Computational Energy Science

Vol. 2, No. 1, p. 17-30, 2025

Invited review

Recent developments in CCUS-EOR for depleted reservoirs

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Keywords:
CCUS-EOR
compositional simulation
geomechanical models
profile control

Cited as:
Yang, Y., Zhao, X., Yang, J., Zhang. Y., Tian, Y. Recent developments in CCUS-EOR for depleted reservoirs. Computational Energy Science, 2025, 2(1): 17-30.
https://doi.org/10.46690/compes.2025.01.04

Abstract:
Carbon capture, utilization, and storage combined with enhanced oil recovery (CCUS-EOR) is recognized as a practical approach to enhance oil recovery while simultaneously reducing CO_2 emissions. Numerical simulation has become an essential tool for guiding the development of CO_2 injection in depleted reservoirs, where the construction of accurate models is fundamental to reliably predicting production performance. This paper first presents an overview of major CCUS-EOR projects worldwide and subsequently provides a detailed discussion of several critical aspects of numerical simulation for CCUS-EOR. Specifically, it includes: The differences between compositional models and black oil models, the detailed computational procedures of compositional simulation, as well as the primary technical challenges currently encountered; mainstream geomechanical models, the application of geomechanics in assessing reservoir sealing capacity in CCUS projects, and further developments in geomechanical coupling techniques; the current research progress on the mechanisms of water-alternating-gas (WAG) injection, the effectiveness of chemical agents for profile control, and microscale gas channeling control studies based on molecular dynamics simulations and pore network modeling. This review provides a solid theoretical foundation for numerical simulation studies of CCUS-EOR in depleted reservoirs and offers constructive suggestions for future research.

1. Introduction

Carbon Capture, Utilization, and Storage (CCUS) is one of the most effective approaches to reducing greenhouse gas emissions and mitigating global climate change. The CCUS-EOR technology enhances oil recovery by injecting CO_2 into reservoirs, replenishing formation energy, and reducing crude oil viscosity. This method enables the capture and geological storage of CO_2 and improves oil recovery, thereby generating greater economic benefits and environmental value.

The development of CCUS-EOR projects involves multiple aspects, with numerical simulation as a critical tool. Currently, CCUS-EOR is primarily applied to depleted oil reservoirs, which typically exhibit significantly reduced formation pressure-often falling below 50% of the original level-due to prolonged water injection or the depletion of natural reservoir energy (Nie, 2021; Kang et al., 2022). This decline in pressure renders natural drive mechanisms insufficient to mobilize crude oil. Additionally, residual oil tends to be heterogeneously distributed in isolated clusters or thin films within micropores or low-permeability zones, mainly due to reservoir heterogeneity and technological limitations, challenging recovery by conventional methods (Yang et al., 2023). Furthermore, continued waterflood in such reservoirs often results in marginal costs, such as energy consumption and maintenance, that exceed the economic return, thereby limiting its viability. To address these challenges, compositional numerical simulation is first employed to perform history matching based on the geological model, ensuring consistency with the reservoir's production history and establishing a foundation for subsequent analyses. Geomechanical simulations are then integrated to predict reservoir responses under various CO_2 injection scenarios, enabling the determination of

Yandy Scientific Press

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Received January 13, 2025; revised February 6, 2025; accepted March 15, 2025; available online March 20, 2025.

safe injection limits and the assessment of potential leakage risks when coupled with compositional modeling. During the development phase, CO_2's high mobility and low viscosity relative to crude oil often lead to gas channeling, undermining sweep efficiency. This issue can be mitigated through water-alternating-gas (WAG) injection or chemical agents to suppress premature breakthrough and improve CO_2 sweep performance.

This review adopts a structured approach, beginning with an overview of the major CCUS-EOR projects worldwide. It then provides a detailed discussion of the key simulation processes involved in CCUS-EOR, the current state of research, and the existing challenges. The review offers valuable guidance for implementing CCUS-EOR in depleted reservoirs and provides direction for future model development and research.

2. Development of CO_2-EOR in China and worldwide

CO_2-EOR mechanisms include oil swelling from CO_2 dissolution, viscosity reduction of crude oil, lowering of oil-water interfacial tension, hydrocarbon extraction, alteration of rock wettability, acidizing and plugging removal, and forming internal solution gas drive. These mechanisms address the technical and economic challenges of producing from depleted reservoirs, enabling continued recovery. Internationally, CO_2-EOR emerged in the 1930s, with lab tests in the 1950s, field pilots in the 1960s, and rapid development in the 1970s. The world's first large-scale commercial CO_2-EOR project began at the SACROC oil field 1972 (Hu et al., 2019). In China, ongoing research has driven CO_2-EOR applications across several basins. Zhongyuan Oilfield implemented CO_2 huff-and-puff in scattered, low-reserve, heavy oil reservoirs with limited water injection feasibility. Daqing Oilfield has tested CO_2 injection for post-waterflood recovery, ultra-low permeability formations, and shale reservoirs. Fields such as Jiangsu, Jingbian, and Daqing have also conducted extensive CO_2-EOR trials.

CO_2 injection has been extensively applied in depleted reservoirs worldwide as a highly effective enhanced oil recovery (EOR) method. It significantly increases production and extends the reservoir's productive life, particularly in cases where conventional recovery techniques fail or yield diminishing returns.

3. Compositional simulation

Numerical simulation is increasingly vital in petroleum engineering, particularly in optimizing and implementing CO_2-EOR (Enhanced Oil Recovery) techniques. By constructing mathematical models that simulate fluid flow, phase behavior, and thermodynamic processes in the reservoir, numerical simulation provides a platform for virtual testing before actual field implementation. In the context of CO_2-EOR, simulations assist researchers in analyzing CO_2 flow pathways, identifying potential oil and gas migration channels, predicting challenges during injection, and supporting the development and optimization of injection-production strategies. Through simulation, engineers can evaluate various injection strategies and operational parameters-such as injection rates, bottom-hole pressures, and injection-production cycles-without conducting costly field trials. This helps improve oil recovery and reduce CO_2 emissions. Additionally, simulation can account for reservoir heterogeneity, fluid phase interactions, and complex multiphase flow behavior, providing theoretical guidance to reduce operational uncertainty.

