

Variational phase-field fracture approach for non-isothermal CO₂-water two-phase flow in deformable porous media

Yuhao Liu^{a,b}, Keita Yoshioka^{c,d}, Tao You^{c,d}, Hanzhang Li^{a,b}, Fengshou Zhang^{a,b}

^aState Key Laboratory of Disaster Reduction in Civil Engineering, Tongji University, Shanghai 200092, China

^bDepartment of Geotechnical Engineering, College of Civil Engineering, Tongji University, Shanghai 200092, China

^cDepartment Geoenergy, Technical University Leoben, Leoben 8700, Austria

^dDepartment of Environmental Informatics, Helmholtz Centre for Environmental Research - UFZ, Leipzig 04318, Germany

Abstract

When CO₂ is injected to induce fracture in rock, the fracture tends to propagate in a more complex pattern and at a lower critical pressure compared to water injection. This study presents a fracture propagation model under CO₂-water two-phase flow, based on the variational thermo-hydro-mechanical phase-field approach. For each constituent (water and CO₂), the mass balance equation is derived while accounting for the capillary effect and the respective equations of state. Meanwhile, the equivalent pressure from two fluids modifies the potential energy description in thermo-poro-elastic media, following our previous micromechanics based model. The proposed model has been verified against the analytical solutions for one-dimensional incompressible, immiscible two-phase flow, and plane strain hydraulic fracture propagation, known as the KGD fracture. Our numerical experiments indicate that fractures propagate at lower breakdown pressures under supercritical CO₂ injection, and their paths are more influenced more by pre-existing weak interfaces due to low viscosity of CO₂.

Keywords: Phase-field; Hydraulic fracturing; Thermo-hydro-mechanical coupling; Two-phase flow; Fixed stress split

1. Introduction

In reservoir stimulation for geothermal and hydrocarbon energy production, fluid injection is required to improve efficiency (Qun et al., 2019), prevent induced seismicity (Bai et al., 2016), and ensure injected fluid containment (Basu et al., 2015). Gao et al. (2024) provided a comprehensive review of field applications of fracturing by CO₂ injection. While hydraulic fracturing remains a widely used reservoir stimulation technique, it faces challenges such as high water consumption (Chen and Carter, 2016), risks of subsurface contamination (Vengosh et al., 2014), and the potential to induce seismicity (Schultz et al., 2020). To address these issues, CO₂ fracturing has emerged as a promising waterless alternative (Zhang et al., 2022; Nianyin et al., 2021; Moridis, 2017; Mojid et al., 2021; Zhang et al., 2021; Zhou and Zhang, 2020). Generally, when the formation depth exceeds 11m, the temperature and pressure surpass the critical values of CO₂ (304.12K and

7.377MPa), bringing it into a supercritical state (Span and Wagner, 1996; Yang et al., 2022). Compared to water-based fracturing fluids, CO₂ exhibits lower dynamic viscosity and higher diffusivity, which can facilitate the formation of more complex fracture geometries (Ishida et al., 2016; Wu et al., 2023; Xie et al., 2021). Its near-zero surface tension results in reduced flow resistance within the fracture, allowing it to reach the tip of the fracture more easily (Zhu et al., 2024). Furthermore, the lower formation breakdown pressure associated with CO₂ may help reduce the risk of fault reactivation (Song et al., 2019; Liu et al., 2017; Ishida et al., 2021), although its low viscosity also leads to greater fluid leak-off. In addition, such operations present an opportunity for the subsurface utilization and storage of CO₂ (Espinoza and Santamarina, 2010; Middleton et al., 2015).

Effective utilization of CO₂ in hydraulic fracturing requires a thorough understanding of the complex mechanisms governing fracture nucleation and propagation. While experimental investigations have explored various aspects of CO₂ fracturing through parametric studies (Zhang et al., 2017, 2019b; Zhou et al., 2018, 2019; Zou et al., 2018; Jiang et al., 2018), these efforts are often constrained by limitations in scale and the difficulty of replicating high-pressure and high-temperature subsurface conditions, which can be addressed by numerical modeling (Adachi et al., 2007; Yew and Weng, 2014). However, current numerical approaches still struggle to fully capture the coupled TH²M processes, where H² denotes the two-phase flow in the thermo-hydro-mechanical system (Grunwald et al., 2022). In deep subsurface environments, elevated confining pressures and in-situ stresses complicate fracture initiation (Zhou et al., 2024), while the presence of natural fractures contributes to more complex fracture geometries (Zhang et al., 2019a; Chen et al., 2018). Additionally, large temperature differences between the injected CO₂ and the surrounding formation may lower the critical pressure required for fracture propagation and lead to wider crack openings (Jiao et al., 2022; Luo et al., 2022). Importantly, injecting CO₂ into saturated porous media creates a two-phase fluid system of water and CO₂, which requires the model to account for capillary effects (Maxwell, 1876), saturation distributions (Brown, 1951), and phase transitions such as evaporation, precipitation, and dissolution (Lu and Connell, 2014; Afanasyev, 2013; Matter and Kelemen, 2009).

Several studies have explored the numerical simulation of CO₂ fracturing. Yan et al. (2019, 2020) developed a finite element hydromechanical (HM) model to simulate supercritical CO₂ fracturing in coal seams, focusing on secondary fracturing triggered by blast loads from CO₂ phase transitions and dynamic interactions between multiple cracks (Yan et al., 2019, 2020). Liu et al. (2020) proposed a hybrid model that integrates unsteady fluid flow with a cohesive solid framework to investigate the fracturing mechanism of supercritical CO₂. Guo et al. (2022) conducted a comprehensive parametric study of fracture propagation, incorporating various geomechanical and operational parameters within a damage mechanics framework. Additional simulations have examined thermal effects and the influence of CO₂ phase states on fracture evolution (Xiao et al., 2024). Despite these advancements, many existing models restrict fracture propagation to predefined paths and lack the capability to capture complex behaviors such as branching and merging. Moreover, representing fractures as sharp discontinuities poses significant challenges for accurate numerical modeling.

Phase-field modeling of fractures (Bourdin et al., 2000, 2008) has seen continuous advancement in the last couple of decades. The first applications of phase-field methods to fluid-driven fractures focused on elastic media (Bourdin et al., 2012; Chukwudozie et al., 2013), and were later extended to poroelastic media (Wheeler et al., 2014; Mikelić et al., 2015). Noii and Wick (2019) expanded the framework to incorporate thermo-hydro-mechanical (THM) coupling. Since then, a growing body of research has developed THM phase-field models (Wang et al., 2023; Li et al., 2021; Yi et al., 2024a; Suh and Sun, 2021; Liu et al., 2024a; Lee et al., 2025b,a), with some models integrating

reactive transport and chemical effects (Dai et al., 2024). Other studies have focused on phase-field modeling of drying-induced fractures in partially saturated porous media (Heider and Sun, 2020; Cajuhi et al., 2018). Yi et al. (2024b) also proposed a coupled phase-field model for a water–oil mixture to predict residual oil saturation.

Regarding phase-field modeling of CO₂ fracturing, Xu et al. (2022) proposed a new energy release rate criterion for rock to simulate supercritical CO₂ fractures under hydro-mechanical (HM) coupling. Feng et al. (2021; 2023) extended this work to include thermo-hydro-mechanical (THM) processes, investigating thermal effects during CO₂ fracturing and validating their results against experimental data. Jiang et al. (2025) analyzed the influence of stress anisotropy on fracture morphology by injecting CO₂ into thermo-poro-elastic media. Despite these advances, current studies still fall short of modeling the complete TH²M fracturing process. The behavior of two-phase fluid flow within the hydraulic process remains insufficiently understood within the THM framework, and phase-field formulations for hydraulic and thermal parameters require further refinement. Additionally, solution algorithms for thermo-hydro-mechanical phase-field fracture models must ensure both efficiency and stability when coupled with two-phase flow.

In this study, we present a fully coupled TH²M phase-field fracture model for CO₂ fracturing. We extend our existing THM phase-field framework to incorporate CO₂–water two-phase flow, involving two immiscible fluid phases. The mass balance equations for each fluid component are formulated with capillary pressure, where water is treated as the wetting phase and CO₂ as the non-wetting phase. Water saturation is determined through capillary pressure, while CO₂ density is computed as a function of pressure and temperature using an appropriate equation of state. A mixed-volume method is employed to compute equivalent hydraulic and thermal material properties. The degradation of thermo-poro-elastic strain energy is governed by a micromechanically derived Biot coefficient, which itself is a function of the phase-field variable (representing damage) and the adopted energy decomposition scheme. Pore fluid energy is reformulated using an equivalent liquid pressure to improve accuracy. To solve the coupled system, we adopt a hybrid monolithic-staggered scheme in which the non-wetting phase pressure and capillary pressure are solved simultaneously in a single iteration step. For the thermal stress analysis, we apply a stabilized fixed-stress split method to enhance numerical robustness.

Section 3 introduces the numerical implementation, including a mixed solution scheme and an adapted fixed-stress split method. In section 4 the proposed model is verified against analytical solutions for one-dimensional two-phase flow in porous media (McWhorter problem) and fluid-driven fracture propagation (KGD problem). Section 5 compares water-based and CO₂ fracturing in terms of single-fracture propagation and investigates CO₂ injection under various temperature differences. Finally, the interaction of hydraulic fractures with weak interfaces—under both water-based and CO₂ injection—is discussed, followed by conclusions and directions for future research.

We use the following notations throughout the paper. The second-order identity tensor is denoted by $\mathbf{I}$. The trace operator $\text{Tr}(\cdot)$ acting on the second-order tensors $\mathbf{A}$ is defined as $\text{Tr}(\mathbf{A}) = \delta : \mathbf{A}$. $\nabla(\cdot)$ is the gradient of $(\cdot)$. A repeated index in subscript follows Einstein’s summation convention i.e., $a_i b_i = a_1 b_1 + a_2 b_2 + a_3 b_3$ for $i = 1, 2, 3$. However, this convention is ignored for an index in parentheses, e.g., $a_{(i)} b_{(i)}$.

2. Mathematical model

Consider a thermo-poro-elastic medium that occupies the domain $\Omega \subset \mathbb{R}^d$, $d = 2, 3$. In Ω , a lower dimensional set of fractures is denoted by Γ (Fig. 1). The body is subjected to a possible flux $\bar{\mathbf{q}}$

124 and a surface force $\bar{\mathbf{t}}$ on the boundary $\partial_N \Omega := \mathcal{C}_N \cup \partial \Gamma$, where $\mathcal{C}_N$ denotes the outer domain boundary
 125 and $\partial \Gamma$ the fracture boundary. The prescribed displacement $\bar{\mathbf{u}}$, pressure $\bar{\mathbf{p}}$ and temperature $\bar{\mathbf{T}}$ can
 126 be applied on the boundary $\partial_D \Omega$. A mixture fluid of component L and component C is considered.
 127 No phase transition is considered; therefore, the two components will each remain in their respective
 128 phases. Furthermore, we assume a local thermal equilibrium in the domain in which the fluid and
 129 porous solid temperatures are equilibrated. The underlying study proceeds from the triphasic
 130 porous material, consisting of a solid phase (S) and two fluid phases (L and C). Regarding their
 131 wetting properties, we consider phase L as the wetting phase and phase C as the non-wetting phase.
 132 The mass density is given as $\rho_\alpha = \phi_\alpha \rho_{\alpha R} = \phi S_\alpha \rho_{\alpha R}$ ($\alpha \in \{S, L, C\}$) where ϕ is the porosity, S_α
 133 is the saturation of phase α and $\rho_{\alpha R}$ is the intrinsic density. The phase volume fraction $\phi_\alpha = \phi S_\alpha$,
 134 where $S_S = 1$, $S_L + S_C = 1$, $\phi_L + \phi_C = \phi$.

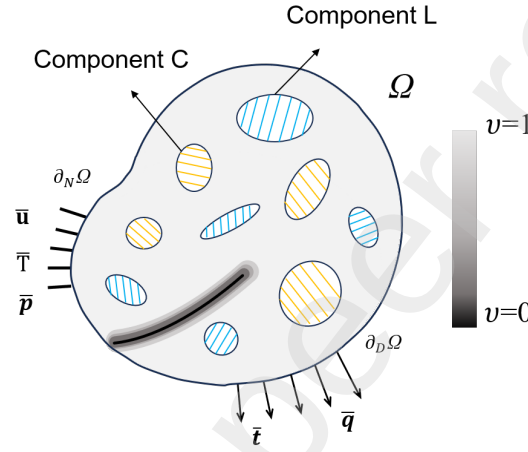


Fig. 1 Schematic of thermo-poroelastic medium with two-phase flow.

135 2.1. Mechanical equilibrium

136 The total energy $\mathcal{E}_\Gamma$ of a homogeneous isotropic and linearly elastic material with a set of
 137 fractures is defined as a sum of the strain energy and the surface energy of fracture:

$$\mathcal{E}_\Gamma(\varepsilon(\mathbf{u}), \Gamma) := \int_{\Omega \setminus \Gamma} \psi(\varepsilon(\mathbf{u})) \, dV + \int_\Gamma G_c \, dS. \quad (1)$$

138 To alleviate the implementational difficulties of the discrete crack, we follow the work of Bourdin
 139 et al. (2000) to regularize the discrete cracks with a phase-field variable v that represents a state of
 140 the material from intact ($v = 1$) to fully broken ($v = 0$) (Fig.1). The total energy of a homogeneous
 141 isotropic and linearly elastic material $\mathcal{E}$ is regularized as

$$\mathcal{E}(\varepsilon(\mathbf{u}), v) := \int_\Omega \psi(\varepsilon(\mathbf{u}), v) \, dV + \int_\Omega \frac{G_c}{4c_n} \left[\frac{(1-v)^n}{\ell} + \ell \nabla v \cdot \nabla v \right] \, dV, \quad (2)$$

142 where ε is the total strain, G_c is the critical energy release rate and c_n is the normalizing parameter
 143 defined as $c_n = \int_0^1 (1-s)^{n/2} \, ds$. For $n = 1$ and $n = 2$, the model is called AT₁ model and AT₂ model.

