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Perspective

CO_2-Enhanced oil recovery in unconventional reservoirs: Motivation, mechanisms, factors, challenges and methods

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Abstract:
CO_2-Enhanced oil recovery and carbon storage in ultra-tight shale reservoirs are governed by multiscale interactions spanning molecular thermodynamics to reservoir engineering. Key mechanisms include CO_2-induced oil swelling and pressure mobilization, diffusion-dominated hydrocarbon transport, viscosity reduction via hydrocarbon plasticization, and competitive adsorption displacing methane from organic surfaces. These processes synergize temporally: Swelling and diffusion dominate early-stage recovery, while viscosity reduction and miscibility prevail later, enhanced by cyclic injection strategies to overcome fracture-limited flow geometries. Supercritical CO_2 optimizes extraction efficiency and pore penetration but elevates operational risks through potential fracture leakage. Challenges persist in reconciling nanoconfinement-altered phase behavior, wettability shifts from carboxylate formation, and adsorption hysteresis impacting long-term storage stability. Emerging machine learning frameworks integrate dimensionless parameters to optimize injection protocols, yet geochemical-geomechanical feedbacks demand dynamic coupling of reactive transport models with fracture stability analyses. Advancing CO_2-EOR-storage co-optimization requires multiscale model integration, combining in-situ spectroscopic characterization of interfacial phenomena with sensor-driven monitoring of plume dynamics. By resolving molecular-to-reservoir asymmetries, shale's inherent complexity can be leveraged for sustainable energy transitions, balancing hydrocarbon recovery with secure carbon sequestration through science-informed engineering innovations.

1. Motivation

Shale oil and gas have emerged as increasingly critical components of the global energy portfolio, representing unconventional hydrocarbon resources characterized by ultra-low permeability and complex nanopore networks (Zhao et al., 2025). These reservoirs, primarily composed of organic-rich mudstones with intricate mineralogical heterogeneity, have revolutionized energy production through technological advancements in horizontal drilling and hydraulic fracturing. However, their unique petrophysical properties result in rapid production decline rates and disappointingly low recovery factors, highlighting fundamental limitations in conventional extraction methodologies. In this context, CO_2-enhanced oil recovery (CO_2-EOR) has emerged as a dual-purpose technological proposition, simultaneously addressing energy production challenges and climate mitigation imperatives (Davoodi et al., 2024). The underlying premise leverages CO_2's unique thermodynamic properties-including its low minimum miscibility pressure (MMP) with light crude oils and superior diffusion capabilities in tight matrices to overcome capillary-dominated flow regimes while achieving permanent carbon sequestration. Mechanistically, CO_2 injection facilitates multiple recovery-enhancing processes: Interfacial tension reduction through partial miscibility, crude oil viscosity reduction via molecular dissolution, and pore-scale swelling effects that enhance relative permeability.

From a carbon storage perspective, shale reservoirs offer exceptional potential due to their vast areal extent, geochemical reactivity conducive to mineral trapping, and naturally occurring sealing mechanisms that minimize vertical migration risks. Current research frontiers focus on resolving funda-

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mental knowledge gaps regarding multiphase flow dynamics under nanoconfinement conditions (Zhang and Sun, 2021), where classical Darcy flow assumptions become invalid and surface forces dominate over viscous forces. Recent experimental studies using nuclear magnetic resonance (NMR) and microfluidic chips have revealed paradoxical behaviors, such as enhanced CO_2 diffusion rates in organic-hosted pores (2-50 nm) compared to inorganic matrices, challenging conventional reservoir simulation paradigms.

The scientific community remains divided on critical aspects of CO_2-shale interactions, particularly regarding the long-term stability of adsorbed carbon in organic matter and the geomechanical impacts of CO_2-induced clay swelling on fracture conductivity. Field-scale pilot projects, such as those conducted in the Eagle Ford and Bakken formations (Grubert, 2018), have demonstrated incremental recovery improvements of 15-25% but simultaneously revealed operational challenges including injectivity limitations and fluid compatibility issues. These practical experiences underscore the urgent need for a comprehensive theoretical framework that integrates molecular-scale interfacial phenomena, core-scale transport mechanics, and reservoir-scale geochemical processes. Current modeling approaches often neglect critical couplings between competitive CO_2-CH_4 sorption dynamics, stress-dependent permeability evolution, and chemical reactions altering pore architecture over time. Furthermore, the dual objectives of maximizing hydrocarbon recovery while optimizing CO_2 storage capacity create complex optimization landscapes requiring advanced machine learning algorithms and multi-objective genetic algorithms for effective parameter space exploration.

