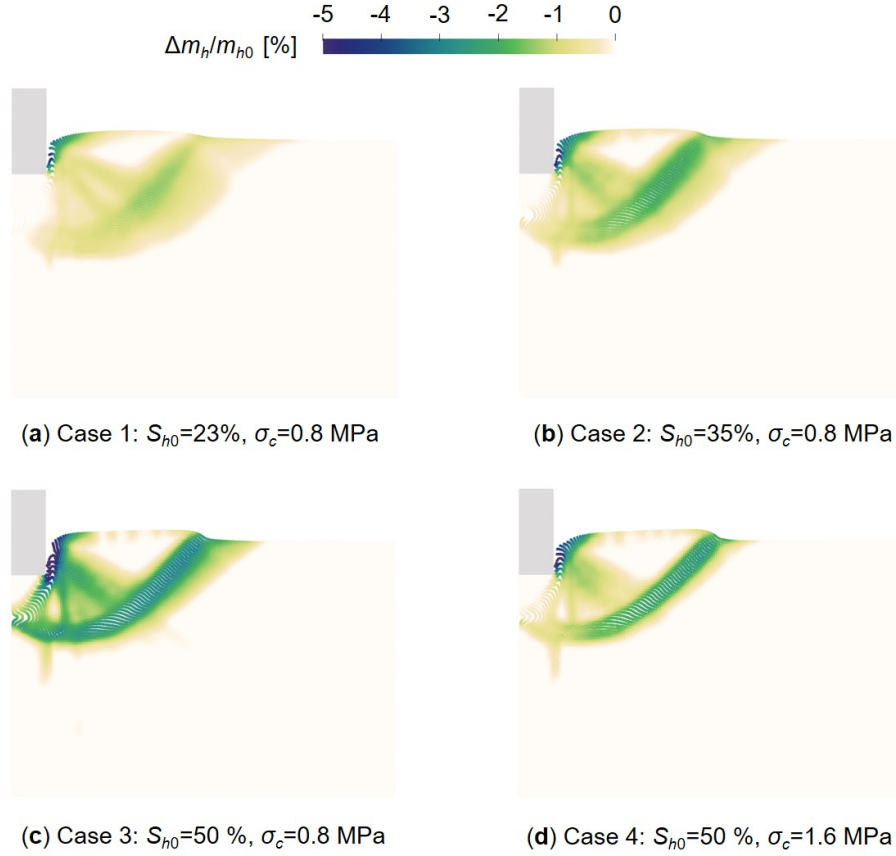


Figure 29: Simulation results of the rigid indenter penetration test: distribution of relative hydrate mass change ($\Delta m_h/m_{h0}$) at $d/B = 0.5$.

by embedding a DEM RVE at each material point. The MPM solver passes the deformation gradient and hydrate saturation information to the DEM solver, which subsequently updates the RVE's material parameters and the effective stress. This updated stress is then returned to the MPM solver for subsequent macroscopic simulation.

2. RVE tests were conducted first with varying hydrate saturations and confining pressures to calibrate the microscopic parameters and validate the hydrate-saturation-dependent bond contact model. Results demonstrate that, with carefully chosen microscopic parameters, the DEM RVE can effectively capture key mechanical characteristics (*e.g.*, Young's modulus, cohesion, friction angle, and dilation angle) of HBS samples under different hydrate saturation conditions. Subsequently, biaxial compression and rigid indenter penetration tests are simulated to demonstrate the framework's capability in capturing shear localization and the corresponding THMC responses of HBS under various conditions.