3.1 Current situation and model

The numerical simulation models commonly used at present mainly include the black oil model and the compositional model. Due to the complex phase behavior involved in the CO_2-EOR process, the black oil model cannot accurately simulate the flow behavior of oil and gas in the reservoir. Compositional simulation recalculates phase behavior at each time step using an equation of state (EOS) and updates the relevant variables accordingly, achieving higher simulation accuracy. It also allows for considering key mechanisms in CO_2-EOR, such as diffusion and CO_2-water-rock chemical reactions. However, due to its computational complexity, field-scale compositional models often consider only a few mechanisms to reduce computation time. More complex mechanism-coupled compositional simulations are typically used in mechanistic model studies.

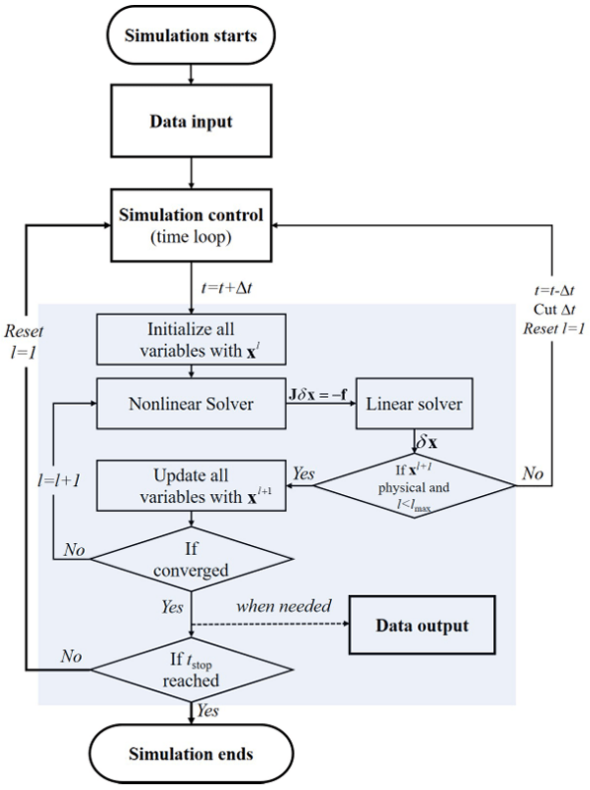

Fig. 1. Schematic diagram of the compositional simulation process (Tian, 2021).

In addition to computational complexity, compositional numerical simulation faces several other challenges. One major issue lies in phase equilibrium calculations. In compositional models, stability testing is required to provide a reliable initial estimate for the subsequent phase-splitting (flash) calculation,

Table 1. The status of CO_2-EOR implementation in China and worldwide.

Oilfield	County	Year	Field result
Daqing (Hu et al., 2019)	China	1965	CO_2 injection after waterflood increased recovery by an estimated 6%-8% compared to continued waterflood.
SACROC (Hosseininoosheri et al., 2018)	USA	1972	Addressed reservoir pressure deficiency; oil production rose from 30,000 to 100,000 barrels per day within 18 months.
Gulf of Mexico (Kuuskraa and Taylor, 2016)	USA	1980s	In late-stage shallow offshore development, trials achieved technical success but were not commercialized.
Wasson (Tanner et al., 1992)	USA	1983	Initial decline during WAG (water-alternating-gas) CO_2 injection, followed by production stabilization and a slight increase after method adjustment.
Midale (Barnhart and Coulthard, 1999)	Canada	1984	Post-waterflood, water cut declined and production dropped; Shell's pilot CO_2 project (1984-1988) achieved good results.
Wasson (Tanner et al., 1992)	USA	1984	CO_2 injection in the continuous injection zone raised daily oil production by 8,000 bbl and increased oil cut from 14% to 31%.
Jiangsu (Wei et al., 2025)	China	1995	71 well cycles of CO_2 huff-and-puff tested in small-block reservoirs; trials suspended due to gas source.
Zhongyuan (Fu et al., 2023)	China	1998	CO_2 injection significantly increased oil rates and altered water cuts across various geological conditions in different reservoir types.
Daqing (Yuan and Wang, 2018)	China	2003	CO_2 flooding trials began in ultra-low permeability formations; pilot projects showed over 9% recovery increase vs. waterflood.
Jingbian (Zhou et al., 2020)	China	2009	Pilot CO_2 injection started in the Qiaojiawa area; by 2016, 59,000 tons of CO_2 had been injected, restoring reservoir pressure to 8.54 MPa.
Jilin (Liang et al., 2024)	China	2012	Full-lifecycle pilot with 10 injectors and 27 producers; production $>$ 6 times of waterflood decline stage; 426,000 tons CO_2 injected.
Shengli (Yang et al., 2024)	China	2013	Pilot in Fan 142-7X4 group raised per-well daily oil from 1 to $>$ 5 tons.
BellCreek (Hamling et al., 2013)	USA	2013	CO_2 injection started in 2013; the projected recovery is an increase of 30-50 million barrels.
East Seminole (Alcorn et al., 2019)	USA	2013	Foam-assisted CO_2 trials improved recovery potential after earlier low-efficiency developments.
Jiangsu (Wei et al., 2025)	China	2015	Pilot miscible and immiscible CO_2 projects in multiple blocks; 23,400 tons of CO_2 injected, 12,200 tons of oil gained.
Jiangsu (Wei et al., 2025)	China	2019	CO_2-EOR promoted in two CCUS hubs; 303,400 tons CO_2 injected, 98,300 tons oil gained.
Jilin (Liang et al., 2024)	China	2020	Industrial-scale CO_2-EOR trials in Hei-125 raised daily production from 12.5 to 50 tons/day.
Shengli (Yang et al., 2024)	China	2022	High-pressure miscible CO_2-EOR in Fan 142 CCUS demo increased daily production from 254.6 to 358.2 tons/day.