The efficacy of CO_2-enhanced oil recovery (CO_2-EOR) in shale reservoirs is fundamentally constrained by their unique petrophysical and geochemical properties. Shale formations exhibit permeability values spanning from sub-nanodarcy (nD) to microdarcy (μD) scales, orders of magnitude lower than conventional sandstone reservoirs. This ultra-low permeability arises from the dominance of nanometer-scale pore throats and the absence of interconnected macropores, rendering Darcy flow assumptions invalid and necessitating stimulation techniques such as hydraulic fracturing to establish artificial fracture networks. These induced fractures temporarily bypass the matrix permeability limitations but introduce challenges in sustaining conductivity due to proppant embedment and stress-sensitive closure. Recent advances in improved EOR emphasize that even post-stimulation, the effective permeability of shale matrices remains insufficient for conventional displacement mechanisms, requiring CO_2 transport to rely on diffusion and imbibition processes rather than viscous displacement.

The pore architecture of shale reservoirs further complicates fluid dynamics, featuring a multimodal distribution of pore sizes ranging from macropores ($>$ 50 nm) to micropores ($<$ 2 nm), with a significant proportion of pores hosted within organic matter (kerogen) and clay-bound water films. Characterization of this dual-porosity system-comprising inorganic mineral-associated pores and organic-hosted pores-demands advanced techniques such as scanning electron microscopy (SEM), nitrogen adsorption isotherms, and small-angle neutron scattering (SANS). Crucially, nanopore confinement effects alter fluid phase behavior, suppressing bubble-point pressures and inducing capillary condensation of hydrocarbons, phenomena now quantifiable through molecular dynamics (MD) simulations. These confinement effects disproportionately influence CO_2 diffusion rates, with recent studies demonstrating that organic-hosted nanopores exhibit a higher CO_2 solubility compared to inorganic pores due to stronger van der Waals interactions with kerogen surfaces.

Minerological heterogeneity, quantified via X-ray diffraction (XRD) and energy-dispersive spectroscopy (EDS), governs shale-CO_2 reactivity and geomechanical stability. Quartzose shales ($SiO_2 > 60\%$) exhibit brittle fracturing conducive to sustained injectivity, whereas micaceous or clay-rich shales (illite, smectite $> 20\%$) face risks of CO_2-induced clay swelling and fracture conductivity loss. Feldspathic shales, with their higher ion-exchange capacity, promote carbonate precipitation during CO_2 injection, potentially enhancing long-term carbon sequestration through mineral trapping. The fissility of shale-controlled by clay alignment and organic matter distribution-directly impacts fracture propagation patterns, as evidenced by acoustic emission monitoring in triaxial compression tests.

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Organic matter content, quantified via total organic carbon (TOC) analysis and Rock-Eval pyrolysis, serves as both a hydrocarbon source and a CO_2 adsorption medium. Kerogen types (I-IV) dictate pore wettability: Carbonaceous organic matter (Type III/IV) tends to be hydrophobic, favoring oil retention, while bituminous shales (Type I/II) exhibit mixed-wet behavior. High-TOC shales ($> 6\%$) demonstrate preferential CO_2 adsorption over methane, with adsorption capacities reaching 2-4 mmol/g at reservoir pressures, as measured by gravimetric adsorption isotherms. However, thermal maturity ($Ro\%$) modulates this behavior-overmature shales ($Ro > 1.3\%$) develop rigid aromatic structures with reduced adsorption potential compared to low-maturity counterparts.