Also, ℓ is the characteristic parameter with the dimension of a length that controls the phase-field profile transition. The strain energy density $\psi(\varepsilon(\mathbf{u}), v)$ in Eq. (2) acknowledges the phase-field variable v and is continuous over Ω for integration. Accounting for the thermo-poro-elastic medium, the energy functional can be extended to

$$\begin{aligned} \mathcal{E}(\varepsilon(\mathbf{u}), \zeta, T, v) := & \int_{\Omega} \psi_e(\varepsilon(\mathbf{u}), T, v) dV + \int_{\Omega} \psi_f(\varepsilon(\mathbf{u}), \zeta, v) dV + \int_{\Omega} \psi_T(T) dV \\ & + \int_{\Omega} \frac{G_c}{4c_n} \left[\frac{(1-v)^n}{\ell} + \ell \nabla v \cdot \nabla v \right] dV. \end{aligned} \quad (3)$$

$\mathbf{u}$, p , and T represent the displacement, the pressure and temperature field, while ζ denotes the incremental content of fluid. The total strain energy density ψ is assumed to be decomposed into elastic $\psi_e(\varepsilon(\mathbf{u}), T, v)$ and hydraulic energies $\psi_f(\varepsilon(\mathbf{u}), \zeta, v)$. Furthermore, we assume that the thermal energy density $\psi_T(T)$ is not contributed by mechanical or hydraulic processes (Suh and Sun, 2021).

With a degradation function $g(v)$ ¹, the elastic strain energy is contributed by the elastic strain ε_e acting on the solid skeleton so that

$$\begin{aligned} \psi_e(\varepsilon(\mathbf{u}), v, T) &= g(v) \psi_+(\mathbf{u}) + \psi_-(\mathbf{u}) \\ &= \frac{1}{2} g(v) \mathbb{C}_+ : \varepsilon_e : \varepsilon_e + \frac{1}{2} \mathbb{C}_- : \varepsilon_e : \varepsilon_e \\ &= \frac{1}{2} \mathbb{C}_{\text{eff}} : \varepsilon_e : \varepsilon_e \\ &= \frac{1}{2} \mathbb{C}_{\text{eff}} : \left(\varepsilon(\mathbf{u}) - \beta \Delta T \mathbf{I} \right) : \left(\varepsilon(\mathbf{u}) - \beta \Delta T \mathbf{I} \right), \end{aligned} \quad (4)$$

where

$$\mathbb{C}_{\text{eff}} = g(v) \mathbb{C}_+ + \mathbb{C}_-. \quad (5)$$

Here the expression for $\mathbb{C}_{\text{eff}}$ is determined by no-tension model (Fredde and Royer-Carfagni, 2010). The total stress can be found by taking the derivative of $\mathcal{E}$ with respect to ε_e as

$$\sigma = \mathbb{C}_{\text{eff}} : \varepsilon(\mathbf{u}) - \alpha(v) p_{FR} \mathbf{I} - 3\beta K_{\text{eff}} \Delta T \mathbf{I}, \quad (6)$$

where K is the drained bulk modulus. The total strain ε is decomposed into the elastic strain and the thermal strain which equals the product of thermal expansion coefficient β and the temperature difference ΔT between the current temperature and initial temperature. $\alpha(v)$ and K_{eff} are the effective Biot's coefficient and the effective bulk modulus. Following the work by You and Yoshioka (2023), the effective Biot coefficient is given as

$$\alpha(v) = 1 - \frac{K_{\text{eff}}}{K_s}. \quad (7)$$

where K_s is the intrinsic bulk modulus. The effective bulk modulus depends not only on the damage

¹In this study, we employed $g(v) = (1-k)v^2 + k$ where k is a phase-field parameter representing residual stiffness, which keeps the system of equations well-conditioned for the partly-broken state.

(v) but also on the type of energy decomposition scheme applied. The expression of K_{eff} for the volumetric-deviatoric energy decomposition (Amor et al., 2009) is given by You and Yoshioka (2023), and the general expression of K_{eff} can also be obtained with the expression of $\mathbb{C}_{\text{eff}}(v)$ and spherical projection $\mathbf{P}_{\text{sph}} = \frac{1}{3}\mathbf{I}$ as

$$K_{\text{eff}}(v) = \frac{1}{9}\text{Tr}(\mathbf{P}_{\text{sph}} : \mathbb{C}_{\text{eff}}(v) : \mathbf{I}). \quad (8)$$

By defining the degradation coefficient g_k with the initial bulk modulus K as

$$g_k = K_{\text{eff}}(v)/K, \quad (9)$$

we can rewrite effective Biot's coefficient in Eq. (7) as

$$\alpha(v) = 1 - \frac{K_{\text{eff}}(v)}{K_s} = 1 - K_{\text{eff}}(v) \frac{1 - \alpha_m}{K} = 1 - g_k(1 - \alpha_m) \quad (10)$$

where α_m is the initial Biot's coefficient.

The hydraulic energy of pore fluid ψ_f is given as

$$\psi_f(\mathbf{u}, v, \zeta) = \frac{M_p}{2} [\alpha(v)\text{Tr}(\varepsilon_e) - \zeta]^2, \quad (11)$$

where M_p denotes the Biot's modulus as

$$\frac{1}{M_p} = \frac{\alpha(v) - \phi}{K_s}, \quad (12)$$

The porosity depends on the deformation as

$$\phi = \phi_m + \varepsilon_1, \quad (13)$$

where ϕ_m is the original porosity and ε_1 is the maximum principal strain (Liu et al., 2024b). The incremental content of fluid ζ is defined without the effect of thermal expansion as

$$\zeta = \alpha(v)\text{Tr}(\varepsilon_e) + \frac{p_{FR}}{M_p} \quad (14)$$

where p_{FR} is the equivalent fluid pressure defined as

$$p_{FR} = S_C p_{CR} + S_L p_{LR}, \quad (15)$$

and p_{CR} and p_{LR} are the non-wetting phase pressure and total fluid pressure. The capillary pressure is defined as the difference between p_{CR} and p_{LR}

$$p_c = p_{CR} - p_{LR}. \quad (16)$$

The thermal energy ψ_T is assumed not to be contributed by mechanical and hydraulic process (Suh and Sun, 2021):

$$\psi_T(T) = (\rho c)_m \left[(T - T_{\text{ref}}) - T \ln \left(\frac{T}{T_{\text{ref}}} \right) \right], \quad (17)$$

where T_{ref} is the reference temperature. $(\rho c)_m$ is the equivalent heat storage for porous medium given by

$$(\rho c)_m = \phi_L c_{p,L} \rho_{LR} + \phi_C c_{p,C} \rho_{CR} + (1 - \phi) c_{p,S} \rho_{SR}, \quad (18)$$

where $c_{p,\alpha}$ $\alpha \in \{S, L, C\}$ is the specific heat capacity of each phase.

2.2. Fluid mass balance

The mass balance equation of each constituent can be expressed as

$$(\rho_\alpha)'_S + \nabla \cdot (\rho_\alpha \mathbf{v}_\alpha) = \hat{p}_\alpha, \quad (19)$$

where ρ_α is the mass density of phase α , $(\bullet)'_s$ denotes the material time derivative of a quantity $\bullet$ with respect to the velocity of the solid skeleton, $\mathbf{v}_\alpha$ is the velocity of phase α , and $\hat{p}_\alpha$ is the mass production term. Accounting for the relative velocity of the fluid with respect to the solid skeleton, we yield

$$(\rho_\alpha)'_S + \rho_\alpha \nabla \cdot \mathbf{v}_S + \nabla \cdot [\rho_\alpha (\mathbf{v}_\alpha - \mathbf{v}_S)] = \hat{p}_\alpha, \quad (20)$$

where $\mathbf{v}_s$ is the velocity of solid skeleton.

For the solid phase ($\alpha = s$), no mass transfer to the solid phase occurs so that $\hat{p}_\alpha = 0$. Thus, the mass balance equation of solid phase simplifies to

$$(\rho_S)'_S + \rho_S \nabla \cdot (\mathbf{u})'_S = 0. \quad (21)$$

For a water component (L) and a CO_2 component (C), their mass balances write

$$(\rho_L)'_S + \rho_L \nabla \cdot (\mathbf{u})'_S + \nabla \cdot [\rho_L (\mathbf{v}_L - \mathbf{v}_S)] = Q_L, \quad (22)$$

and

$$(\rho_C)'_S + \rho_C \nabla \cdot (\mathbf{u})'_S + \nabla \cdot [\rho_C (\mathbf{v}_C - \mathbf{v}_S)] = Q_C. \quad (23)$$

Eq. (22) can be expanded into

$$(n S_L \rho_{LR})'_S + n S_L \rho_{LR} \nabla \cdot (\mathbf{u})'_S + \nabla \cdot [\rho_L (\mathbf{v}_L - \mathbf{v}_S)] = Q_L. \quad (24)$$

Defining $\rho_L (\mathbf{v}_L - \mathbf{v}_S) = \mathbf{q}_L$ as the advective liquid flux and neglecting the diffusive liquid flux Eq. (24) can be expanded into

$$S_L \rho_{LR} (n)'_S + n \rho_{LR} (S_L)'_S + n S_L (\rho_{LR})'_S + n S_L \rho_{LR} \nabla \cdot (\mathbf{u})'_S + \nabla \cdot \mathbf{q}_L = 0. \quad (25)$$

Recalling Eq. (21), with $S_S = 1$, we have

$$\begin{aligned} & ((1 - \phi) \rho_{SR})'_S + (1 - \phi) \rho_{SR} \nabla \cdot (\mathbf{u})'_S \\ & = (1 - \phi) (\rho_{SR})'_S - \rho_{SR} (\phi)'_S + (1 - \phi) \rho_{SR} \nabla \cdot (\mathbf{u})'_S = 0. \end{aligned} \quad (26)$$

Solving for the rate of porosity change yields

$$(\phi)'_S = (1 - \phi) \left(\frac{(\rho_{SR})'_S}{\rho_{SR}} + \nabla \cdot (\mathbf{u})'_S \right). \quad (27)$$

200 Substituting Eq. (27) into Eq. (25) gives

$$\phi\rho_{LR}(S_L)'_S + \phi S_L(\rho_{LR})'_S + S_L\rho_{LR}\frac{1-\phi}{\rho_{SR}}(\rho_{SR})'_S + S_L\rho_{LR}\nabla \cdot (\mathbf{u})'_S + \nabla \cdot \mathbf{q}_L = Q_L. \quad (28)$$

201 Similarly, we get the expanded mass balance of CO₂ as

$$\phi\rho_{CR}(S_C)'_S + \phi S_C(\rho_{CR})'_S + S_C\rho_{CR}\frac{1-\phi}{\rho_{SR}}(\rho_{SR})'_S + S_C\rho_{CR}\nabla \cdot (\mathbf{u})'_S + \nabla \cdot \mathbf{q}_C = Q_C. \quad (29)$$

202 The rate of solid density change can be written as

$$\frac{(\rho_{SR})'_S}{\rho_{SR}} = \frac{1}{1-\phi} \left[(\alpha(v)-1)\nabla \cdot (\mathbf{u})'_S - 3\beta(\alpha(v)-\phi)(T)'_S + \frac{\alpha(v)-\phi}{K_s}(p_{FR})'_S \right], \quad (30)$$

203 where $\alpha(v)$ is Biot's coefficient, β is thermal expansive coefficient, T is global temperature and K_s
204 is the intrinsic bulk modulus. Substituting Eq. (30) into Eq. (28), we obtain

$$\begin{aligned} & S_L\rho_{LR} \left[(\alpha(v)-1)\nabla \cdot (\mathbf{u})'_S - 3\beta(\alpha(v)-\phi)(T)'_S + \frac{\alpha(v)-\phi}{K_s}(p_{FR})'_S \right] \\ & + \phi\rho_{LR}(S_L)'_S + \phi S_L(\rho_{LR})'_S + S_L\rho_{LR}\nabla \cdot (\mathbf{u})'_S + \nabla \cdot \mathbf{q}_L \\ & = S_L\rho_{LR}\alpha(v)\nabla \cdot (\mathbf{u})'_S - 3S_L\rho_{LR}\beta(\alpha(v)-\phi)(T)'_S + S_L\rho_{LR}\frac{\alpha(v)-\phi}{K_s}(p_{FR})'_S \\ & + \phi\rho_{LR}(S_L)'_S + \phi S_L(\rho_{LR})'_S + \nabla \cdot \mathbf{q}_L = Q_L. \end{aligned} \quad (31)$$