3. Simulation results show that (a) shear-induced dilation within shear bands generates

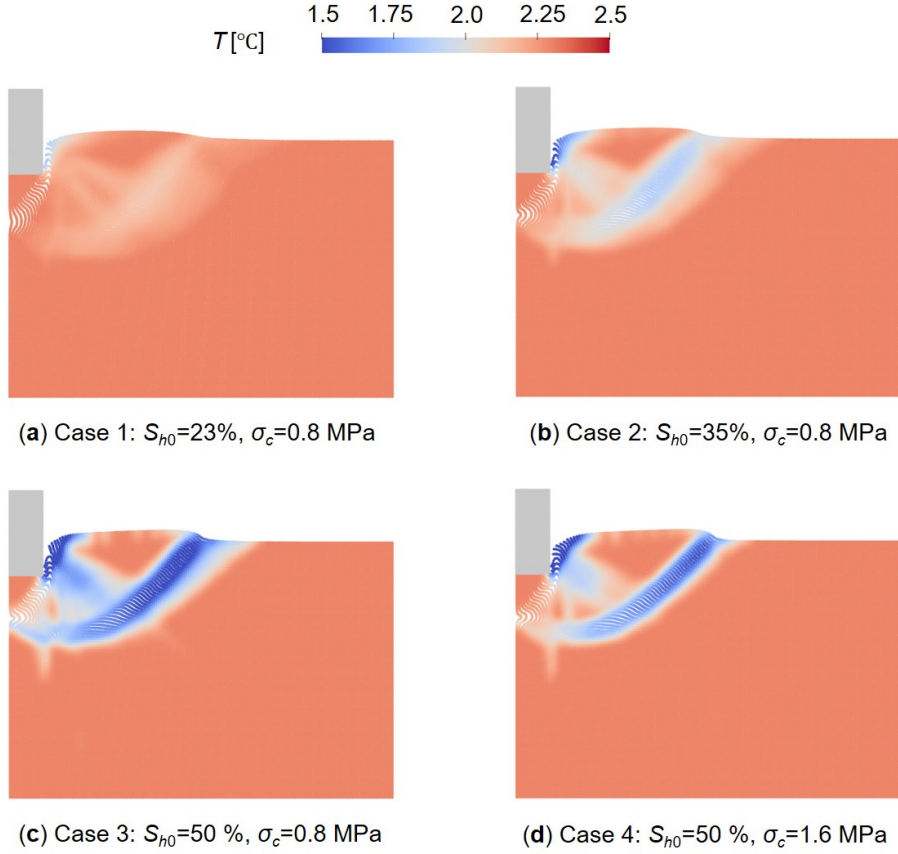


Figure 30: Simulation results of the rigid indenter penetration test: distribution of temperature at $d/B = 0.5$.

negative pore pressure, triggering localized hydrate dissociation; (b) specimens with higher initial hydrate saturation produce more pronounced negative pore pressure and consequently experience greater dissociation; (c) elevated confining pressures suppress volumetric dilation and the development of negative pore pressure; (d) plastic heating within shear bands further promotes hydrate dissociation; and (e) high-saturation HBS exhibits a trend of brittle failure mode under biaxial compression and general shear failure under indenter penetration.

In summary, the proposed multiscale, multiphysics framework effectively bypasses the need for traditional elastoplastic constitutive models for HBS. It demonstrates that even a relatively simple DEM model can replicate hallmark behaviors of hydrate-bearing soils. By leveraging the strengths of MPM for large-deformation multiphysics problems, this method provides a powerful and versatile tool for investigating hydrate-related granular mechanics and geohazards across multiple length scales, from laboratory specimens to engineering-scale problems.

Notwithstanding its capabilities, the current model has some limitations for future refinement. First, the use of a 2D RVE, although computationally efficient, may lead

to an overestimation of dilation due to the absence of out-of-plane particle mobility and its inability to represent the true 3D porosity of sediments. The 2D examples presented here are intended as a necessary first step to demonstrate the feasibility and effectiveness of the proposed multiscale framework prior to undertaking computationally prohibitive 3D simulations. Nevertheless, these limitations do not compromise the validity of the present findings, and extension of the current 2D model to 3D is conceptually straightforward. Furthermore, the current RVE model is specifically designed for cementing-type hydrate-bearing sediment; its applicability to pore-filling habits remains to be investigated. Future research will therefore focus on integrating advanced DEM models that explicitly account for various hydrate occurrence modes and incorporate particle-scale dissociation mechanics (Zhang et al., 2025). To enable large-scale 3D simulations, we will also explore the integration of machine learning and data-driven surrogate modeling techniques to supplant computationally intensive DEM calculations, thereby enhancing efficiency (Qu et al., 2023; Wang et al., 2025).