Fluid property characterization reveals critical distinctions between shale hydrocarbons and conventional oils. Shale oils typically exhibit API gravities $> 40^\circ$ (light oils) but suffer from abnormally high bubble-point pressures due to nanopore confinement. CO_2 injection must therefore be optimized for both miscibility (via minimum miscibility pressure, MMP, determinations using vanishing interfacial tension techniques) and viscosity reduction, particularly in gas-condensate shales where retrograde behavior exacerbates liquid dropout. Supercritical CO_2 ($scCO_2$) emerges as the optimal injection phase, combining liquid-like density (600-800 kg/m^3) with gas-like diffusivity, though its reactivity with brine introduces scaling risks that demand geochemical modeling using PHREEQC or TOUGHREACT codes.

2. Mechanistic framework of CO_2-Enhanced oil recovery in unconventional reservoirs

The effectiveness of CO_2-enhanced oil recovery (CO_2-EOR) in ultra-tight shale reservoirs arises from synergistic interactions among molecular-scale thermodynamics, nanoconfined transport phenomena, and reservoir-scale fluid dynamics. CO_2 dissolution into crude oil induces volumetric swelling, reducing capillary trapping forces and generating localized pressure gradients that mobilize hydrocarbons. This process is amplified in organic-hosted nanopores due to enhanced interfacial contact but suppressed in mineral-bound regions by competitive water adsorption. Diffusion dominates hydrocarbon transport in ultra-low permeability matrices, with advanced multicomponent models integrating Knudsen and surface diffusion pathways to address pore geometry heterogeneity. Concurrently, viscosity reduction through CO_2-induced plasticization of heavy hydrocarbon chains and selective extraction of lighter fractions alters oil composition, particularly under supercritical conditions. Miscibility, though operationally challenged by fracture-dominated flow geometries, is optimized through cyclic injection strategies to prolong interfacial contact. Competitive adsorption further displaces methane and liquid hydrocarbons from kerogen surfaces, driven by CO_2's higher adsorption affinity, yet irreversible pore deformation in low-maturity shales underscores the need for geomechanical coupling in predictive models.

The temporal evolution of these mechanisms dictates recovery dynamics, with swelling and diffusion governing early production stages, while viscosity reduction, extraction, and miscibility dominate later phases. Machine learning frameworks leverage dimensionless groups to optimize injection parameters across spatiotemporal scales, yet critical uncertainties persist. These include the role of dissolved CO_2 in altering shale wettability through surface chemical modifications and the long-term stability of adsorbed CO_2 under biogeochemical interactions. Such uncertainties highlight the gap between laboratory-scale observations and field-scale predictability, necessitating advanced monitoring technologies to validate plume behavior and storage security.

To advance CO_2-EOR in shale systems, future research must prioritize multiscale model integration, combining reactive transport simulations with in-situ spectroscopic techniques to resolve confinement-altered phase behavior. Dynamic geomechanical coupling is essential to address adsorption hysteresis and fracture stability under cyclic stresses, while sensor networks must be developed to track interfacial phenomena and storage integrity. By harmonizing molecular insights with reservoir engineering, the dual objectives of hydrocarbon recovery and carbon storage can be co-optimized, transforming shale's nanoscale complexity into a strategic asset for sustainable energy transitions.

3. Factors governing CO_2-EOR efficacy and storage potential in shale reservoirs

The efficacy of CO_2-enhanced oil recovery (CO_2-EOR) and subsurface carbon storage in shale reservoirs is governed by a complex interplay of geological architecture, petrophysical constraints, and multiphase fluid dynamics. Shale's inherent ultra-low permeability and porosity create fundamental injectivity challenges, necessitating engineered fracture networks with hierarchical connectivity to overcome capillary barriers in organic-rich nanopores. Hydraulic and reactivated natural fractures collectively dictate CO_2 plume distribution, where fracture density and spatial arrangement critically influence sweep efficiency. Reservoir pressure and temperature gradients further modulate CO_2 phase behavior: Supercritical CO_2 ($scCO_2$) at greater depths exhibits enhanced pore penetration due to its liquid-like density and gas-like diffusivity, while subcritical CO_2 in shallower reservoirs suffers from limited solvation capacity (Chen et al., 2022). Thermal maturity amplifies wettability shifts toward CO_2-wet conditions, promoting imbibition but risking asphaltene destabilization in organically hosted pores.