205 Expanding the rate of equivalent pressure change with Eqs. (15) and (16), we have

$$\begin{aligned} (p_{FR})'_S &= (S_C p_{CR} + S_L p_{LR})'_S \\ &= [(S_L p_{CR})'_S - (S_L p_c)'_S + (S_C p_{CR})'_S] \\ &= S_L(p_{CR})'_S - (S_L)'_S p_c - (p_c)'_S S_L + S_C(p_{CR})'_S \\ &= (p_{CR})'_S - (S_L)'_S p_c - (p_c)'_S S_L. \end{aligned} \quad (32)$$

206 As for advective terms $\mathbf{q}_\alpha$ ($\alpha \in \{L, C\}$), the seepage velocity relates to pressure changes through
207 Darcy's law

$$\mathbf{q}_L = \phi_L(\mathbf{v}_L - \mathbf{v}_s) = -\frac{k_L^{rel}\mathbf{k}_s}{\mu_{LR}}(\nabla p_{LR} - \rho_{LR}\mathbf{b}) \quad (33)$$

208

$$\mathbf{q}_C = \phi_C(\mathbf{v}_C - \mathbf{v}_s) = -\frac{k_C^{rel}\mathbf{k}_s}{\mu_{CR}}(\nabla p_{CR} - \rho_{LR}\mathbf{b}) \quad (34)$$

209 where k_α^{rel} is relative permeability, $\mathbf{k}$ is the intrinsic permeability of the porous medium, $\mu_{\alpha R}$ is
210 viscosity and $\mathbf{b}$ is the body force. The saturation and relative permeability are calculated by Brooks
211 Corey model (Brooks, 1965):

$$S_L(p_c) = \begin{cases} S_L^{max}, & p_c \leq p_b \\ \left(\frac{p_b}{p_c}\right)^\lambda (S_L^{max} - S_L^r) + S_L^r, & p_c > p_b \end{cases} \quad (35)$$

$$k_L^{rel} = (S_e)^{\frac{2+3\lambda}{\lambda}}, k_C^{rel} = (1 - S_e)^2(1 - S_e^{\frac{2+\lambda}{\lambda}}) \quad (36)$$

$$S_e = \frac{S_L - S_L^r}{S_L^{max} - S_L^r} \quad (37)$$

where S_L^{max} and S_L^r represent the maximum and residual saturation of water and S_e the effective saturation. p_b in the saturation model is the entry pressure concerning with the density and Biot's coefficient while λ is Brooks Corey's pore size distribution index. Substituting Eqs. (32), (33) and (34) into Eqs. (28) and (29) leads to

$$\begin{aligned} & \phi S_L(\rho_{LR})'_S + \alpha(v)S_L\rho_{LR}\nabla \cdot (\mathbf{u})'_S - 3\beta S_L\rho_{LR}(\alpha(v) - \phi)(T)'_S + n\rho_{LR}(S_L)'_S \\ & + S_L\rho_{LR}\frac{\alpha(v) - \phi}{K_s}(p_{CR})'_S - S_L\rho_{LR}\frac{\alpha(v) - \phi}{K_s}(S_L)'_Sp_c - S_L\rho_{LR}\frac{\alpha(v) - \phi}{K_s}(p_c)'_SS_L \\ & - \nabla \cdot \left(\rho_{LR}\frac{k_L^{rel}\mathbf{k}_s}{\mu_{LR}}(\nabla p_{CR} - \nabla p_c - \rho_{LR}\mathbf{b}) \right) = Q_L \end{aligned} \quad (38)$$

$$\begin{aligned} & \phi S_C(\rho_{CR})'_S + \alpha(v)S_C\rho_{CR}\nabla \cdot (\mathbf{u})'_S - 3\beta S_C\rho_{CR}(\alpha(v) - \phi)(T)'_S - \phi\rho_{CR}(S_L)'_S \\ & + S_C\rho_{CR}\frac{\alpha(v) - \phi}{K_s}(p_{CR})'_S - S_C\rho_{CR}\frac{\alpha(v) - \phi}{K_s}(S_L)'_Sp_c - S_C\rho_{CR}\frac{\alpha(v) - \phi}{K_s}(p_c)'_SS_L \\ & - \nabla \cdot \left(\rho_{CR}\frac{k_C^{rel}\mathbf{k}_s}{\mu_{CR}}(\nabla p_{CR} - \rho_{CR}\mathbf{b}) \right) = Q_C \end{aligned} \quad (39)$$

For the dependency of permeability on the fracture deformation, we employ the model from Liu et al. (2024b). The altered permeability should be anisotropic, accounting for the the Poiseuille-type flow in fractures (Miehe et al., 2015; Miehe and Mauthe, 2016):

$$\mathbf{K} = \mathbf{k}_s\mathbf{I} + (1 - v)^\xi \frac{\omega^2}{12} (\mathbf{I} - \mathbf{n}_\Gamma \otimes \mathbf{n}_\Gamma), \quad (40)$$

where $\xi \geq 1$ is a weighting exponent and $\mathbf{n}_\Gamma$ is the fracture unit normal vector, and the fracture width ω as calculated as

$$\omega = h_e \varepsilon_1, \quad (41)$$

where h_e is the element size. We refer to Liu et al. (2024a) for details of the width computation and its verification against fracture opening problems.

2.3. Energy balance

The energy conservation in porous medium is given as

$$3\beta K_{eff}T\nabla \cdot (\mathbf{u})'_S + (\rho c)_m \frac{\partial T}{\partial t} + \nabla \cdot (\mathbf{q}_T) = Q_T, \quad (42)$$

where the first term denotes the thermal effect due to the deformation and Q_T is the source term. We assume that the thermal dilation due to deformation is neglected. $\mathbf{q}_T$ denotes the heat flux which is decomposed into advective and conductive terms using Fourier's law:

$$\mathbf{q}_T = \rho_{LR}\mathbf{q}_{Lc_{p,L}}T + \rho_{CR}\mathbf{q}_{Cc_{p,C}}T - \lambda_{eff}\nabla T, \quad (43)$$

where the effective thermal conductivity is the summation of the partial parts of solid skeleton, water and CO₂ weighted by porosity:

$$\lambda_{\text{eff}} = (1 - \phi)\lambda_s + \phi_L\lambda_L + \phi_C\lambda_C. \quad (44)$$

3. Numerical implementation

Our theoretical framework consists of four processes: the hydraulic, the thermal, the mechanical, and the phase-field evolution processes. These four processes involve five primary variables as the hydraulic process has the two mass balance equations for each component with non-wetting phase pressure p_{CR} and capillary pressure p_c . To solve all the primary variables, a nested staggered scheme is applied as outlined in Algorithm 1. A global loop is set between v and the sub-loop $[T, [p_{CR}, p_c], u]$ where the two pressure variables (p_{CR}, p_c) are solved in a monolithic scheme because of their strong dependency. To stabilize the sub-loop, we adopt the fixed-stress splitting method (Kim et al., 2011) by freezing the volumetric stress in the hydraulic process. Detailed discretization forms are given in Appendix A.

Algorithm 1 A staggered solution of TH²M phase-field modeling

Require: Tolerance: $\delta_v, \delta_T, \delta_{p_c}, \delta_{p_{CR}}, \delta_u$, maximum number of iteration for global loop m_{max}^g , maximum number of iteration for subloop m_{max}^s , total time step n etc.

Ensure: Displacement u , temperature T , capillary pressure p_c , non-wetting phase pressure p_{CR} and phase-field v .

```

1: for  $k \leftarrow 1$  to  $n$  do
2:   /* Alternate minimization algorithm */
3:   while  $\Delta v \geq \delta_v$  and  $n \leq m_{\text{max}}^g$  do
4:
5:      $v^{k,n} = \text{Step\_v}(T^{k,n-1}, p_c^{k,n-1}, p_{CR}^{k,n-1}, u^{k,n-1})$ ;
6:     UpdateFractureWidth( $u, v$ );
7:      $\Delta v = |v^{k,n} - v^{k,n-1}|$ ;
8:     /* TH2M coupling algorithm */
9:     while  $\Delta T \geq \delta_T, \Delta p_c \geq \delta_{p_c}, \Delta p_{CR} \geq \delta_{p_{CR}}, \Delta u \geq \delta_u$  and  $m \leq m_{\text{max}}^s$  do
10:       $T^{k,m} = \text{Step\_T}(p_c^{k,m}, p_{CR}^{k,m}, v^{k,m})$ ;
11:       $\Delta T = |T^{k,m} - T^{k,m-1}|$ ;
12:      /* fixed stress splitting method */
13:       $(p_c^{k,m}, p_{CR}^{k,m}) = \text{Step\_p}(T^{k,m}, u^{k,m-1}, p_c^{k,m-1}, p_{CR}^{k,m-1}, v^{k,m})$ ;
14:       $\Delta p_c = |p_c^{k,m} - p_c^{k,n-i}|$ ;
15:       $\Delta p_{CR} = |p_{CR}^{k,m} - p_{CR}^{k,n-i}|$ ;
16:       $u^{k,m} = \text{Step\_u}(T^{k,m}, p_c^{k,m}, p_{CR}^{k,m}, v^{k,m})$ ;
17:      UpdateFractureWidth( $u, v$ );
18:       $\Delta u = |u^{k,m} - u^{k,m-1}|$ ;
19:       $m = m + 1$ ;
20:
21:    $n = n + 1$ ;
22: 
```

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4. Model verification

To the best of our knowledge, no closed-form solution is available for the non-isothermal fracture propagation with two-phase flow. Therefore, this section presents verifications of two subsets of the whole process: one-dimensional incompressible, immiscible two-phase flow problem and the plane strain hydraulic fracture propagation, i.e., KGD problem. For verification of the thermo-hydro-mechanical part, we refer to our previous work (Liu et al., 2024b).

4.1. McWorther problem

Firstly, we verified the two-phase flow module against the analytical solution proposed by McWhorter and Sunada (1990). Fig. 2 illustrates the one-dimensional flow of two incompressible, immiscible fluids through a porous medium, where the wetting phase displaces the non-wetting fluid in the horizontal direction. The initial non-wetting phase pressure p_{GR} is 0.1 MPa and the initial saturation is 0.05. On the left boundary the saturation for the wetting phase is set to 0.8 with a fixed capillary pressure to displace the non-wetting phase. Other parameters are listed in Table 1. The saturation profile along the horizontal direction at $t=1000$ s is shown in Fig. 3, which closely matches the analytical solution.

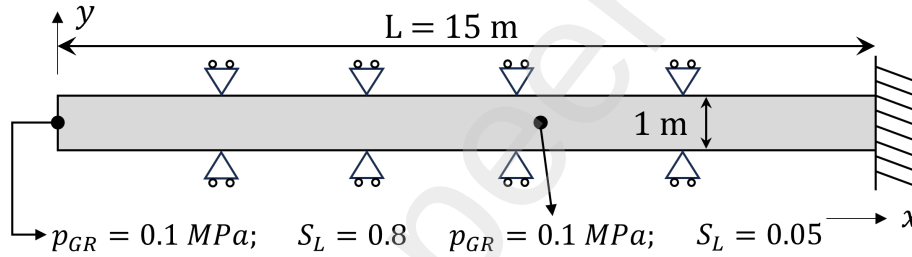


Fig. 2 Schematic of McWorther problem.

4.2. KGD problem

The second benchmark is to verify the hydromechanical module of our model with a propagating fracture (phase field) in the plane strain condition against a so-called KGD model (Kristianovich-Geertsma-de Klerk (Garagash, 2006)) without fluid leak-off. Assuming a symmetry over the y -axis, a line fracture $[0 \text{ m}, 2 \text{ m}] \times \{30 \text{ m}\}$ is considered in a domain $[0 \text{ m}, 45 \text{ m}] \times [0 \text{ m}, 60 \text{ m}]$ (Fig. 4). We consider the injection of an incompressible fluid ($c_f = 0$) into an impermeable elastic medium ($\alpha_m = 0$ and $\phi_m = 0$) to induced propagation of the line fracture. Regarding the injected fluid as a wetting phase, we set the non-wetting phase pressure to 0 in the entire domain so that the fluid mass remains single-phase. The smallest element size is 0.05 m and $\ell/h_e = 2$. In the first 10 time steps, $\Delta t = 0.01$ s and then $\Delta t = 0.1$ s in the remaining simulation time. Table 2 lists the mechanical and flow parameters.

The hydraulic fracture propagation in this setting is considered a toughness-dominated regime (Detournay and Garagash, 2003) in which the fluid viscous dissipation is negligible compared to the energy release by fracture propagation. To judge the fracture propagation regime, we can use the

Table 1 Parameters for McWorther problem.