Daqing (Hu et al., 2019)	China	2022	Pilot in the Aonan shale reservoir raised oil from 14.0 to 34.3 tons/day. CO_2-EOR projects overview (domestic & international)
Daqing (Hu et al., 2019)	China	2023	Pilot test on shale reservoir CO_2 injection increased daily oil production from 14.0 to 34.3 tons.

guiding optimization algorithms to converge toward the global minimum from this initial guess. Physically, the stability test determines whether the system is stable under given pressure, temperature, and composition conditions. If the system is unstable, the test provides initial guesses for the equilibrium constants used in the phase-splitting calculation. However, the results of such calculations are often susceptible to the choice of initial guess values. If the initial guess significantly deviates from the proper solution, it can lead to long computation times or even convergence failure. During the phase equilibrium calculation, flash calculations are typically performed to determine individual components' distribution and phase behavior. Currently, the Peng-Robinson Equation of State (PR EOS), developed by Peng and Robinson, is the most widely used cubic EOS for calculating the phase behavior of hydrocarbon fluids. The molar density of any phase can be determined by solving the PR EOS, making it a fundamental tool in compositional modeling:

$$Z^3-(1-B)Z^2+(A-2B-3B^2)Z-(AB-B^2-B^3)=0 \quad (1)$$

For multicomponent mixtures, the Peng-Robinson equation of state (PR EOS) utilizes the mixing rules proposed by Zudkevitch and Joffe (1970):

$$a=\sum_{i=1}^{\pi}\sum_{j=1}^{\pi}x_i x_j\sqrt{a_i a_j}\left(1-\mathscr{S}_{ij}^{BC}\right), \quad b=\sum_{i=1}^{\pi}x_i b_i \quad (2)$$

$$a_i=\frac{\Omega_a R^2 T_{ci}^2}{P_{ci}}\left[1+\kappa_i\left(1-\sqrt{T/T_{ci}}\right)\right]^2, \quad b_i=\frac{\Omega_b R T_{ci}}{P_{ci}} \quad (3)$$

$$\kappa_i=0.37464+1.54226\omega_i-0.26992\omega_i^2 \quad (4)$$

3.2 Current issues

The standard Peng-Robinson (PR) equation of state becomes less applicable when dealing with shale oil reservoirs characterized by extensive micropores and nanopores, where nanoscale confinement effects significantly influence fluid behavior. Many researchers have proposed modifications to the PR EOS to account for these effects in response to these limitations. For example, Dong et al. (2016) developed a modified PR EOS by coupling it with equations incorporating capillary pressure and adsorption effects. Yang et al. (2020) proposed a modified PR EOS by adjusting the parameters for molecular-wall interactions and geometric constraints. Similarly, Hao et al. (2023) introduced another parameter-modified PR EOS considering pore size and shape. Despite these advances, accurate phase behavior prediction in compositional simulations under confined conditions remains a significant challenge, particularly for complex shale systems.

Compared with reservoir depletion or waterflood development, CO_2-EOR involves more complex physico-chemical processes, including variations in thermal, flow, stress, and chemical fields. Due to the complexity of thermal and chemical field variations, current CCUS-EOR numerical simulation studies often neglect these two fields, resulting in discrepancies between simulation results and actual production data. For thermal fields, substantial research has already been conducted, and thermo-hydro-mechanical (THM) coupling models have been developed to accurately describe heat transfer, fluid flow, and stress variations within the formation. However, most of these studies have focused on Enhanced Geothermal Systems (EGS), with research primarily addressing the influence of engineering parameters on geothermal extraction performance. Investigations specifically targeting the impact of thermal field variations on EOR processes remain limited. Moreover, the commonly used flow equations in petroleum engineering often assume isothermal conditions, meaning that introducing thermal effects into compositional simulation would invalidate these assumptions, complicating the modeling process. Regarding the chemical field, some current models can account for chemical reactions and the associated ion concentration changes to a certain extent. Nevertheless, due to high computational cost and methodological limitations, most numerical simulations incorporating chemical field variations can only consider a limited number of significant reactions, failing to capture the full range of chemical interactions following CO_2 injection into the reservoir. These models are primarily mechanistic, and when applied at the field scale, simulations that incorporate chemical field dynamics often encounter issues such as non-convergence or extremely slow computation.

Most current compositional simulations are based on the pseudo-steady-state assumption. This results in low accuracy when predicting mass transfer between fractures and matrix, especially in cases where the matrix is highly tight and significantly different in physical properties from the fractures. Three main approaches have been proposed to improve simulation accuracy. The first involves treating the transfer function as a time-dependent dynamic function. For example, Zimmerman et al. (1993) introduced a time-varying correction factor to describe transient (non-steady-state) flow driven by pressure gradients. The second approach uses fine grid systems to characterize the matrix; although still based on the PSS assumption, it improves accuracy to some extent, as shown by Moortgat and Firoozabadi (2013). However, this method significantly increases simulation time and computational cost, making applying to large-scale field models difficult. The third approach subdivides the matrix according to reservoir characteristics. It applies multiple interacting continua (MINC) methods, as proposed by Wu and Pruess (1988), to improve the physical realism of the simulation. Despite these advances,

each method still has unresolved issues, and incorporating non-steady-state mechanisms into compositional simulation remains a key area for further research.

4. Geomechanical modeling of CO_2 geological storage and enhanced oil/gas recovery

Geological storage of CO_2 unfolds over extensive timescales-ranging from centuries to millions of years-making it inherently difficult to replicate or assess through short-duration lab experiments or field trials (Zhao et al., 2024). These processes operate across vast spatial and temporal domains, which early analytical methods (Bedrikovetsky et al., 1996; Mathias et al., 2011; Azizi and Cinar, 2013) attempted to simplify to forecast CO_2 plume behavior during and after injection. However, such methods are typically constrained to one-or two-dimensional frameworks and fall short of capturing the full spectrum of physical and chemical interactions involved in subsurface CO_2 dynamics. Rutqvist et al. (2007) pointed out that the simple analytical solutions could underestimate or overestimate the maximum injection pressure. In contrast, numerical modeling is fundamental to CO_2 sequestration studies, enabling the simulation of multiphase flow, geochemical reactions, and geomechanical responses over extended timescales (Zhou et al., 2024; Li et al., 2025).