Minerological heterogeneity introduces geochemical reactivity that dynamically reshapes storage and flow pathways. Clay-rich lithologies experience permeability reduction through swelling mechanisms triggered by CO_2 adsorption, whereas carbonate-cemented systems undergo dissolution-reprecipitation cycles that reconfigure pore-throat geometries. Organic content inversely correlates with effective diffusion rates due to molecular sieving within kerogen matrices but enhances CO_2 adsorption via aromatic carbon interactions. Natural fracture networks, characterized through advanced seismic and discrete fracture modeling, amplify storage potential by increasing accessible surface area but risk leakage if connectivity exceeds critical percolation thresholds.

Fluid dynamics introduce nonlinear optimization challenges. Light crude oils achieve miscibility at lower pressures

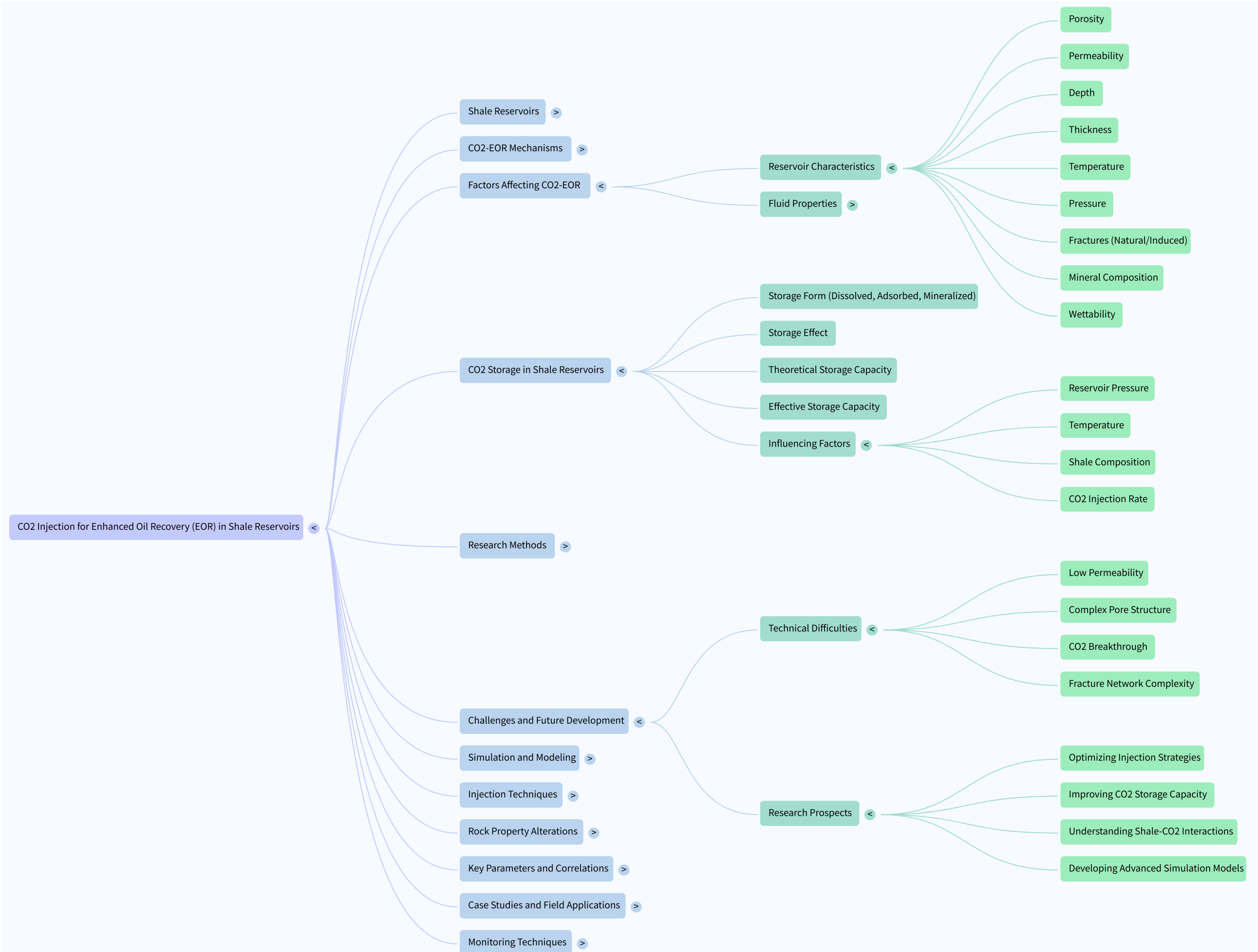

Fig. 1. Mind map of CO_2-Enhanced oil recovery in unconventional reservoirs.