Input parameters	Value	Unit
Porosity (ϕ_m)	0.15	-
Intrinsic permeability ($\mathbf{k}_s$)	1e-10	m ²
Residual saturation of wetting phase (S_L^r)	0.02	-
Maximum saturation of wetting phase (S_L^{max})	0.999	-
Dynamic viscosity of wetting phase (μ_L)	1e-3	Pa·s
Dynamic viscosity of non-wetting phase (μ_C)	5e-3	Pa·s
Brooks and Corey model: entry pressure (p_b)	5000	Pa
Brooks and Corey model: pore size distribution index (λ)	3	-

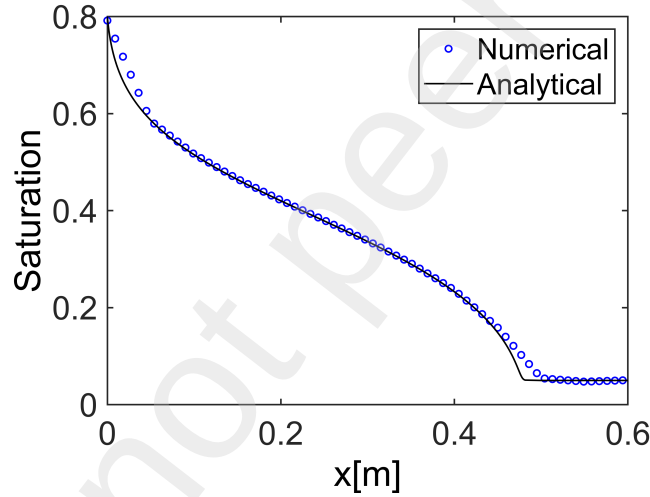


Fig. 3 Comparison of numerical solution and analytical solution of McWorther problem.

dimensionless viscosity $\mathcal{M}$ defined for the KGD fracture as (Garagash, 2006)

$$\mathcal{M} = \frac{\mu' Q}{E'} \left(\frac{E'}{K'} \right)^4, \quad (45)$$

with $K' = \sqrt{\frac{32G_c E'}{\pi}}$, $\mu' = 12\mu$, $E' = \frac{E}{1-\nu^2}$. And if $\mathcal{M} < \mathcal{M}_c = 3.4 \times 10^{-3}$, the KGD fracture

is toughness dominated. In our setting, $\mathcal{M} = 3.8 \times 10^{-7}$ and $\mathcal{M} < \mathcal{M}_c^2$. Fig. 5 compares the numerical results against the analytical solution (Garagash, 2006). The pressure of injection point, fracture length and fracture width all demonstrate a good agreement.

Table 2 Mechanical and flow parameters for KGD problem.

Input parameters	Value	Unit
Young's modulus (E)	17	GPa
Poisson's ratio (ν)	0.2	-
Permeability ($\mathbf{K}_m$)	1×10^{-18}	m^2
Fluid viscosity (μ)	1×10^{-8}	Pa·s
Injection rate (Q)	2×10^{-3}	m^3/s
Critical surface energy release rate (G_c)	300	N/m

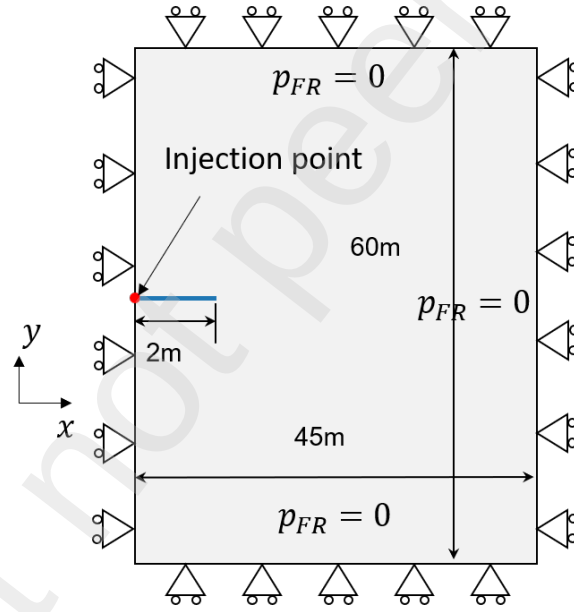


Fig. 4 Schematic of KGD problem.

²The effective critical surface energy release rate G_c in the phase-field model needs to be adjusted to account for the discretization (Bourdin et al., 2008; Tanné et al., 2018; Yoshioka et al., 2020). With the mesh size h_e and the characteristic length ℓ , the modification is given by

$$G_c^{\text{eff}} = G_c \left(1 + \frac{h_e}{4c_n \ell} \right).$$

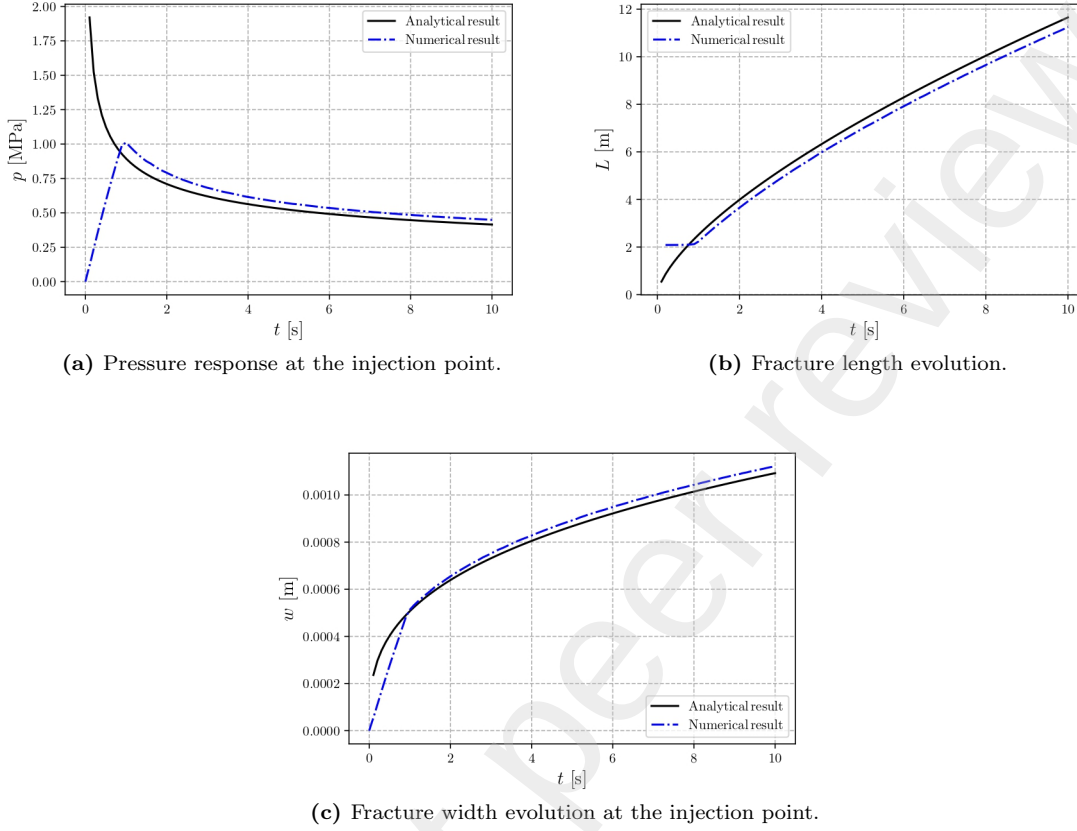


Fig. 5 Comparisons of numerical solutions and analytical solutions of KGD problem.

5. Numerical experiments

In this section, we highlight the differences between water-based and CO₂-based fracturing through a series of numerical experiments. We begin by comparing fracturing with the two fluids under isothermal conditions, followed by cases involving varying injection temperatures. Next, we emphasize the importance of two-phase flow modeling by comparing the two-phase flow model against a simulation of the same scenario based on a single-phase CO₂ flow assumption. Finally, we compare water-based and CO₂ fracturing in the presence of natural fractures. To capture the dependence of CO₂ density on temperature and pressure, we employ the Peng–Robinson equation of state (Peng and Robinson, 1976) (see Appendix A for details).

5.1. Comparison between water-based and supercritical CO₂ fracturing

We simulated water and CO₂ injection into a pre-existing crack $[3.98 \text{ m}, 4.02 \text{ m}] \times \{0 \text{ m}\}$ in the domain $[0 \text{ m}, 8 \text{ m}] \times [-2 \text{ m}, 2 \text{ m}]$ (Fig. 6) with an injection rate of $2\text{e-}5 \text{ m}^3/\text{s}$. The initial pressure in the domain is 15 MPa, and the in-situ stresses of $\sigma_{xx} = 22 \text{ MPa}$ and $\sigma_{yy} = 20 \text{ MPa}$ were imposed

through traction loadings on all the boundaries except $y = 0$, where the normal displacement was constrained. For hydraulic and thermal processes, all the boundaries were set as drained and isothermal conditions. Table 3 lists all the material properties in this example.

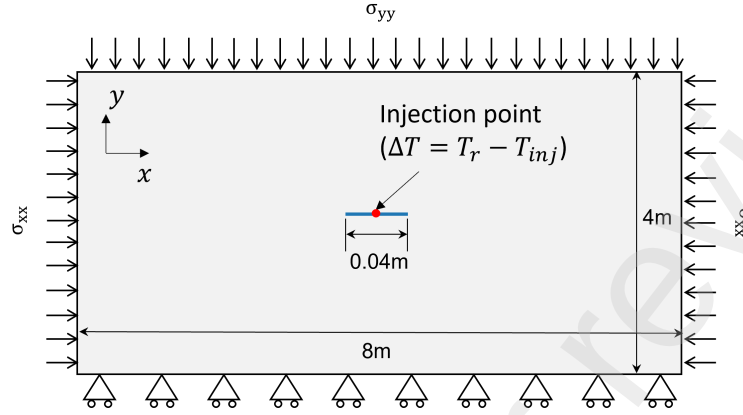


Fig. 6 The schematic of a single fracture in the middle of the domain.

Table 3 Parameters for single-cracked model.

Input parameters	Value	Unit
Young's modulus (E)	25	GPa
Poisson's ratio (ν)	0.2	-
Biot's coefficient (α_m)	0.6	-
Permeability (K_m)	4e-16	m ²
Thermal conductivity of solid, water and CO ₂ (λ)	3, 0.5, 0.03	W/(m·K)
Thermal expansivity (α_s)	8×10^{-6}	-
Fluid viscosity of water and CO ₂ (μ)	5×10^{-4} , 5×10^{-5}	Pa·s
Critical surface energy release rate (G_c)	50	N/m
Initial temperature (T_r)	353.15	K
Injection temperature (T_{inj})	313.15	K

The first simulation cases compare water injection to CO₂ injection under isothermal conditions, i.e., $\Delta T = 0$ (Fig 7). For the water injection case, the pressure reaches the critical pressure³ (Fig 7a),

³The critical pressure will be 31.2 MPa based on the analytical solution $\left(\sigma_{yy} + \sqrt{\frac{E'G_c}{l_o\pi}}\right)$ (Bourdin et al., 2012),

and the fracture begins to propagate (Fig. 7b). However, in the CO₂ injection case, the pressure does not build up enough even after 300 s, due to the low viscosity of CO₂ (Fig. 7), and the fracture does not grow (Fig. 7b).

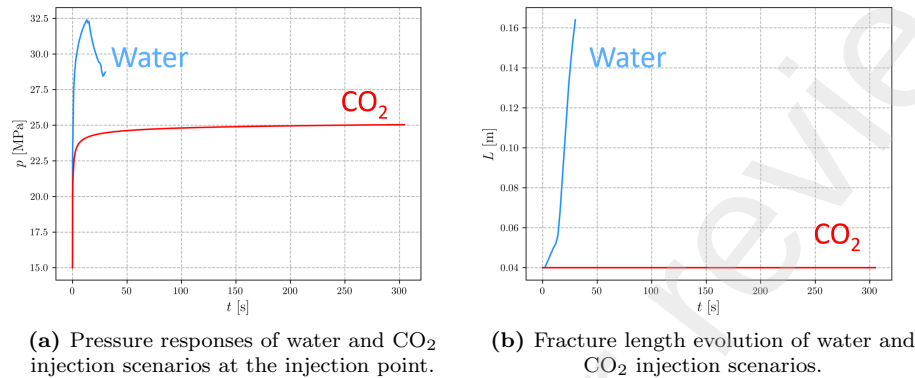


Fig. 7 Simulated pressure responses (a) and fracture length evolution (b) of water and CO₂ injection scenarios under isothermal condition.

Next, we repeated the same simulations with a lower injection temperature of 313.15 K (i.e., $\Delta T = 40$ K). For the water injection case, the peak pressure is lower (Fig. 8) compared to the isothermal case, as the cold injection temperature causes the rock to contract, thereby reducing the compressive stress. Again, in CO₂ injection case, the pressure does not build up as much as the water injection case. However, due to the cold injection fluid, the fracture begins to gradually propagate right from the beginning despite the subcritical fluid pressure build-up within the fracture. When its growth accelerates around 100 s, the injection pressure drops slightly.

For the water injection case, the temperature decreases predominantly along the fracture while the reduced temperature profile is more diffused in the CO₂ injection case due to the strong diffusion and the weak surface tension of CO₂ (Fig. 9). Prior to the onset of fracture propagation, CO₂ diffuses into the reservoir formation from the initial fracture. Once the fracture starts to propagate, the CO₂ travels faster along the growing fracture, developing an advection-diffusion mixed CO₂ saturation profile.

5.2. CO₂ fracturing under non-isothermal conditions

This section explores the fracturing behavior under CO₂ injection at three different injection temperatures ($\Delta T = 40$ K, 50 K, 60 K), using the same setup as in Sec. 5.1. As before, pressure does not build up significantly at the injection point (Fig. 10a), and no clear break-down is observed. However, whenever the pressure drops slightly (around 100 s for $\Delta T = 40$ K, around 40 s for $\Delta T = 50$ K, and around 30 s for $\Delta T = 60$ K cases), the fracture growth accelerates similarly to the previous CO₂ injection case. The greater the temperature difference (ΔT), the earlier the acceleration in

assuming no leak-off and infinite domain boundaries.