For CCUS processes, introducing significant amounts of CO_2 into deep geological formations may trigger a range of geomechanical challenges, including seismicity, caprock sealing performance, and potential fault reactivation (Kopp et al., 2009; Polak et al., 2011). These deformations depend on variations in the stress field, as well as the thermal and mechanical properties of the host rock and the frictional behavior of faults-factors that are often not directly observable or intuitive (Furre et al., 2017; Wang et al., 2017). In such cases, geomechanically coupled models support not only the prediction of plume migration and estimation of adequate storage capacity, but also evaluation of injection feasibility and containment integrity under site-specific geological conditions (Zhao et al., 2024).

4.1 Mathematical model

Cross-coupling of hydrological and geomechanical models is a common choice for modeling CCUS-related processes. The fluid flow can be described using a typical transport equation (Zhang et al., 2017):

$$\frac{\partial}{\partial t}\left(\phi \sum_{k=1}^{P} \rho^{\beta} x_i^{\beta} S^{\beta}\right) - \sum_{k=1}^{P} \nabla\left(x_i^{\beta}\mathbf{u}^{\beta} + S^{\beta} J_i^{\beta}\right) - q_i = 0 \quad (5)$$

where t is time, β is the phase index, P is the number of co-existing phases, ρ is the density, x_i^{β} denotes the mole fraction of component i in phase β, S is the saturation, $\mathbf{u}$ is the Darcy velocity, ϕ is the porosity, q is the sink/source term. The second term combines convection ($x_i^{\beta}\mathbf{u}^{\beta}$) and diffusive flux ($S^{\beta} f_i^{\beta}$), the latter of which is often ignored as a result of secondary significance and lack of data.

Geomechanical equations can be developed using linear elastic theory for poroelastic systems. Winterfeld et al. developed a geomechanical governing equation based on Hooke's law for thermos-multiporoelastic media:

$$\left[\frac{3(1-\nu)}{1+\nu}\right]\nabla\sigma_m + \nabla\cdot\mathbf{F} - \frac{2(1-2\nu)}{1+\nu}\left(\alpha\nabla^2 P + 3\widetilde{\beta}K\nabla^2 T\right) = 0 \quad (6)$$

where ν is Poisson's ratio, σ_m is the mean value of the three principal stresses, $\mathbf{F}$ is the body force vector, α is the Biot's coefficient, $\widetilde{\beta}$ is the linear thermal expansion coefficient, and K is the bulk modulus. Ongoing discussion exists about whether incorporating heat transfer should be included, given the trade-off between computational cost and its potential significance. On one hand, thermal coupling could enable us to account for thermal stresses (Shi et al., 2012; Rutqvist et al., 2010), associated near-wellbore effects, and more accurate phase behavior calculations. Others, however, believe that the cooling effect due to CO_2 injection occurs only in the vicinity of the injector, of which the impact could be considered minimal (Arjomand et al., 2024). For field-scale simulations, neglecting thermal effects from a computational cost perspective is probably preferable.

The geomechanical model is usually fully or sequentially coupled with a hydrological model to understand geomechanical response to CO_2 injections (Rutqvist et al., 2010; Vilarrasa et al., 2010). The fully coupled models solve coupled nonlinear equations simultaneously using fully implicit finite difference methods. Even though they have been reported to be unconditionally stable in some cases (Kim et al., 2011), applying them to large-scale field simulations tends to be cumbersome due to excessively high computation cost. At the same time, sequentially coupled hydromechanical (HM) models provide more flexibility by linking separate simulators (Mainguy and Longuemare, 2002; Jha and Juanes, 2014).

4.2 Failure criteria and maximum sustainable CO_2 injection pressure

For CO_2 geological storage (excluding EOR/EGR), the capacity greatly depends on the caprock sealing capacity, which is dominated by tensile and shear failure. In some early modeling studies (Rutqvist and Tsang, 2002; Rutqvist et al., 2007), the critical pore pressure at which the tensile failure (tensile fracture or reactivation of pre-existing fracture) occurs can be estimated as the sum of minimum principal stress (σ_3) and reservoir tensile strength (T_0):

$$P_{fc} = \sigma_3 + T_0 \quad (7)$$

The shear or slip failure occurs when the shear stress acting upon the fault plane exceeds the shear strength (Hajiabadi et al., 2021). The effective stress law and Mohr-Coulomb failure criteria can describe such relationships:

$$\tau = C + \mu_s \sigma_n^i \quad (8)$$

where τ is the shear stress, C is the internal cohesion coefficient, μ_s is the coefficient of static friction ($\tan\varphi$), σ_n^i is the effective normal stress, which can be expressed as:

$$\sigma_n^i = \sigma_n - \alpha P_p \quad (9)$$

where P_p is the pore pressure. By manipulating the two equations above, and ignoring cohesion ($C = 0$), the maximum sustainable CO_2 injection pressure to prevent fault slip can be derived as (Khazaei and Chalaturnyk, 2017):

$$P_{sc} = \sigma_n - \frac{\tau}{\mu_s} \tag{10}$$

Rutqvist et al. (2006) proposed the critical pressure for fault slip with non-zero cohesion:

$$P_{sc} = -\sigma_{m2} + S_0 \cot\varphi - \frac{|\tau_{m2}|}{\sin\varphi} \tag{11}$$

where S_0 is the fault coefficient of internal cohesion and φ is the angle of internal friction. Also, τ_{m2} and σ_{m2} are the two-dimensional maximum shear stress and mean stress in the plane σ_1 and σ_3, respectively, can be denoted as:

$$\tau_{m2} = \frac{1}{2}(\sigma_1 - \sigma_3) \tag{12}$$

$$\sigma_{m2} = \frac{1}{2}(\sigma_1 + \sigma_3) \tag{13}$$

Other geomechanical responses to CO_2 injections might impact the development plan, such as induced seismicity, ground surface uplift, and wellbore integrity. Rutqvist (2012) systematically discussed these problems.

4.3 Applications of the coupled geomechanical model

Before executing any CCUS-related projects, numerical modeling should be carried out to avoid the aforementioned geomechanical risks and estimate the maximum sustainable injection pressure and storage capacity. Under such circumstances, coupled geomechanical models provide much more reasonable solutions compared to uncoupled hydrological models as they account for the stress change with reservoir pore pressure (Khan et al., 2024).