but are prone to gas stripping, whereas heavier oils require higher pressures for viscosity reduction. Residual oil saturation post-injection reflects nanoconfinement trapping effects, as revealed by advanced nuclear magnetic resonance techniques. CO_2 storage mechanisms in shales operate through multiscale trapping: Free-phase CO_2 occupies fractures and macropores, dissolved CO_2 enriches formation brines, and adsorbed CO_2 binds preferentially to organic surfaces. Mineral trapping, though thermodynamically favorable in specific lithologies, progresses slowly and may compromise fracture integrity through secondary cementation. Emerging integrated models employ machine learning to balance injection parameters, optimizing recovery and storage efficiency while accounting for geochemical feedbacks such as permeability reduction via clay alteration. Field-scale pilots highlight critical trade-offs: elevated injection pressures enhance miscibility but escalate leakage risks, while high organic content maximizes adsorption capacity at the expense of injectivity due to pore-throat occlusion.

4. Challenges in CO_2-EOR for shale reservoirs

The deployment of CO_2-enhanced oil recovery (CO_2-EOR) in shale reservoirs is constrained by nanoscale geological complexity and subsurface heterogeneity, presenting multifaceted technical and economic challenges. A critical barrier lies in the ultra-low permeability of shale matrices, which imposes inherent limitations on fluid transport even after hydraulic fracturing. Stimulated fracture networks, though initially effective, suffer from progressive conductivity degradation due to proppant crushing and stress-sensitive closure, necessitating advanced stimulation techniques such as plasma pulse fracturing and microbial-induced permeability enhancement to sustain injectivity. Beyond fracture dynamics, multiphase flow in dual-porosity systems deviates from conventional Darcy-flow regimes, as Knudsen diffusion, adsorption hysteresis, and capillary condensation dominate transport mechanisms within nanopores. Microfluidic studies reveal significant deviations in CO_2-oil miscibility under nanoconfinement compared to bulk-phase predictions, while confinement-induced interfacial tension reduction remains inadequately quantified. These pore-scale uncertainties propagate into field-scale models, where discrepancies between simulated and observed CO_2 breakthrough times highlight the inadequacy of existing upscaling frameworks to reconcile multiscale transport phenomena.

Premature CO_2 breakthrough, driven by fracture channeling and viscous fingering, compromises both recovery efficiency and storage integrity. Conformance control strategies, including salinity-tailored water-alternating-gas (WAG) injection and surfactant-stabilized CO_2 foams, demonstrate improved sweep efficiency in laboratory settings but face operational challenges under extreme salinity and low-pH conditions. Economic optimization requires balancing capital-intensive compression and recycling costs against incremental recovery gains, with machine learning workflows now integrating reservoir heterogeneity and real-time monitoring data to forecast economic thresholds. However, the energy penalties associated with CO_2 recycling in low-permeability systems remain a critical bottleneck.

Future research must address multiscale knowledge gaps through interdisciplinary integration. At the molecular scale, synchrotron X-ray tomography coupled with molecular dynamics simulations is elucidating confinement-altered phase behavior, particularly capillary condensation thresholds in kerogen-hosted nanopores. Concurrently, hybrid finite element-lattice Boltzmann models are advancing pore-to-reservoir upscaling by incorporating stress-dependent adsorption and geochemical reaction kinetics. Long-term geomechanical risks, such as CO_2-induced clay swelling and fracture network cementation, demand coupled thermo-hydro-mechanical-chemical (THMC) models validated against decade-scale field trials. Additive engineering innovations-including nanoparticle-stabilized foams and ionic liquid-enhanced miscibility-show transformative potential but require rigorous field testing to evaluate stability and compatibility with reservoir geochemistry. Hybrid strategies integrating CO_2-EOR with in-situ resistive heating or microbial methane generation further aim to synergize recovery and emissions mitigation, though asphaltene deposition and regulatory gaps in monitoring technologies pose persistent risks.