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Derivation of mass balance equations

Further derivation of the mass balance equations requires the equation of state for each phase. For the solid, liquid, and hydrate phases, the linear equation of state is adopted, given by,

$$\frac{1}{\rho_\pi} \frac{D^\pi \rho_\pi}{Dt} = \alpha_\pi \frac{D^\pi p_\pi}{Dt} - \beta_\pi \frac{D^\pi T}{Dt}, \quad \pi = s, h, w, \quad (\text{A.1})$$

where α_π and β_π are respectively the compressibility and the thermal conductivity of π phase; T is the temperature; and p_π is the phase pressure. The solid and hydrate phases

are considered to be incompressible, i.e., $\alpha_s = \alpha_h = 0$. For the gas phase, the equation for an ideal gas is adopted, given by,

$$\rho_g = \frac{M_g p_g}{RT}, \quad (\text{A.2})$$

where M_g is the gas molar mass and R is the universal gas constant.

By applying the chain rule for Eqs. (3) to (6) and introducing the equation of state of each phase, the mass balance equations can be reformulated as follows,

Solid phase:

$$\frac{D^s \phi}{Dt} = -(1 - \phi) \beta_s \frac{D^s T}{Dt} + (1 - \phi) \nabla \cdot \mathbf{v}_s, \quad (\text{A.3})$$

Hydrate phase:

$$\phi \frac{D^s S_h}{Dt} = \frac{\dot{m}_h}{\rho_h} + \beta_{sh} \frac{D^s T}{Dt} - S_h \nabla \cdot \mathbf{v}_s, \quad (\text{A.4})$$

Water phase:

$$\left(\phi \frac{\partial S_w}{\partial p_w} + \frac{\phi S_w}{K_w} \right) \frac{D^s p_w}{Dt} - \phi \frac{\partial S_w}{\partial p_w} \frac{D^s p_g}{Dt} - \beta_{ws} \frac{D^s T}{Dt} + S_w \nabla \cdot \mathbf{v}_s + \nabla \cdot \mathbf{J}_w = \frac{\dot{m}_w}{\rho_w}, \quad (\text{A.5})$$

Gas phase:

$$\left(\frac{\phi S_g}{\rho_g} \frac{M_g}{RT} + \phi \frac{\partial S_w}{\partial p_w} \right) \frac{D^s p_g}{Dt} - \phi \frac{\partial S_w}{\partial p_w} \frac{D^s p_w}{Dt} - \beta_{ghs} \frac{D^s T}{Dt} + (S_g + S_h) \nabla \cdot \mathbf{v}_s + \nabla \cdot \mathbf{J}_g = \frac{\dot{m}_g}{\rho_g} + \frac{\dot{m}_h}{\rho_h}, \quad (\text{A.6})$$

where $\beta_{sh} = (1 - \phi) S_h \beta_s + \phi S_h \beta_h$, $\beta_{ws} = (1 - \phi) S_w \beta_s + \phi S_w \beta_w$, $\beta_{ghs} = (1 - \phi) (S_g + S_h) \beta_s + \phi S_h \beta_h + \frac{\phi S_g}{\rho_g} \frac{M_g p_g}{RT^2}$, and $K_w = 1/\alpha_w$ is the liquid bulk modulus.

Eqs. (A.3) and (A.4) describe the rate of porosity ϕ and hydrate saturation S_h , respectively, whereas Eqs. (A.5) and (A.6) describe the rate of pore water pressure and pore gas pressure.

Appendix B. Matrices in discretized governing equations

The matrices in Eq. (35) are given by,

$$\tilde{K}_{ww} = K_{ww} + \Delta t \frac{N_h M_w}{\rho_w} K_d A_s \chi_w, \quad (\text{B.1a})$$

$$\tilde{K}_{wg} = K_{wg} + \Delta t \frac{N_h M_w}{\rho_w} K_d A_s \chi_g, \quad (\text{B.1b})$$

$$\tilde{K}_{gg} = K_{gg} + \Delta t \left(\frac{M_g}{\rho_g} - \frac{M_h}{\rho_h} \right) K_d A_s \chi_g, \quad (\text{B.1c})$$