Pruess et al. (2004) conducted a code comparison for geological disposal of CO_2. Their study shows the possibility of using numerical simulation tools to evaluate the feasibility of CO_2 geological disposal, and design and monitor CO_2 disposal operations. Later, TOUGH2-FLAC3D was developed at Lawrence Berkeley National Laboratory (LBNL), which allows HM or thermo-hydrological-mechanical (THM) modeling for CO_2 geological storage. Rutqvist et al. (2006) utilized TOUGH2-FLAC3D for a study where CO_2 was injected into a hypothetical saline aquifer. The study demonstrated that the risk for CO_2 leakage is relatively small if substantial upward migration of CO_2 can be prevented. Rutqvist et al. (2007) estimated the reservoir's maximum sustainable injection pressure based on its potential to trigger fault slip. These early simulation efforts underscored the value of geomechanical coupling in CO_2 geological storage, motivating further model development, perfection of the commercial software, and follow-up studies.

Choi et al. (2023) conducted a 3D geomechanical simulation for the Smeaheia fault block in the Norwegian North Sea using a finite element model (Abaqus). The simulation results were compared with the analytical solution with a simplified uniaxial strain assumption. The investigation showed that the uniaxial strain assumption could underestimate effective horizontal stress change, especially when there is a significant change in pore pressure near the bounding fault. Arjomand et al. (2024) also used Abaqus to investigate ground surface deformation caused by CO_2 injection at In Salah, Algeria. The simulation results agreed well with the interferometric synthetic aperture radar (InSAR) measurements.

Ouellet et al. (2011) used ECLIPSE for dynamic flow simulation and VISAGE for geomechanical simulation using a one-way partial coupling scheme, as illustrated in Fig. 2. They used the model to study the possibility and location of caprock failure, fault reactivation, and ground surface elevation. The one-way coupled model will not be as accurate as fully coupled or sequentially coupled models. Still, it will provide quick simulations and allow one to link simulators with different numerical discretization methods, such as finite difference and finite element. Saffou et al. (2023) utilized the same approach to evaluate the geological response of CO_2 disposal into a depleted gas reservoir, through reservoir and fault stability.

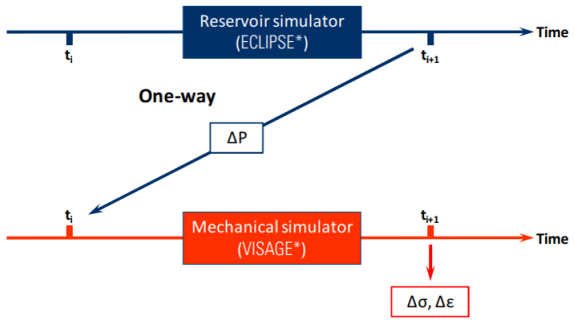

Fig. 2. Schematic diagram for partial coupling scheme (Ouellet et al., 2011).

Over the years, researchers have also put tremendous effort into improving the model to have more realistic rock mechanical behavior. For example, trials use isotropic and anisotropic constitutive models instead of assuming linear poroelasticity and isotropic properties to evaluate fault reactivation induced by CO_2 injection (Cappa and Rutqvist, 2011). An emerging body of research has recently focused on the application of the extended finite element method (X-FEM) to coupled THM problems (Wang et al., 2020; Cheng et al., 2022).

5. Gas channeling control during CO_2 injection in enhanced oil recovery

CO_2 displacement is a promising approach to enhance oil recovery, but may raise severe gas channeling issues, especially when the pressure constraints of miscible displacement cannot be fulfilled. An unfavorable mobility ratio between displacing CO_2 and reservoir fluids would lead to early gas breakthrough and ineffective gas circulation. Thus, additional profile control in CO_2-EOR projects is necessary to compensate for the restricted sweep efficiency (Lei et al., 2016; Zhou et al., 2022).

5.1 Profile control methods

Due to its flexibility and relatively low cost, the water-alternating-gas (WAG) process has been considered a standard gas channeling control approach during the immiscible CO_2 injection. Key mechanisms of the WAG process include mobility adjustment via restraining continuous gas flow and gravity segregation (Yan et al., 2017). Alternating injection of water and gas slug results in pressure maintenance among the displaced region, effectively stabilizing the invading front of injected fluids with multiple mechanisms like IFT adjustment, promoting Jamin effect, etc (Massarweh and Abushaikha, 2022). Systematic studies on the investigation of mechanisms and the field application of WAG have lasted for decades, from early-stage quantification of sweep efficiency based on classic Buckley-Leverett theory to novel AI boosted optimization that connects pore-scale phenomena to field-scale predictions (Dong et al., 2013; Dang et al., 2020; Wei et al., 2021). Yan et al. (2017) had investigated the mechanism of WAG processes with injection of the supercritical CO_2 that dissolves the polar components of oil and the water, providing the stable interfaces, displacing the CO_2-oil mixture away from micro or even nanopores. Lei et al. (2016) had presented the possibilities and potentials of WAG processes with multi-level core flooding experimental studies that either miscible or immiscible conditions of gas-liquid alternating injection result in an increment of recovery factor in low to medium permeable regions. Cao et al. (2023) investigated the contribution of fracture distribution in the CO_2 displacement, suggesting that more fractures may lead to earlier and severe gas channeling. Still, the results have shown that the oil-producing pore size is being expanded with a limited reduction of the overall recovery factor. The experiments have further confirmed the effectiveness of CO_2 flooding in enhancing local displacement, indicating the potential of CO_2 displacement when gas channeling is further controlled.