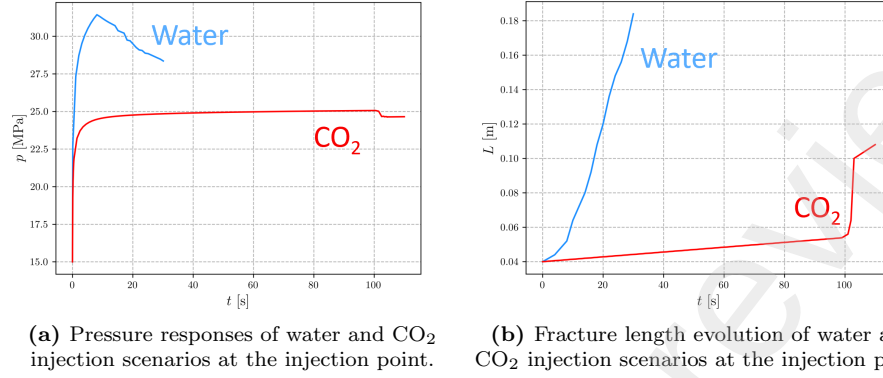


Fig. 8 Simulated pressure responses (a) and fracture length evolution (b) of water and CO₂ injection scenarios under non-isothermal condition.

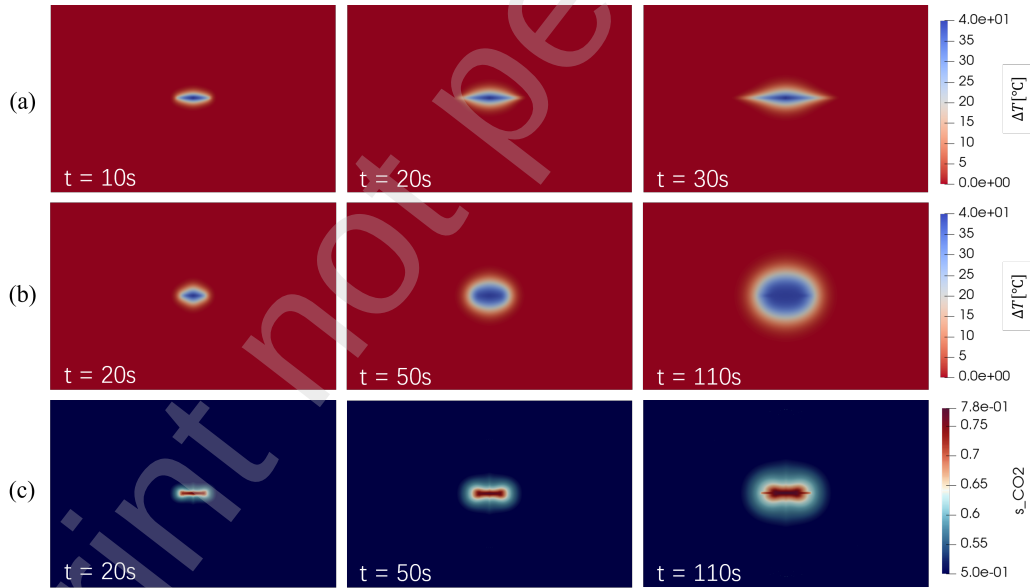


Fig. 9 Temperature difference (ΔT) profiles of (a) water injection and (b) CO₂ injection cases, and (c) CO₂ saturation profiles over time.

fracture propagation begins (Fig. 10b), and the wider the fracture openings are at the injection point (Fig. 10c).

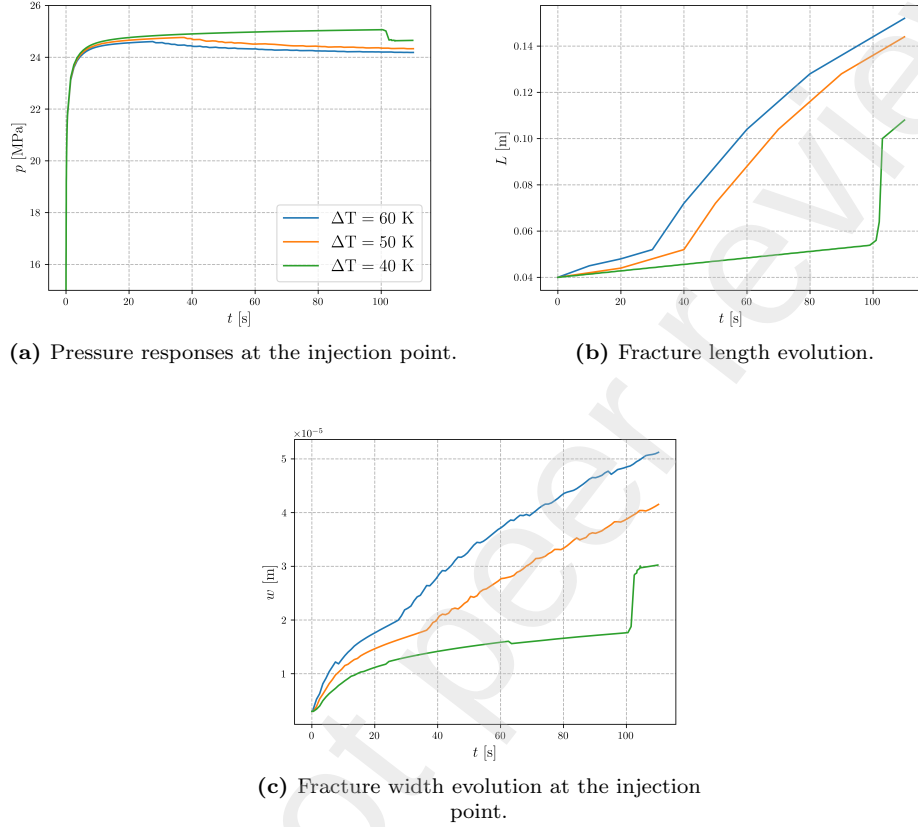


Fig. 10 Simulated CO₂ injection into a fracture under three different injection temperatures ($\Delta T = 40$ K, 50 K, 60 K).

With the increasing temperature difference, the mode of CO₂ transport shifts from diffusion-dominated to advection-dominated. As the fracture propagation accelerates, CO₂ transport becomes more strongly influenced by the fracture. This shift reduces the average CO₂ saturation in the reservoir, which may be beneficial in terms of CO₂ storage (Fig. 11).

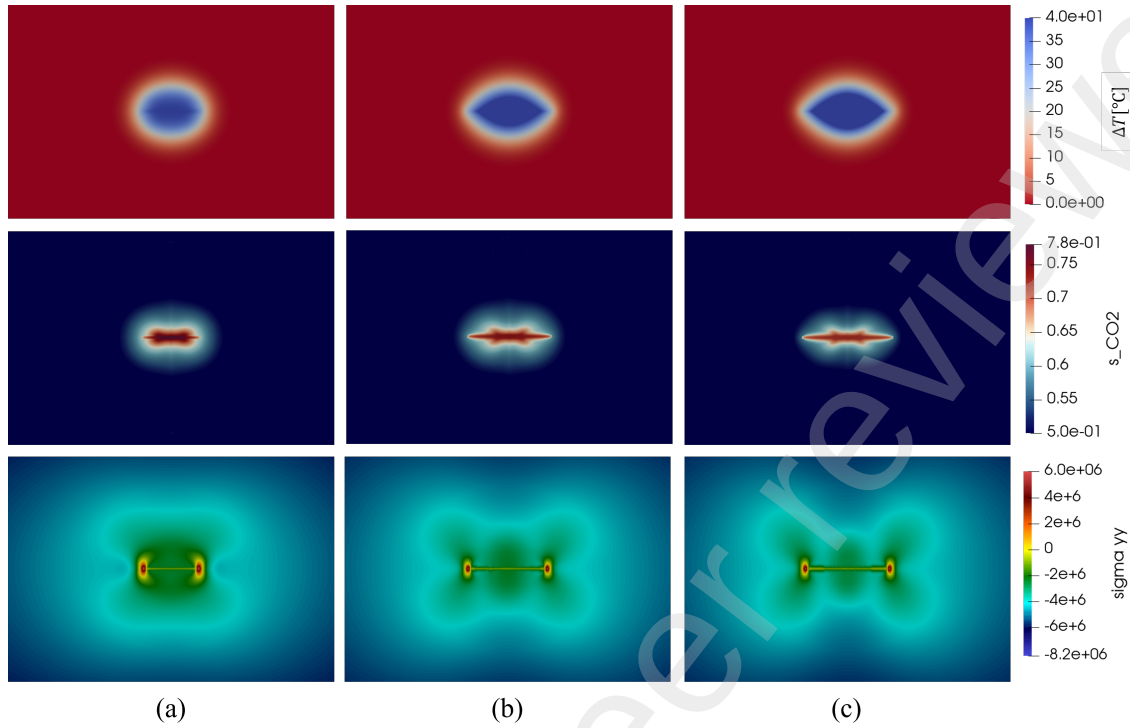


Fig. 11 Comparison of temperature, saturation and vertical stress distribution in the cases with $\Delta T = 40$ K (a), 50 K (b) and 60 K (c) at the end of the simulation time (110 s).

Lower injection temperatures also reduce the effective stress along the propagating fracture in the y -direction (Fig. 10(c)). Compared to the reduction of effective stress during water fracturing discussed in (Liu et al., 2024a), the temperature decreases more near the tip of the fracture, which results from uniform thermal diffusion with low-viscosity fluid.

5.3. Two-phase flow effects

This section emphasizes the importance of properly modeling two-phase fluid flow by comparing it with a simplified single-phase flow model. Assuming single-phase CO_2 flow, we simulated the same fracturing scenarios using the parameters listed in Table 3 with a temperature difference of $\Delta T = 40$ K. In the single-phase case, the pressure build-up is significantly lower than in the two-phase flow scenario (Fig. 12a), and fracture propagation does not occur (Fig. 12b). This difference highlights a key aspect of CO_2 fracturing: as a low-viscosity, non-wetting phase, CO_2 injected into water-saturated porous media has a relative permeability much smaller than one as the water saturation is high in the beginning. This leads to a higher pressure required to induce fracture propagation. In contrast, the single-phase model neglects capillary effects, resulting in insufficient pressure to propagate the fracture.

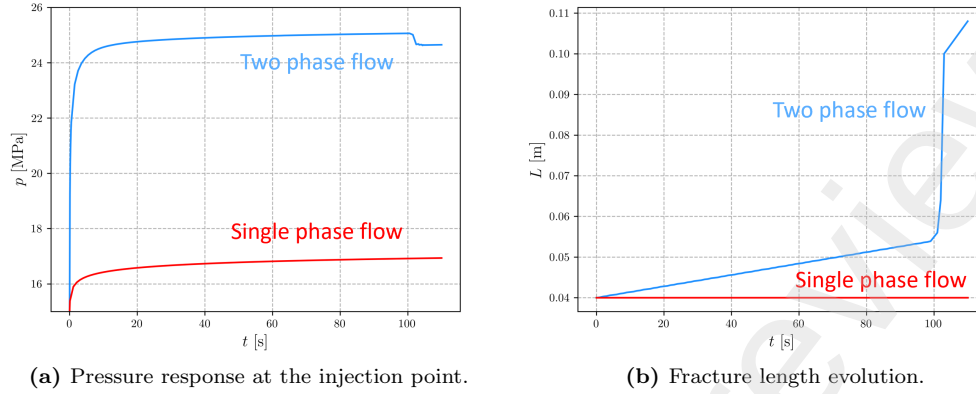


Fig. 12 Propagation of a single fracture under the assumptions of two phase and single phase flow.

5.4. Interactions with weak interfaces

In this section, we highlight the differences between water and CO₂ injection induced fracturing in the presence of weak interfaces (e.g., defects or natural fractures). Weak interfaces in our simulation were modeled as planes with reduced fracture toughness (G_c), following the approach proposed by Yoshioka et al. (2020). As shown in Fig. 13, a weak interface is placed at each end of the initial crack, inclined at 45° to the x -direction. The fracture toughness of the weak interfaces is set to 40% of that of the bulk rock formation, and no frictional shear slippage is considered along the interfaces under compression. The in-situ stresses in the x - and y -directions (σ_{xx} and σ_{yy}) are 23 MPa and 20 MPa, respectively. The temperature difference between the injection fluid and the reservoir formation is 50 K, and all other parameters are the same as the previous numerical examples.

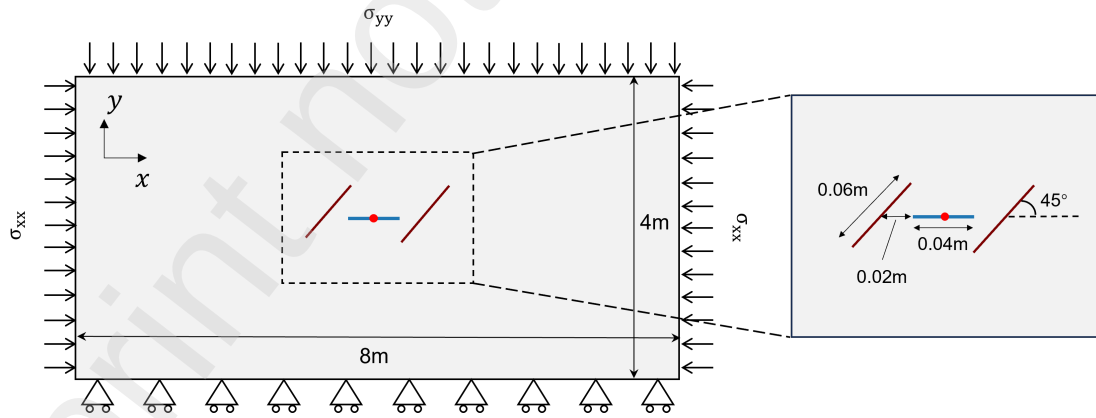


Fig. 13 The schematic of a single fracture with natural fractures.