$$\tilde{K}_{gw} = K_{gw} + \Delta t \left(\frac{M_g}{\rho_g} - \frac{M_h}{\rho_h} \right) K_d A_s \chi_w, \quad (\text{B.1d})$$

$$\tilde{f}_w = \frac{N_h M_w}{\rho_w} K_d A_s (p_e - p^k) + \beta_{ws} \dot{T}_p^{k+1} + S_w \varepsilon_{sp}^{k+1} + \phi_p S_w (\dot{\varepsilon}_{wp}^{k+1} - \dot{\varepsilon}_{sp}^{k+1}) , \quad (\text{B.1e})$$

$$\tilde{f}_g = \left(\frac{M_g}{\rho_g} - \frac{M_h}{\rho_h} \right) K_d A_s (p_e - p^k) + \beta_{ghs} \dot{T}_p^{k+1} + (S_h + S_g) \dot{\varepsilon}_{sp}^{k+1} + \phi_p S_g (\dot{\varepsilon}_{gp}^{k+1} - \dot{\varepsilon}_{sp}^{k+1}) . \quad (\text{B.1f})$$

The matrices in Eq. (38) are given by,

$$(M_\pi)_I = \sum_p V_p \phi_p S_{\pi p} \rho_{\pi p} S_{Ip}, \quad \pi = w, g , \quad (\text{B.2a})$$

$$(M_{sh})_I = \sum_p V_p \rho_{shp} S_{Ip}, \quad (\text{B.2b})$$

$$(Q_\pi^d)_I = - \sum_p V_p (\phi_p S_{\pi p})^2 \frac{\mu_{\pi p}}{k_{ap} k_{r\pi p}} S_{Ip}, \quad \pi = w, g , \quad (\text{B.2c})$$

$$(\mathbf{f}_\pi^{ext})_I = \sum_p V_p h_p^{-1} \hat{\mathbf{t}}_{\pi p} S_{Ip} + \sum_p V_p \phi_p S_{\pi p} \rho_{\pi p} \mathbf{b} S_{Ip}, \quad \pi = w, g , \quad (\text{B.2d})$$

$$(\mathbf{f}_\pi^{int})_I = \sum_p V_p \phi_p S_{\pi p} p_{\pi p} \nabla S_{Ip}, \quad \pi = w, g , \quad (\text{B.2e})$$

$$(\mathbf{f}_m^{ext})_I = \sum_p V_p h_p^{-1} \hat{\mathbf{t}} S_{Ip} + \sum_p V_p \rho_m \mathbf{b} S_{Ip}, \quad (\text{B.2f})$$

$$(\mathbf{f}_m^{int})_I = - \sum_p V_p \boldsymbol{\sigma}_p : \nabla S_{Ip}. \quad (\text{B.2g})$$

The matrices in Eq. (39) are given by,

$$(\tilde{C}_m)_I = \sum_p V_p \left(C_{mp} + \Delta t \frac{\partial q_e}{\partial T} \right) S_{Ip}, \quad (\text{B.3a})$$

$$(\mathbf{Q}_w^{conv})_I = - \sum_p V_p \phi_p S_{wp} \rho_{wp} c_{wp} \nabla T_p S_{Ip}, \quad (\text{B.3b})$$

$$(\mathbf{Q}_g^{conv})_I = - \sum_p V_p \phi_p S_{gp} \rho_{gp} c_{gp} \nabla T_p S_{Ip}, \quad (\text{B.3c})$$

$$(\mathcal{E}_T^{source})_I = \sum_p V_p q_{ep} S_{Ip}, \quad (\text{B.3d})$$

$$(\mathcal{E}_T^{ext})_I = - \sum_p V_p h^{-1} \hat{q}_{ep} S_{Ip} + \sum_p V_p (\theta \boldsymbol{\sigma}' : \dot{\boldsymbol{\varepsilon}}^p) S_{Ip}, \quad (\text{B.3e})$$

$$(\mathcal{E}_T^{int})_I = \sum_p V_p (-\kappa_m \nabla T_p) \cdot \nabla S_{Ip}. \quad (\text{B.3f})$$

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