Chemical profile control has been introduced to respond to more complicated reservoir conditions with natural or hydraulic fractures, where regular WAG becomes less effective (Bai et al., 2022; Yang et al., 2024). Multiple studies have reported the effectiveness of anti CO_2 channeling attempts inside the fractured tight core samples using crosslinking polymer gel with spatial network structure, which provides over 95% of the plugging rate and around 35% of incremental oil recovery at reservoir temperature and salinity conditions of over 100 ℃ and 20,000 mg/L (Zhang et al., 2020; Yang et al., 2024). Jiang et al. (2024) had developed a novel acid-resistant polymer microsphere (DCNPM-A) with 13.5 of swelling rate, 95% of plugging rate, and 21% of incremental oil recovery while being applied in the core flooding scenarios with tight oil condition of relative high temperature (80 ℃), high salinity (85,000 mg/L), and acid environment (pH = 3). The experimental studies of the DCNPM-A with delayed swelling properties and stable expandability have shown the potential of realizing controllable deep plugging on post-CO_2 injection applications. Song et al. (2022) had developed a novel self-healing polymer gel for CO_2 channeling control during CO_2 storage and CO_2 flooding, which has shown incredible plugging performance and mechanical strength with comprehensive experimental evaluation on multiple aspects like swelling kinetics, self-healing behavior, thermal stability, in-situ rheology, etc. The breakthrough pressure gradient of supercritical CO_2 has been raised to 5.48 MPa/m after the stable sealing of gel within the fracture. Saifullin et al. (2022) studied the feasibility of treating gas breakthroughs with polymer-stabilized foam injections from production wells. The experimental results had shown an effective gas block in the presence of polymer without introducing additional negative impacts on the relative permeability of the oil phase.

5.2 Research status of profile control methods

For either non-chemical WAG processes or chemical profile control methods with strategic injection of polymer, gel, or foam, the corresponding numerical simulation studies on gas channeling control during the CO_2 displacement are essential for micro-mesoscale mechanisms investigation and field-scale application design, which fills the gap between numerous experimental results and guidance on field application. Multiple-scale numerical simulation studies, from micro-scale molecular dynamics (MD) simulation to field-scale reservoir simulation, have successfully incorporated the mechanisms and patterns collected from experimental investigations of the profile control during CO_2 displacement. Molecular simulation has been widely applied in multiple studies on revealing micro-scale interaction during CO_2 injection and relevant profile control attempts, which has become a common and practical approach to quantify the interfacial behavior under the impacts of various factors like displacing velocity, wettability, oil components, rock type, etc (Yu et al., 2012; Sun et al., 2018; Zhao et al., 2024). Results and patterns resulting from the MD simulation can be used as a reference for the corresponding CO_2 channeling control processes, such as unknown interfacial properties or optimization in defining relevant energy or interfacial terms, for model development at a larger scale.

Pore-scale models can be developed with necessary properties on pore structure and interfacial behavior of CO_2 involved multiphase displacement processes, which on the one hand utilizes the mechanisms discovered at lower scale to describe invading or trapping rules inside pores or throats, on the other hand provides necessary parameters quantifying multiphase fluid flow inside porous media that are difficult to collect via current experimental technologies (Zhao et al., 2020). Wang et al. (2022) had proposed a pore-scale discrete phase model of micro-bubble CO_2 flooding that couples the motions of continuous gas flow with the independent trajectory of discrete micro-scale CO_2 bubbles within the heterogeneous porous media. The simulation results had been matched with core flooding tests and suggested the benefits of oil displacement efficiency with smaller micro-bubble sizes and higher micro-bubble injection rates. Recent developments in pore network modeling have gradually installed multiple pore-scale events encountered during the chemical-related displacement processes, including surfactant, polymer, and foam (Chen et al., 2005; Blunt et al., 2013; Almajid and Kovscek, 2020). For the convenience of capturing multiphasic or interfacial

mechanisms inside the pore network, the classic modeling framework of invasion percolation is widely adopted, which simplifies immiscible displacement into the manner of quasi-static processes (Hammond and Pearson, 2010; Affandi et al., 2024). Hammond and Unsal (2012) had proposed a pore network model that incorporates the dynamic advection and diffusion of surfactant into the quasi-static displacement processes inside the pore network. The modeling results illustrated the effects of surfactant and the interaction between rock and fluid during the displacement in the pore network.

Quantifying the variable shearing thinning features is the key to capturing characteristics of polymer-involved immiscible displacement processes. Rodríguez de Castro et al. (2023) presented a pore network modeling study of rheology and displacement of fluids with shear-thinning features, which provides a comprehensive evaluation of the impacts of the rheology of fluids and the morphology of pore network configuration on the pore-scale flow with shear-thinning characteristics. Suo et al. (2025) revealed three types of layered flow regime configurations as the responses of flow dynamics among the pore networks. The modeling results quantitatively described the impacts of heterogeneity and dynamic rheology on flow conductance of various polymer systems, which brought insightful understanding for upscaling polymer injection processes in field-scale reservoir simulations.

The simulation of foam displacement in a pore network combines the features of complicated interfacial events resulting in generation, mobilization, and coalescence of foam lamellae, as well as the non-linear foam flow patterns due to temporary blockage from the gas trapping (Chen et al., 2006; Yang et al., 2023). To track the expanding foam bank and quantify the local pressure thresholds of foam mobilization, a memory term has been proposed to modify the classic invasion percolation process, which became the invasion percolation with memory (IPM) that counts the changes of pressure threshold of foam bank explicitly (Kharabaf and Yortsos, 1998). The IPM method gradually became a common and practical model framework in simulating foam behavior inside pore network for decades of iteration, that multiple features and mechanisms had been incorporated, from the viscous effects caused by yield stress of foam bank to the quantification of flowing foam fraction (Chen et al., 2005; Almajid and Kovscek, 2020). Zhao et al. (2020) proposed a modified framework of the IPM method for foam displacement inside the pore network model by adding a "scaled" time dependency to couple continuous film thinning and rupture caused by capillary suction into the quasi-static invasion event of foaming gas. Later, the effects of grain configuration and surface wettability are quantified by distinguishing interfacial events like burst, touch, and overlap during the foaming gas drainage with designated pressure constraints (Yang et al., 2023; Zhao et al., 2023). Thus, with a pore network model of foam displacement, flowing and trapped gas can be identified. In contrast, the relative permeability of gas phase can be estimated accordingly as shown in Fig. 3, which provides a dependable upscaling approach connecting pore-scale mechanisms and field-scale prediction and optimization as shown in Fig. 4 (Zhao et al., 2021). Pore-scale models of enhanced CO_2 displacement work as the bridge connecting the understanding based on micro-scale mechanism studies along interfacial behaviors, with macro-scale application and optimization of CO_2 injection with non-chemical or chemical profile control attempts. Classic model parameters quantifying multiphase fluid flow in porous media, like relative permeability curves and capillary force curves, can be defined reasonably based on the prediction given by the pore-scale model.