Fig. 14 compares fracture interactions with weak interfaces in the water and CO₂ injection cases.

350 In the water injection case, fracture propagation is only slightly influenced by the interfaces, and the
 351 fracture essentially propagates straight through the interfaces (Fig.14(a)). With CO₂ injection, the
 352 fracture is more receptive to weak interfaces; its propagation is disturbed when encountering them
 353 (Fig.14(b)). In both cases, however, the stress differential (3MPa) is sufficient for the fractures to
 354 propagate in the direction of the maximum in-situ stress, i.e., the x -direction.

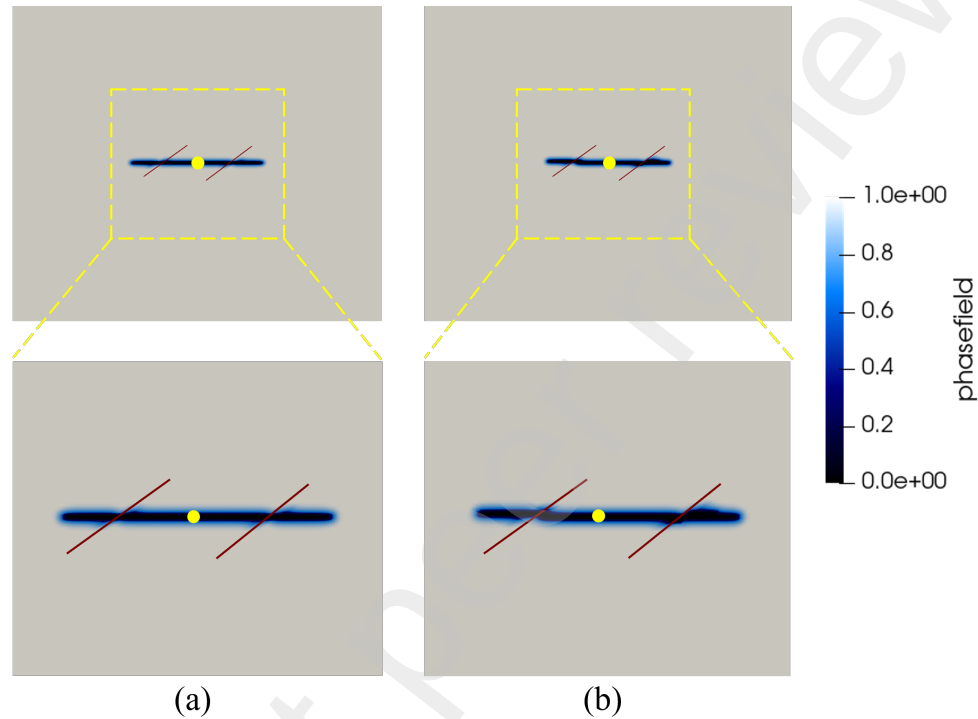


Fig. 14 The fracture interacting with weak interfaces in water (a) and CO₂ (b) fracturing.

355 When the fracture passes through the interface after approximately 12.5 s of water injection,
 356 the pressure drops after the peak while, in the CO₂ fracturing, the pressure drops only slightly and
 357 exhibits oscillations which indicates the interaction with the natural fractures (Fig. 15).

358 The CO₂ injection simulation was repeated with the stress difference of 0 MPa. Fig. 16 shows
 359 that the fracture changes its direction when it hits the weak interfaces and propagates along the
 360 interfaces. The fracture also begins to propagate earlier with a lower critical pressure (Fig. 17).

361 The saturation profiles of CO₂ under different stress differentials are compared in Fig.18.
 362 When interacting with natural fractures, the injected CO₂ flows along the deflected fracture path
 363 (Fig.18(a)) and leaks into the branching fractures (Fig. 18(b)).

364 6. Discussion

365 Our proposed numerical approach overcomes the limitations of previous models that relied on
 366 partially coupled hydro-mechanical (HM) formulations or assumed single-phase flow. By imple-
 367 menting a fully coupled TH²M framework, we enable a more realistic and comprehensive analysis

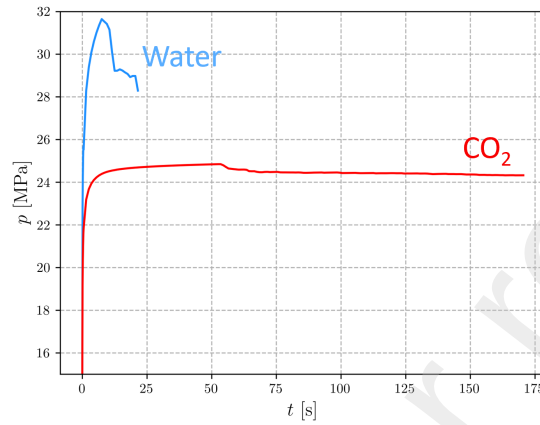


Fig. 15 Pressure response at injection point with weak interfaces in water and CO₂ fracturing.

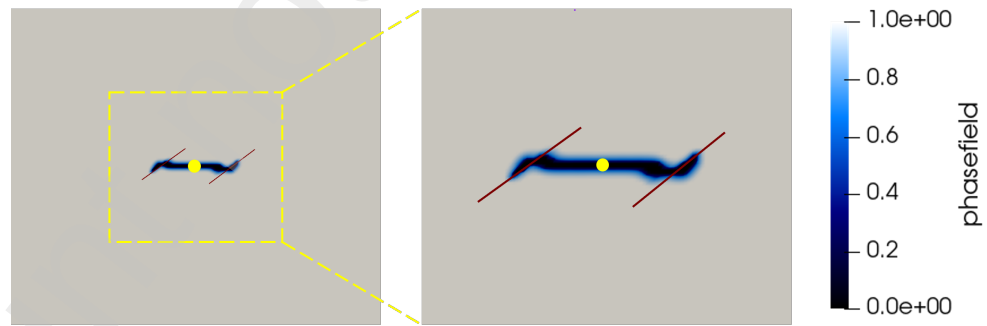


Fig. 16 The fracture interacting with weak interfaces under $\Delta\sigma = 0$ MPa.

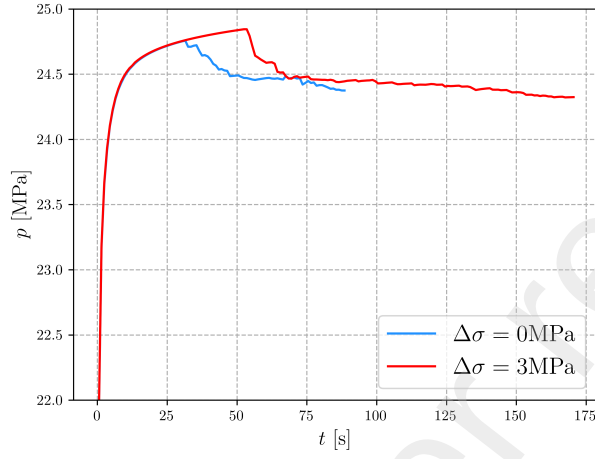


Fig. 17 Pressure response at injection point with weak interfaces in CO₂ fracturing under $\Delta\sigma = 0$ MPa and 3 MPa.

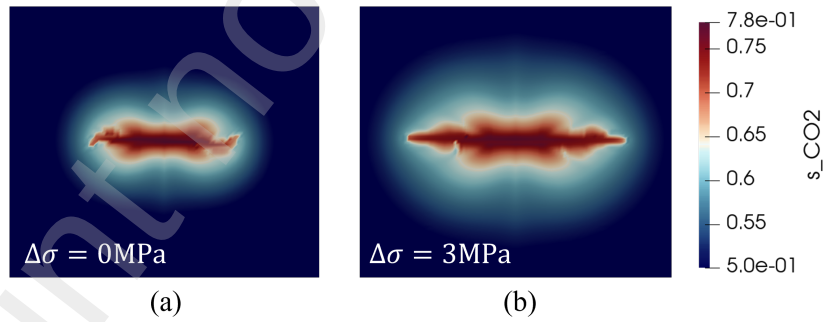


Fig. 18 CO₂ saturation with weak interfaces under $\Delta\sigma = 0$ MPa and 3 MPa.

of fracture initiation and propagation mechanisms during subsurface CO₂ injection. Our numerical results show that CO₂ injection does not lead to the high pressure build-up or subsequent pressure drop as observed in experimental studies (Song et al., 2019; Liu et al., 2017; Ishida et al., 2021). We also find that the interaction between hydraulic fractures and pre-existing weak interfaces becomes more complex with CO₂ injection. Due to its low viscosity and slow flow rate, CO₂ more readily infiltrates these features, promoting branching and complex fracture geometries. As demonstrated in Section 5.4, in-situ stress differences significantly influence fracture propagation paths. These findings underscore the importance of accurately characterizing the in-situ stress field during early site assessments to improve predictions of fracture behavior in naturally fractured reservoirs.

In this study, weak interfaces are represented by assigning a lower fracture toughness than that of the surrounding rock. However, additional factors may need to be considered. For instance, natural fractures typically exhibit a Biot coefficient close to 1, significantly higher than that of intact rock, which can induce greater tensile stress, as shown analytically in You and Yoshioka (2025). When injecting low-viscosity fluids such as supercritical CO₂, the pressure front can travel farther, potentially triggering fracture initiation at distant natural fractures, a phenomenon referred to as “remote fracturing” (You and Yoshioka, 2025). Compared to water-based fracturing, remote fracturing is more likely with CO₂ injection due to its ability to reach supercritical conditions under typical subsurface environments. This highlights the importance of monitoring for remote fracturing during field operations involving CO₂. Another critical factor is the permeability of natural fractures. High-permeability fractures tend to attract the propagating fracture front and dissipate pressure, promoting the formation of complex fracture networks.

A potential future study is to extend the current TH²M phase-field model to incorporate other fracturing fluids, such as liquid nitrogen (Yang et al., 2024), liquefied petroleum gas (Gandossi and Von Estorff, 2015), or high-energy gas (Yang et al., 1992). This would likely require the use of fluid-specific equations of state to accurately model two-phase flow behavior. Moreover, these thermally sensitive fluids may undergo phase transitions near the fracture tip, where temperature and pressure can change rapidly. Such conditions can cause complex flow environments in which multiple fluid phases (supercritical, gaseous, and liquid) coexist (Osipov, 2017).

7. Conclusions

This paper proposes a novel variational phase-field fracture approach that considers non-isothermal CO₂-water two-phase flow in deformable porous media. Building on our previous thermo-hydro-mechanical (THM) phase-field model, the fluid flow component has been extended to the two-phase case by incorporating capillary effects. Saturation is determined from the capillary pressure relationship. Furthermore, the equivalent liquid pressure is used to represent the pore fluid energy within the total energy functional. A hybrid monolithic-staggered scheme has been implemented to solve the TH²M phase-field system, incorporating an adapted fixed-stress split method that accounts for thermal stress, within the open-source finite element code OpenGeoSys (Bilke et al., 2023). The proposed model has been verified against analytical solutions for one-dimensional two-phase flow transport (McWhorter problem) and plane-strain hydraulic fracture propagation (KGD problem).

Through numerical experiments, we compared CO₂ fracturing with water-based fracturing to highlight the distinct characteristics of CO₂ injection. The following conclusions can be drawn:

1. Cold CO₂ injection can initiate fracture propagation at a low injection rate, even below the critical pressure.

2. A single-phase assumption is inadequate for simulating CO₂ fracturing, as it neglects capillary effects and changes in relative permeability.
3. Fracture growth becomes more pronounced with colder CO₂ injection.
4. When interacting with weak interfaces, fracture propagation induced by CO₂ tends to develop a more complex morphology.

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

No data was used for the research described in the article.

Acknowledgement

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Appendix

Appendix A. Peng-Robinson equation for the state of CO₂

Peng-Robinson equation of state (PR-EOS) is a widely used cubic equation of state for describing the behaviour of real gases, particularly hydrocarbons. It accounts for non-ideal behaviour of fluids over a range of temperatures and pressures. The equation is given in terms of the molar density ρ as:

$$P = \frac{RT\rho}{1 - b\rho} - \frac{a\rho^2}{1 + 2b\rho - b^2\rho^2} \quad (\text{A.1})$$

where P is the pressure, T the temperature, ρ the molar density, R the universal gas constant, and a , b are substance-specific parameters.

The parameters a and b are computed from the critical temperature T_c in Kelvin, critical pressure p_c in Pascal, and (dimensionless) acentric factor ω as follows:

$$a = 0.457235 \frac{R^2 T_c^2}{p_c} \quad (\text{A.2})$$

$$b = 0.077796 \frac{RT_c}{p_c} \quad (\text{A.3})$$

The Peng-Robinson equation is applicable for a wide range of substances (gases and liquids), particularly hydrocarbons, at conditions ranging from subcritical to supercritical. The EOS is not suitable for solid phases or very low-temperature applications where real gases behave ideally.