A coordinated roadmap for shale reservoir optimization must prioritize three frontiers: (1) Nanoscale wettability modulation through in-situ chemical mapping. (2) Fracture self-healing mechanisms under cyclic injection stresses. (3) Integration of renewable-sourced CO_2 to enhance lifecycle sustainability. Bridging these gaps will require physics-informed AI models trained on multiscale datasets from targeted field pilots across diverse shale plays. By harmonizing molecular insights, engineered additives, and intelligent monitoring systems, the vision of co-optimized EOR and secure carbon storage in shale reservoirs transitions from theoretical ambition to scalable reality, contingent on resolving persistent technical, economic, and regulatory asymmetries.

5. Integrated methodologies and fndings in CO_2-EOR and storage research

The scientific understanding of CO_2-enhanced oil recovery and storage in shale reservoirs integrates multiscale modeling, experimental characterization, and computational optimization (Wang et al., 2024). Diffusion modeling employs correlations to calculate CO_2 diffusion coefficients in oil and gas phases, accounting for temperature, pressure, and molecular interactions, with deviations observed in organic-rich systems due to surface diffusion along nanopores. Fracture-matrix permeability relationships are quantified using pore-throat characteristics and cementation factors, where fracture networks dominate flow dynamics while matrix properties govern long-term storage. Reservoir simulations utilize discrete fracture and dual-porosity models to capture heterogeneity, incorporating parameters such as fracture apertures, matrix porosity, and spacing to optimize CO_2 penetration. Geochemical studies reveal CO_2-induced mineral dissolution and clay transformations, altering pore structures and mechanical properties, while advanced imaging techniques characterize these changes. Phase behavior modeling adapts equations of state to account for confinement effects in nanopores, resolving shifts in miscibility thresholds and interfacial interactions. Experimental studies on carbonated water injection and nanoparticle-stabilized foams demonstrate enhanced oil recovery through combined solubility trapping and viscosity reduction, with molecular dynamics simulations elucidating confinement-driven flow restrictions in kerogen-hosted pores. Optimization challenges are addressed via machine learning and metaheuristic algorithms (Zhuang et al., 2025), balancing injection strategies with fracture stability and leakage risks. Emerging sensor networks improve monitoring efficiency, though discrepancies persist between pore-scale models and reservoir-scale predictions, particularly in organic porosity and gas slippage effects. Future advancements require integrating molecular-scale insights with field-scale simulations, validated through targeted pilots to bridge gaps in predictive accuracy and operational reliability. This synthesis highlights the interplay of theoretical frameworks, experimental validations, and computational tools in advancing CO_2-EOR and storage, emphasizing the need for holistic approaches to address multiscale complexity.

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Conflict of interest

The authors declare no competing interest.

References

Chen, Z., Zhou, Y., Li, H. A review of phase behavior mechanisms of CO_2 EOR and storage in subsurface formations. Industrial & Engineering Chemistry Research, 2022, 61(29): 10298-10318.

Davoodi, S., Al-Shargabi, M., Wood, D. A., et al. Carbon dioxide sequestration through enhanced oil recovery: A review of storage mechanisms and technological applications. Fuel, 2024, 366: 131313.

Grubert, E. The Eagle Ford and Bakken shale regions of the United States: A comparative case study. The Extractive

Industries and Society, 2018, 5(4): 570-580.
Wang, Y., Cao, R., Jia, Z., et al. A multi-mechanism numerical simulation model for CO_2-EOR and storage in fractured shale oil reservoirs. Petroleum Science, 2024, 21(3): 1814-1828.
Zhao, J., Ren, L., Lin, C., et al. A review of deep and ultra-deep shale gas fracturing in China: Status and directions. Renewable and Sustainable Energy Reviews, 2025, 209: 115111.
Zhang, T., Sun, S. An exploratory multi-scale framework to reservoir digital twin. Advances in Geo-Energy Research, 2021, 5(3): 239-251.
Zhuang, X., Wang, W., Su, Y., et al. Deep learning-assisted optimization for enhanced oil recovery and CO_2 sequestration considering gas channeling constraints. Petroleum Science. 2025.