For decades, numerous studies have been conducted to develop the framework of modeling foam flow with the population balance method that quantifies the impacts of generation and coalescence behaviors on foam texture and the mobility reduction of the gaseous phase (Izadi et al., 2021). After fitting with experimental results of core-scale laboratory investigations, the foam flow model incorporating mechanistic features can be used in the optimization of field-scale foam injection processes for chemical EOR or foam-assisted CO_2 sequestration. Li et al. (2022) had introduced a mathematical model to identify and characterize the gas channeling processes with consideration of initial injection concentration, dispersion, and adsorption. The entire CO_2 flowing region is divided into three sections, including CO_2, miscible, and crude oil regions, via tracking the CO_2 and miscible region fronts. The model had successfully incorporated the mass transfer during the adsorption and dispersion, which reveals their impacts on CO_2 displacement efficiency. Jia et al. (2024) had proposed a numerical simulation method of gel treatment by quantifying the inaccessible pore volume (IAPV) from rheological properties and the size exclusion effect. Multiple mechanisms of gel performance are considered, including the dynamic polymer adsorption and disproportionate permeability reduction due to oil & gas blocking. The simulation results suggest that the gel treatment in fractured gas reservoirs benefited from higher fracture permeability, lower water production, and lower bottom water connectivity based on gray relation analysis of impact. As a benchmark simulator in modeling chemical enhanced oil recovery, UTCHEM has been developed for decades in capturing the phenomena and mechanisms of chemical processes involved, like polymer, foam, and gel. Recently, the in-situ polymer viscosity model has been incorporated with the impacts from varying salinity, hardness, and temperature. Also, the hydrolysis of polyacrylamide polymers, the relevance between inaccessible pore volume and reservoir properties, and the cation exchange among the aqueous phase are included in the model development. Improvements in UTCHEM based on the latest experimental results effectively assist the optimization of polymer-involved processes in profile control from the polymer selection to operation design. Izadi and Kam (2019) fitted the population balance model, which has been established with pore-scale foaming/defoaming events, to the supercritical CO_2 foam experimental data, extracting the core-scale mechanisms and features, and then applied it to the field-scale performance evaluation of profile control. Such a mechanistic modeling approach provides theoretical reasoning on the optimization of foam injection strategy and demonstrates how supercritical CO_2 foam outperforms gaseous CO_2 foam in propagation range and blockage state.

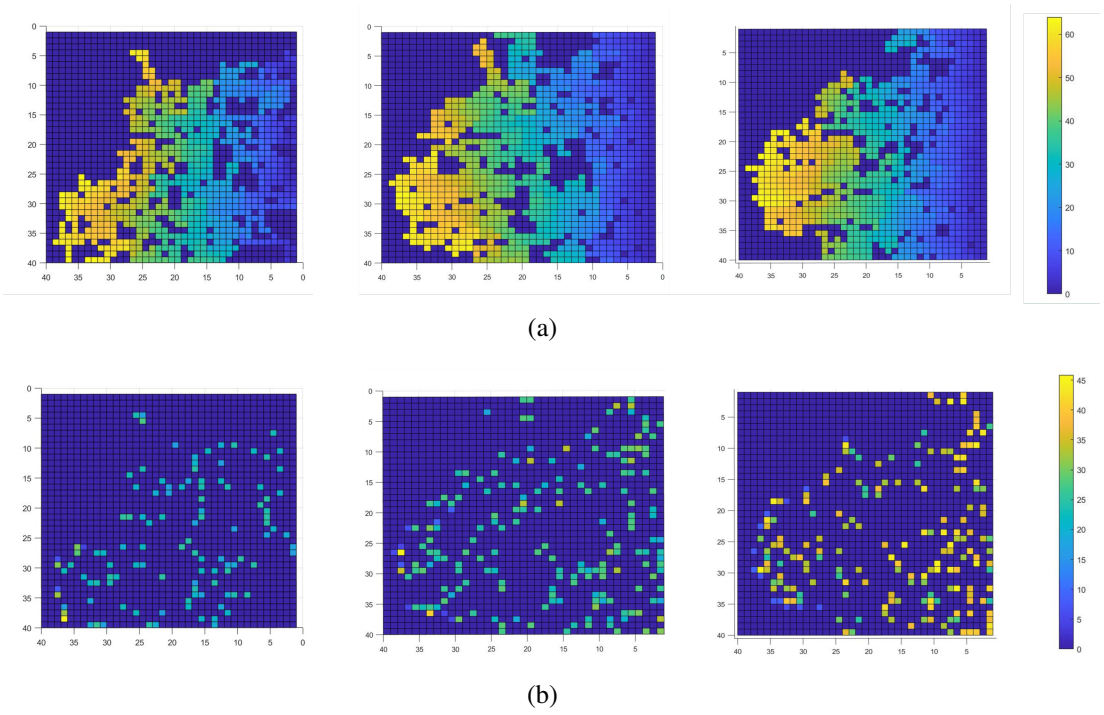

Fig. 3. (a) Heatmap of frontal invasion history of foam displacement inside pore network at varying snap-off probability (P_{SO}= 0.3, 0.5, 0.7 from left to right). (b) Heatmap of immobile foam bank distribution and foam blockage degree at foam breakthrough inside pore network at varying snap-off probability (P_{SO} = 0.3, 0.5, 0.7 from left to right). (Generated based on the method introduced in Yang et al., 2023).