439 Appendix B. Discretization of TH²M phase-field modeling with FEM

440 The variables v , T , p_c , p_{CR} and $\mathbf{u}$ are defined at integration points as nodal values so that the
441 field discretization form for the variables themselves and the respective gradients can be written as

$$\begin{aligned}
 \mathbf{u} &= \sum_{i=1}^n N_i^u u_i = \mathbf{N}_u \hat{\mathbf{u}}, \quad v = \sum_{i=1}^n N_i^v v_i = \mathbf{N}_v \hat{v}, \quad p_c = \sum_{i=1}^n N_i^p p_{c,i} = \mathbf{N}_p \hat{p}_c \\
 p_{CR} &= \sum_{i=1}^n N_i^p p_{CR,i} = \mathbf{N}_p \hat{p}_{CR}, \quad T = \sum_{i=1}^n N_i T_i = \mathbf{N}_T \hat{T}, \quad \varepsilon = \sum_{i=1}^n B_i^u u_i = \mathbf{B}_u \hat{\mathbf{u}} \\
 \nabla v &= \sum_{i=1}^n B_i^v v_i = \mathbf{B}_v \hat{v}, \quad \nabla p_c = \sum_{i=1}^n B_i^p p_{c,i} = \mathbf{B}_p \hat{p}_c, \quad \nabla p_{CR} = \sum_{i=1}^n B_i^p p_{CR,i} = \mathbf{B}_p \hat{p}_{CR} \\
 \nabla T &= \sum_{i=1}^n B_i^T T_i = \mathbf{B}_T \hat{T}
 \end{aligned} \tag{B.1}$$

442 where $\hat{T}$, $\hat{p}_c$, $\hat{p}_{CR}$, $\hat{\mathbf{u}}$ and $\hat{v}$ represent the vectors of the integration point values in one element.
443 Note that ε is a vector of independent strain variables but not a tensor, e.g., $\varepsilon = [\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy}]^T$ in
444 2D problem. Shape functions $\mathbf{N}_u$, $\mathbf{N}_T$, $\mathbf{N}_{p_c}$, $\mathbf{N}_{p_{CR}}$ and $\mathbf{N}_v$ are represented as matrixes for vector
445 field $\mathbf{u}$ and a vector for scalar field like p , v and T and they are also used as test functions for each
446 process:

$$\begin{cases}
 \mathbf{N}_u = \begin{bmatrix} N_1^u & 0 & \dots & N_i^u & 0 & \dots & N_n^u & 0 \\ 0 & N_1^u & \dots & 0 & N_i^u & \dots & 0 & N_n^u \end{bmatrix} \\
 \mathbf{N}_T = \begin{bmatrix} N_1^T & \dots & N_i^T & \dots & N_n^T \end{bmatrix} \\
 \mathbf{N}_{p_c} = \begin{bmatrix} N_1^{p_c} & \dots & N_i^{p_c} & \dots & N_n^{p_c} \end{bmatrix} \\
 \mathbf{N}_{p_{CR}} = \begin{bmatrix} N_1^{p_{CR}} & \dots & N_i^{p_{CR}} & \dots & N_n^{p_{CR}} \end{bmatrix} \\
 \mathbf{N}_v = \begin{bmatrix} N_1^v & \dots & N_i^v & \dots & N_n^v \end{bmatrix}
 \end{cases} \tag{B.2}$$

447 The Galerkin finite element method considers the same shape functions in the present work, i.e.,
448 $N_i^u = N_i^T = N_i^{p_c} = N_i^{p_{CR}} = N_i^v$.

$$\{\mathbf{T}\}_m = \{\mathbf{T}\}_{m-1} - [\mathbf{K}^{TT}]_{m-1}^{-1} \{\mathbf{r}^T\}_{m-1}, \tag{B.3}$$

$$\begin{Bmatrix} \mathbf{p}_{CR} \\ \mathbf{p}_c \end{Bmatrix}_m = \begin{Bmatrix} \mathbf{p}_{CR} \\ \mathbf{p}_c \end{Bmatrix}_{m-1} - \begin{bmatrix} \mathbf{K}^{C\mathbf{p}_{CR}} & \mathbf{K}^{C\mathbf{p}_c} \\ \mathbf{K}^{C\mathbf{p}_{CR}} & \mathbf{K}^{W\mathbf{p}_c} \end{bmatrix}_{m-1}^{-1} \begin{Bmatrix} \mathbf{r}^C \\ \mathbf{r}^W \end{Bmatrix}_{m-1}, \tag{B.4}$$

$$\begin{Bmatrix} \mathbf{u} \\ \mathbf{v} \end{Bmatrix}_m = \begin{Bmatrix} \mathbf{u} \\ \mathbf{v} \end{Bmatrix}_{m-1} - \begin{bmatrix} \mathbf{K}^{uu} & 0 \\ 0 & \mathbf{K}^{vv} \end{bmatrix}_{m-1}^{-1} \begin{Bmatrix} \mathbf{r}^u \\ \mathbf{r}^v \end{Bmatrix}_{m-1}. \tag{B.5}$$

451 The residuals of each field are given as

$$\begin{aligned}
 \mathbf{r}_m^T = & \int_{\Omega} 3\beta K_{\text{eff}} \mathbf{N}_T^T \mathbf{N}_T \hat{T}^{k,m} \frac{\varepsilon_v(\hat{\mathbf{u}}^{k,m-1}) - \varepsilon_v(\hat{\mathbf{u}}^{k-1})}{\Delta t} dV \\
 & + \int_{\Omega} \mathbf{N}_T^T \mathbf{N}_T (\rho c)_m \frac{\hat{T}^{k,m} - \hat{T}^{k-1}}{\Delta t} dV - \int_{\Omega} \mathbf{B}_T^T \mathbf{N}_T \rho_{LR} c_{p,L} \hat{\mathbf{q}}_L^{k,m-1} T^{k,m} dV \\
 & - \int_{\Omega} \mathbf{B}_T^T \mathbf{N}_T \rho_{CR} c_{p,C} \hat{\mathbf{q}}_C^{k,m-1} T^{k,m} dV + \int_{\Omega} \mathbf{B}_T^T \mathbf{B}_T \lambda_{\text{eff}} \hat{T}^{k,m} dV \\
 & - \int_{\Omega} \mathbf{N}_T^T Q_T dV + \int_{\partial_N \Omega} \mathbf{N}_T^T \mathbf{q}_{Tn} dS
 \end{aligned} \tag{B.6}$$

452

$$\begin{aligned}
 \mathbf{r}_m^W = & \int_{\Omega} \alpha S_L^{k,m-1} \rho_{LR} \mathbf{N}_p^T \frac{\varepsilon_v(\hat{\mathbf{u}}^{k,m-1}) - \varepsilon_v(\hat{\mathbf{u}}^{k-1})}{\Delta t} dV + \int_{\Omega} S_L^{k,m-1} \rho_{LR} \mathbf{N}_p^T \frac{1}{M_p} \mathbf{N}_p \frac{\hat{p}_{CR}^{k,m} - \hat{p}_{CR}^{k-1}}{\Delta t} dV \\
 & - \int_{\Omega} S_L^{k,m-1} \rho_{LR} \mathbf{N}_p^T \frac{1}{M_T} \mathbf{N}_T \frac{\hat{T}^{k,m} - \hat{T}^{k-1}}{\Delta t} dV + \int_{\Omega} \rho_{LR} \mathbf{B}_p^T \frac{k_L^{\text{rel}} \mathbf{k}_s}{\mu_{LR}} \mathbf{B}_p dV (\hat{p}_{CR}^{k,m} - \hat{p}_c^{k,m} - \mathbf{b}) \\
 & + \int_{\Omega} \phi S_L^{k,m-1} \mathbf{N}_p^T \frac{\rho_{LR}^{k,m} - \rho_{LR}^{k-1}}{\Delta t} dV + \int_{\Omega} \frac{\alpha^2}{K} S_L^{k,m-1} \rho_{LR} \mathbf{N}_p^T \mathbf{N}_p dV \frac{\hat{p}_{FR}^{k,m} - \hat{p}_{FR}^{k,m-1}}{\Delta t} \\
 & + \int_{\Omega} \phi \rho_{LR} \mathbf{N}_p^T \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} dV - \int_{\Omega} \mathbf{N}_p^T S_L^{k,m-1} \rho_{LR} p_c \frac{1}{M_p} \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} dV \\
 & - \int_{\Omega} S_L^{k,m-1} \mathbf{N}_p^T \mathbf{N}_p \rho_{LR} \frac{1}{M_p} \frac{\hat{p}_c^{k,m} - \hat{p}_c^{k-1}}{\Delta t} S_L^{k,m-1} dV + \int_{\Omega} 3\alpha \alpha_s S_L^{k,m-1} \rho_{LR} \mathbf{N}_p^T \mathbf{N}_T \frac{\hat{T}^{k,m} - \hat{T}^{k,m-1}}{\Delta t} dV \\
 & - \int_{\Omega} \mathbf{N}_p^T Q_L dV + \int_{\partial_N \Omega} \mathbf{N}_p^T q_n dS
 \end{aligned} \tag{B.7}$$

453

$$\begin{aligned}
 \mathbf{r}_m^C = & \int_{\Omega} \alpha S_C^{k,m-1} \rho_{CR} \mathbf{N}_p^T \frac{\varepsilon_v(\hat{\mathbf{u}}^{k,m-1}) - \varepsilon_v(\hat{\mathbf{u}}^{k-1})}{\Delta t} dV + \int_{\Omega} S_C^{k,m-1} \rho_{CR} \mathbf{N}_p^T \frac{1}{M_p} \mathbf{N}_p \frac{\hat{p}_{CR}^{k,m} - \hat{p}_{CR}^{k-1}}{\Delta t} dV \\
 & - \int_{\Omega} S_C^{k,m-1} \rho_{CR} \mathbf{N}_p^T \frac{1}{M_T} \mathbf{N}_T \frac{\hat{T}^{k,m} - \hat{T}^{k-1}}{\Delta t} dV + \int_{\Omega} \rho_{CR} \mathbf{B}_p^T \frac{k_C^{\text{rel}} \mathbf{k}_s}{\mu_{CR}} \mathbf{B}_p dV (\hat{p}_{CR}^{k,m} - \mathbf{b}) \\
 & + \int_{\Omega} \phi S_C^{k,m-1} \mathbf{N}_p^T \frac{\rho_{CR}^{k,m} - \rho_{CR}^{k-1}}{\Delta t} dV + \int_{\Omega} \frac{\alpha^2}{K} S_C^{k,m-1} \rho_{CR} \mathbf{N}_p^T \mathbf{N}_p dV \frac{\hat{p}_{FR}^{k,m} - \hat{p}_{FR}^{k,m-1}}{\Delta t} \\
 & - \int_{\Omega} \phi \rho_{CR} \mathbf{N}_p^T \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} dV - \int_{\Omega} \mathbf{N}_p^T S_C^{k,m-1} \rho_{CR} p_c \frac{1}{M_p} \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} dV \\
 & - \int_{\Omega} S_C^{k,m-1} \mathbf{N}_p^T \mathbf{N}_p \rho_{CR} \frac{1}{M_p} \frac{\hat{p}_c^{k,m} - \hat{p}_c^{k-1}}{\Delta t} S_L^{k,m-1} dV + \int_{\Omega} 3\alpha \alpha_s S_C^{k,m-1} \rho_{CR} \mathbf{N}_p^T \mathbf{N}_T \frac{\hat{T}^{k,m} - \hat{T}^{k,m-1}}{\Delta t} dV \\
 & - \int_{\Omega} \mathbf{N}_p^T Q_C dV + \int_{\partial_N \Omega} \mathbf{N}_p^T q_n dS
 \end{aligned} \tag{B.8}$$

454

$$\begin{aligned} \mathbf{r}_m^u &= \int_{\Omega} g(v) \mathbf{B}_u^T \sigma_e^{k,m} dV - \int_{\Omega} \mathbf{B}_u^T \alpha(v) \mathbf{N}_p \hat{p}_{FR}^{k,m} \mathbf{I} dV \\ &\quad - \int_{C_N} \mathbf{N}_u^T \bar{\mathbf{t}} dS \end{aligned} \quad (\text{B.9})$$

455

$$\begin{aligned} \mathbf{r}_m^v &= \int_{\Omega} 2(1-k) \mathbf{N}_v^T \mathbf{N}_v \psi_+(\mathbf{u})^{k,m-1} dV \hat{v} + \frac{G_c}{4c_n} \int_{\Omega} \left[-\frac{n}{\ell} (1 - \mathbf{N}_v \hat{v})^{n-1} \mathbf{N}_v^T + 2\ell \mathbf{B}_v^T \mathbf{B}_v \hat{v} \right] dV \\ &\quad + \int_{\Omega} 2(1-k) \mathbf{N}_v^T \frac{\mathbf{N}_p \hat{p}_{FR}}{2} H(\text{Tr}(\varepsilon_e)) (1 - \alpha_m) dV \hat{v} \end{aligned} \quad (\text{B.10})$$

456 and the Jacobian matrices for each field are given as

$$\begin{aligned} \mathbf{K}^{TT} &= \frac{\partial \mathbf{r}^T}{\partial \hat{T}} = \int_{\Omega} 3\beta K_{\text{eff}} \mathbf{N}_T^T \mathbf{N}_T \frac{\varepsilon_v(\hat{\mathbf{u}}^{k,m-1}) - \varepsilon_v(\hat{\mathbf{u}}^{k-1})}{\Delta t} dV \\ &\quad + \int_{\Omega} \mathbf{N}_T^T \mathbf{N}_T (\rho c)_m \frac{1}{\Delta t} dV + \int_{\Omega} \mathbf{B}_T^T \lambda_{\text{eff}} \mathbf{B}_T dV \\ &\quad - \int_{\Omega} \mathbf{B}_T^T \mathbf{N}_T \rho_{LR} c_{p,L} \hat{\mathbf{q}}_L^{k,m-1} dV - \int_{\Omega} \mathbf{B}_T^T \mathbf{N}_T \rho_{CR} c_{p,C} \hat{\mathbf{q}}_C^{k,m-1} dV \end{aligned} \quad (\text{B.11})$$

457

$$\begin{aligned} \mathbf{K}^{Wp_c} &= \frac{\partial \mathbf{r}^W}{\partial \hat{p}_c} = - \int_{\Omega} \rho_{LR} \mathbf{B}_p^T \frac{k_L^{\text{rel}} \mathbf{k}_s}{\mu_{LR}} \mathbf{B}_p dV \\ &\quad - \int_{\Omega} \frac{\alpha^2}{K} S_L^{k,m-1} \rho_{LR} \mathbf{N}_p^T \mathbf{N}_p dV \frac{1}{\Delta t} - \int_{\Omega} \phi S_L^{k,m-1} \rho_{LR} c_{f,L} \mathbf{N}_p^T \mathbf{N}_p \frac{1}{\Delta t} dV \\ &\quad - \int_{\Omega} \mathbf{N}_p^T \mathbf{N}_p S_L^{k,m-1} \rho_{LR} \frac{1}{M_p} \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} dV - \int_{\Omega} S_L^{k,m-1} \mathbf{N}_p^T \mathbf{N}_p \rho_{LR} \frac{1}{M_p} \frac{1}{\Delta t} S_L^{k,m-1} dV \end{aligned} \quad (\text{B.12})$$

458

$$\mathbf{K}^{Wp_c} = \frac{\partial \mathbf{r}^W}{\partial \hat{p}_c} = -\mathbf{M}_{pc}^W - \mathbf{L}_{pc}^W + \mathbf{A}_{pc}^W + \mathbf{S}_{pc}^W + \mathbf{D}_{pc}^W - \mathbf{F}_{pc}^W \quad (\text{B.13})$$

459

$$\mathbf{K}^{Wp_{CR}} = \frac{\partial \mathbf{r}^W}{\partial \hat{p}_{CR}} = \mathbf{M}_{pCR}^W + \mathbf{L}_{pCR}^W + \mathbf{A}_{pCR}^W + \mathbf{S}_{pCR}^W + \mathbf{D}_{pCR}^W + \mathbf{F}_{pCR}^W \quad (\text{B.14})$$

460

$$\mathbf{K}^{Cp_c} = \frac{\partial \mathbf{r}^C}{\partial \hat{p}_c} = -\mathbf{M}_{pc}^C + \mathbf{L}_{pc}^C + \mathbf{A}_{pc}^C - \mathbf{S}_{pc}^C + \mathbf{D}_{pc}^C - \mathbf{F}_{pc}^C \quad (\text{B.15})$$

461

$$\mathbf{K}^{Cp_{CR}} = \frac{\partial \mathbf{r}^C}{\partial \hat{p}_{CR}} = \mathbf{M}_{pCR}^C + \mathbf{L}_{pCR}^C + \mathbf{A}_{pCR}^C - \mathbf{S}_{pCR}^C + \mathbf{D}_{pCR}^C + \mathbf{F}_{pCR}^C \quad (\text{B.16})$$

$$\mathbf{K}^{uu} = \frac{\partial \mathbf{r}^u}{\partial \hat{\mathbf{u}}} = \int_{\Omega} g(v) \mathbf{B}_u^T \mathbf{C}_+ \mathbf{B}_u dV \quad (\text{B.17})$$

$$\begin{aligned} \mathbf{K}^{vv} &= \frac{\partial \mathbf{r}^v}{\partial \hat{\mathbf{v}}} = \int_{\Omega} 2(1-k) \psi_+(\mathbf{u})^{k,m-1} \mathbf{N}_v^T \mathbf{N}_v dV \\ &+ \int_{\Omega} 2(1-k) \mathbf{N}_v^T \frac{\mathbf{N}_p \hat{p}_{FR}}{2} H(\text{Tr}(\varepsilon_e)) (1 - \alpha_m) dV \\ &+ \frac{G_c}{4c_n} \int_{\Omega} \left[\frac{n(n-1)}{\ell} (1 - \mathbf{N}_v \hat{v})^{n-2} \mathbf{N}_v^T \mathbf{N}_v + 2\ell \mathbf{B}_v^T \mathbf{B}_v \right] dV \end{aligned} \quad (\text{B.18})$$

$$\mathbf{M}_{pc}^W = \int_{\Omega} S_L^{k,m-1} \mathbf{N}_p^T \mathbf{N}_p \rho_{LR} \frac{1}{M_p} \frac{1}{\Delta t} S_L^{k,m-1} dV \quad (\text{B.19})$$

$$\mathbf{M}_{pCR}^W = \int_{\Omega} S_L^{k,m-1} \rho_{LR} \mathbf{N}_p^T \frac{1}{M_p} \mathbf{N}_p \frac{1}{\Delta t} dV \quad (\text{B.20})$$

$$\mathbf{M}_{pc}^C = \int_{\Omega} S_C^{k,m-1} \mathbf{N}_p^T \mathbf{N}_p \rho_{CR} \frac{1}{M_p} \frac{1}{\Delta t} S_L^{k,m-1} dV \quad (\text{B.21})$$

$$\mathbf{M}_{pCR}^C = \int_{\Omega} S_C^{k,m-1} \rho_{CR} \mathbf{N}_p^T \frac{1}{M_p} \mathbf{N}_p \frac{1}{\Delta t} dV \quad (\text{B.22})$$

$$\mathbf{L}_{pc}^W = \mathbf{L}_{pCR}^W = \int_{\Omega} \rho_{LR} \mathbf{B}_p^T \frac{k_L^{\text{rel}} \mathbf{k}_s}{\mu_{LR}} \mathbf{B}_p dV \quad (\text{B.23})$$

$$\mathbf{L}_{pc}^C = 0 \quad (\text{B.24})$$

$$\mathbf{L}_{pCR}^C = \int_{\Omega} \rho_{CR} \mathbf{B}_p^T \frac{k_C^{\text{rel}} \mathbf{k}_s}{\mu_{CR}} \mathbf{B}_p dV \quad (\text{B.25})$$

$$\mathbf{A}_{pc}^W = \int_{\Omega} \mathbf{B}_p^T \left(\frac{\partial \rho_{LR}}{\partial p_c} \frac{k_L^{\text{rel}} \mathbf{k}_s}{\mu_{LR}} + \rho_{LR} \frac{k_L^{\text{rel}}}{\partial p_c} \frac{\mathbf{k}_s}{\mu_{LR}} \right) \mathbf{B}_p \left(\hat{p}_{CR}^{k,m} - \hat{p}_c^{k,m} \right) \mathbf{N}_p dV \quad (\text{B.26})$$

$$\mathbf{A}_{pCR}^W = \int_{\Omega} \mathbf{B}_p^T \left(\frac{\partial \rho_{LR}}{\partial p_{CR}} \frac{k_L^{\text{rel}} \mathbf{k}_s}{\mu_{LR}} \right) \mathbf{B}_p \left(\hat{p}_{CR}^{k,m} - \hat{p}_c^{k,m} \right) \mathbf{N}_p dV \quad (\text{B.27})$$

473

$$\mathbf{A}_{pc}^C = \int_{\Omega} \mathbf{B}_p^T \left(\rho_{CR} \frac{k_C^{\text{rel}}}{\partial p_c} \frac{\mathbf{k}_s}{\mu_{CR}} \right) \mathbf{B}_p \hat{p}_{CR}^{k,m} \mathbf{N}_p dV \quad (\text{B.28})$$

474

$$\mathbf{A}_{pCR}^C = \int_{\Omega} \mathbf{B}_p^T \left(\frac{\partial \rho_{CR}}{\partial p_{CR}} \frac{k_C^{\text{rel}}}{\mu_{CR}} \mathbf{k}_s \right) \mathbf{B}_p \hat{p}_{CR}^{k,m} \mathbf{N}_p dV \quad (\text{B.29})$$

475

$$\begin{aligned} \mathbf{S}_{pc}^W = \int_{\Omega} \mathbf{N}_p^T & \left(\left(\phi \frac{\partial \rho_{LR}}{\partial p_c} - \left(\frac{\partial S_L^{k,m-1}}{\partial p_c} \rho_{LR} + S_L^{k,m-1} \frac{\partial \rho_{LR}}{\partial p_c} \right) p_c \frac{1}{M_p} \right. \right. \\ & \left. \left. - S_L^{k,m-1} \rho_{LR} \frac{1}{M_p} \right) \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} + \left(\phi \rho_{LR} - S_L^{k,m-1} \rho_{LR} p_c \frac{1}{M_p} \right) \frac{\partial S_L^{k,m-1}}{\partial p_c} \frac{1}{\Delta t} \right) \mathbf{N}_p dV \end{aligned} \quad (\text{B.30})$$

476

$$\mathbf{S}_{pCR}^W = \int_{\Omega} \mathbf{N}_p^T \left(\phi \frac{\partial \rho_{LR}}{\partial p_{CR}} - S_L^{k,m-1} \frac{\partial \rho_{LR}}{\partial p_{CR}} p_c \frac{1}{M_p} \right) \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} \mathbf{N}_p dV \quad (\text{B.31})$$

477

$$\begin{aligned} \mathbf{S}_{pc}^C = \int_{\Omega} \mathbf{N}_p^T & \left(\left(\phi \frac{\partial \rho_{CR}}{\partial p_c} + \left(\frac{\partial S_C^{k,m-1}}{\partial p_c} \rho_{CR} + S_C^{k,m-1} \frac{\partial \rho_{CR}}{\partial p_c} \right) p_c \frac{1}{M_p} \right. \right. \\ & \left. \left. + S_C^{k,m-1} \rho_{CR} \frac{1}{M_p} \right) \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} + \left(\phi \rho_{CR} + S_C^{k,m-1} \rho_{CR} p_c \frac{1}{M_p} \right) \frac{\partial S_L^{k,m-1}}{\partial p_c} \frac{1}{\Delta t} \right) \mathbf{N}_p dV \end{aligned} \quad (\text{B.32})$$

478

$$\mathbf{S}_{pCR}^C = \int_{\Omega} \mathbf{N}_p^T \left(\left(\phi \frac{\partial \rho_{CR}}{\partial p_{CR}} + S_C^{k,m-1} \frac{\partial \rho_{CR}}{\partial p_{CR}} p_c \frac{1}{M_p} \right) \frac{S_L^{k,m-1} - S_L^{k-1}}{\Delta t} \right) \mathbf{N}_p dV \quad (\text{B.33})$$

479

$$\mathbf{D}_{pc}^W = \int_{\Omega} \phi \mathbf{N}_p^T \left(\frac{\partial S_L^{k,m-1}}{\partial p_c} \frac{\rho_{LR}^{k,m} - \rho_{LR}^{k-1}}{\Delta t} + S_L^{k,m-1} \frac{\partial \rho_{LR}^{k,m}}{\partial p_c} \frac{1}{\Delta t} \right) \mathbf{N}_p dV \quad (\text{B.34})$$

480

$$\mathbf{D}_{pCR}^W = \int_{\Omega} \phi S_L^{k,m-1} \mathbf{N}_p^T \frac{\partial \rho_{LR}^{k,m}}{\partial p_{CR}} \frac{1}{\Delta t} \mathbf{N}_p dV \quad (\text{B.35})$$

481

$$\mathbf{D}_{pc}^C = \int_{\Omega} \phi \mathbf{N}_p^T \left(\frac{\partial S_C^{k,m-1}}{\partial p_c} \frac{\rho_{CR}^{k,m} - \rho_{CR}^{k-1}}{\Delta t} + S_C^{k,m-1} \frac{\partial \rho_{CR}^{k,m}}{\partial p_c} \frac{1}{\Delta t} \right) \mathbf{N}_p dV \quad (\text{B.36})$$

482

$$\mathbf{D}_{pCR}^C = \int_{\Omega} \phi S_C^{k,m-1} \mathbf{N}_p^T \frac{\partial \rho_{CR}^{k,m}}{\partial p_{CR}} \frac{1}{\Delta t} \mathbf{N}_p dV \quad (\text{B.37})$$

$$\mathbf{F}_{pc}^W = \int_{\Omega} S_L^{k,m-1} \rho_{LR} \frac{\alpha^2}{K} \mathbf{N}_p^T \mathbf{N}_p S_L^{k,m-1} dV \frac{1}{\Delta t} \quad (\text{B.38})$$

$$\mathbf{F}_{pCR}^W = \int_{\Omega} S_L^{k,m-1} \rho_{LR} \frac{\alpha^2}{K} \mathbf{N}_p^T \mathbf{N}_p dV \frac{1}{\Delta t} \quad (\text{B.39})$$

$$\mathbf{F}_{pc}^C = \int_{\Omega} S_C^{k,m-1} \rho_{LR} \frac{\alpha^2}{K} \mathbf{N}_p^T \mathbf{N}_p S_L^{k,m-1} dV \frac{1}{\Delta t} \quad (\text{B.40})$$

$$\mathbf{F}_{pCR}^C = \int_{\Omega} S_C^{k,m-1} \rho_{LR} \frac{\alpha^2}{K} \mathbf{N}_p^T \mathbf{N}_p dV \frac{1}{\Delta t} \quad (\text{B.41})$$

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