Over decades of development and application, gas channeling control techniques during CO_2 injection have evolved substantially, from non-chemical methods like Water-Alternating-Gas (WAG) to multiple chemical strategies. However, for the numerical simulation studies of various gas channeling control strategies, except for the global issues in efficiency and convergence issues encountered in chemical involved problem, there are several critical problems remaining unsolved for now, including capturing the mechanisms of further reduction of trapped defending phase after the gas breakthrough when viscous force is not negligible for the immiscible displacement processes, as well as the appropriate coupling of lamellae coalescence caused by gas diffusion within the current modeling framework of foam injection in pore network based on invasion percolation with memory.

6. Summary

Compositional simulation, geomechanical modeling, and profile control are critical for the effective implementation of CCUS-EOR. This review summarizes the main models, methodologies, and limitations associated with these key simulation approaches, as outlined below:

1) Compared with black oil models, compositional simulation accounts for the dynamic variation of fluid components during the simulation, thus providing higher accuracy. However, achieving accurate phase behavior calculations and reliably simulating mass transfer between fractures and matrix remains a major challenge and a critical requirement for effectively guiding CCUS-EOR projects.
2) CO_2 injection into subsurface formations may induce various geomechanical risks, including seismic activity, caprock integrity issues, and the potential reactivation of sealed faults. Coupled geomechanical simulation is essential for predicting CO_2 migration behavior and assessing the safety of CCUS-EOR operations.
3) Gas channeling after CO_2 injection in depleted reservoirs is a critical factor affecting oil recovery. Techniques such as water-alternating-gas (WAG) injection and injecting chemical agents have shown potential in mitigating gas channeling. At the microscale, the underlying mechanisms are primarily investigated through molecular dynamics simulations and pore network modeling.

Acknowledgements

The authors are grateful for funding from the National Natural Science Foundation of China (Grant No. 52304048, 52004032, 12302329), the National Science and Technology Major Project (No. 2024ZD1406601).

Conflict of interest

The authors declare no competing interest.

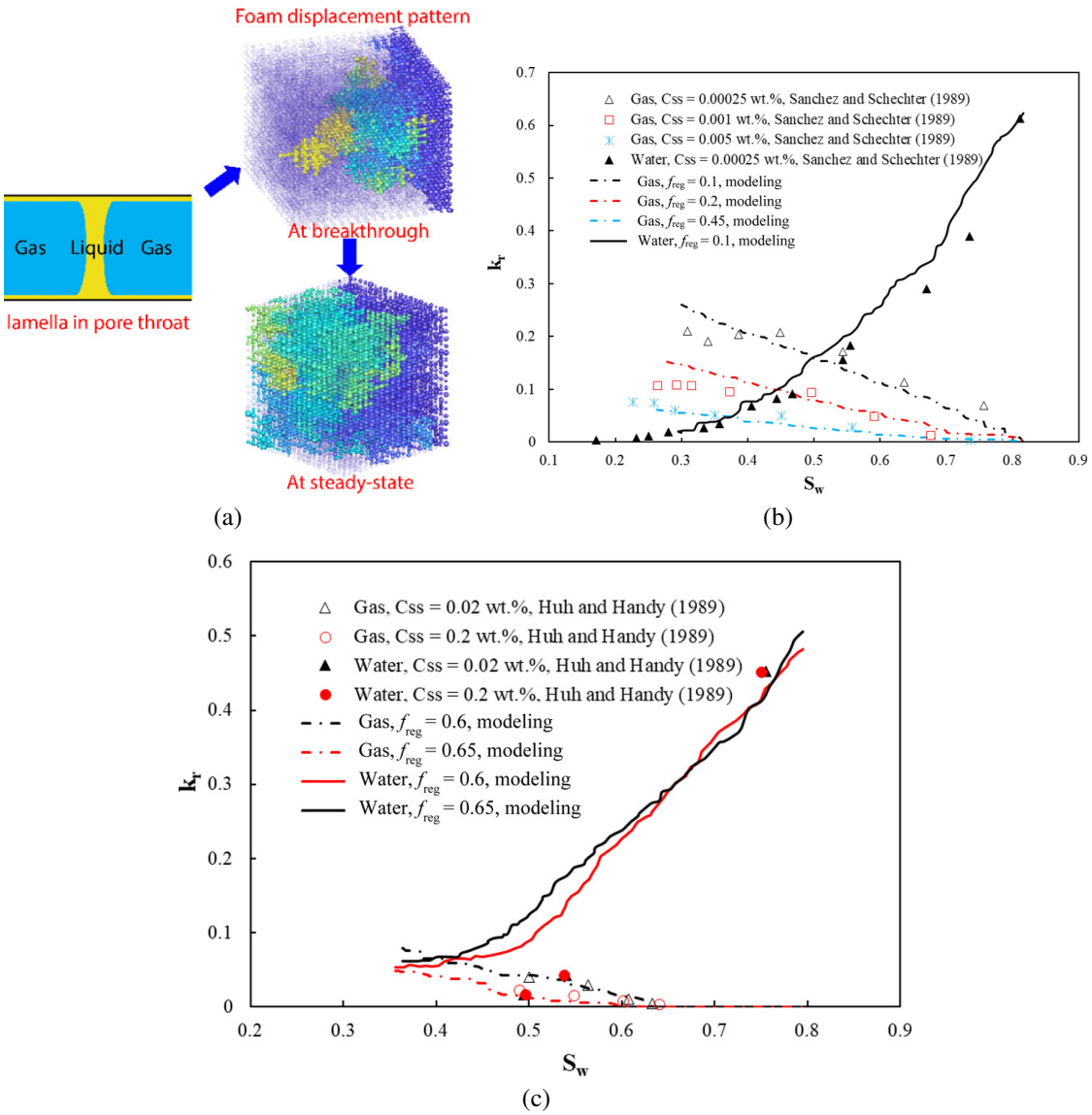

Fig. 4. (a) Modeling foam displacement incorporated with pore-scale lamellae behaviors and post-breakthrough viscous effects of foam. (b) Steady-state relative permeability of liquid and foaming gas in Ottawa sandpack of Sanchez and Schechter (1989) and the fitted curves computed with pore network simulation. (c) Relative permeability of liquid and foaming gas in Berea sandstone of Huh and Handy (1989) at varying surfactant concentrations (C_{ss}) and the fitted curves computed with pore network simulation (Figures cited from Zhao et al., 2021).

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