




## Research article

# Leakage and Sealing in CO<sub>2</sub> Geological Storage: Driving Forces, Resistance and Mechanisms

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### Abstract:

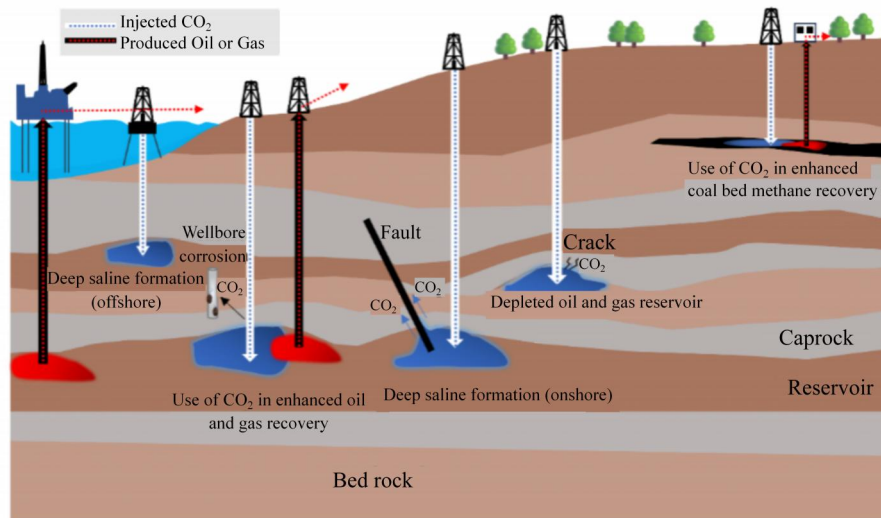
As a key strategy for achieving carbon neutrality, the safety and effectiveness of CO<sub>2</sub> geological storage depend on a thorough understanding of leakage dynamics and sealing mechanisms. Adopting a multi-scale perspective spanning pore, core, reservoir, site, and basin levels, this review systematically examines the structural characteristics of storage and migration spaces, identifies primary leakage pathways governed by faults, caprocks, and wellbores, and classifies dominant leakage modes. To address common conceptual ambiguities and scale disconnect issues in conventional studies, we propose a unified multi-scale definition framework based on the “object–process–boundary” concept, which clearly distinguishes among migration, transformation, sealing, and leakage behaviors. On this basis, we elucidate the dynamic coupling between driving mechanisms (e.g., buoyancy, pressure perturbation) and resistance mechanisms (e.g., capillary sealing, mineral reactions), and clarify their variations across scales and dimensions. Finally, a closed-loop “monitoring–prediction–regulation–intervention” framework, centered on stress management, is developed to provide systematic concepts and practical methodologies for risk assessment, monitoring design, and engineering control. This study provides a systematic synthesis across multiple scales, from pores to basins, forming a comprehensive foundation for assessing and ensuring the safety and efficiency of geological carbon storage projects.

## 1 Introduction

With the continuous increase in global energy demand and the intensification of climate change, carbon capture, utilization, and storage (CCUS) has become increasingly important for achieving carbon neutrality and has gradually progressed toward large-scale deployment (Bachu, 2008; Davis et al., 2018), being applied across diverse regions and multiple scales. By early 2025, the global operational CCUS capture and storage capacity had exceeded 50 million tons per year. Based on the current project pipeline, the capture capacity is projected to reach approximately 430 million tons per year by 2030, with a corresponding storage capacity of about 670 million tons per year (IEA, 2025). On the one hand, large-scale deployment

highlights the core value of CCUS; on the other hand, it inevitably increases system complexity and potential risks. The risk of CO<sub>2</sub> leakage during storage remains a major obstacle to the widespread deployment of this technology.

CO<sub>2</sub> leakage is a critical issue for the safety of large-scale geological storage, and its prevention and control rely on well-sealed reservoir systems. The ideal reservoir is typically located at depths greater than 800 m (temperature >31.1 °C and pressure >72.8 bar), with sufficient pore space and high permeability to facilitate CO<sub>2</sub> injection and distribution, and is overlain by low-permeability caprock that prevents upward migration (Orr, 2009) (Fig. 1). Common storage media include deep saline



**Fig. 1** Overview of geological storage options (modified after (Orr, 2009))

aquifers, depleted oil and gas reservoirs, salt or crystalline rock caverns, unminable coal seams, unconventional reservoirs, and igneous rocks (Jin et al., 2017; Raza et al., 2022; Sun et al., 2023; Davoodi et al., 2024). Through mechanisms such as structural and lithologic trapping, residual trapping, dissolution, mineralization, and coal-bed adsorption, these storage media enable CO<sub>2</sub> to remain for extended periods and effectively prevent escape (Dooley et al., 2006; Raza et al., 2016; Aminu et al., 2017).

However, there exists a dynamic interplay between sealing mechanisms and leakage pathways, which can essentially be attributed to a competitive process between driving and resistance forces. This mechanism operates across multiple scales (pores, cores, reservoirs, basins), and although specific parameters vary, they collectively determine the evolutionary outcomes of leakage and sealing (Luo et al., 2025). The process strongly depends on the multi-scale characteristics of storage and migration spaces and their dynamic evolution (De Silva et al., 2015; Yang et al., 2024). Among these, fault systems are particularly complex, as their discontinuities and associated fracture networks significantly increase the diversity and uncertainty of leakage pathways (Xu et al., 2022). Therefore, the long-term security of geological sequestration fundamentally depends on the precise definition and understanding of “leakage” and “sealing” behaviors. At present, there is still no unified and clear definition within academia and engineering for concepts such as “leakage” and related terms, including “migration”, “transformation” and “sealing”. Conceptual ambiguities not only hinder academic communication but also result in unreliable criteria for risk assessment and engineering design. Particularly in a multi-scale context, defining leakage behaviors across different levels—from pore and core to reservoir, site, and basin—has become a prerequisite for accurate modeling, monitoring, and management.

This review aims to systematically delineate the issues of leakage and sealing in CO<sub>2</sub> geological storage, beginning with

fundamental concepts and focusing on the driving resistance force mechanisms and their multi-scale characteristics. The specific objectives are: (1) to reveal the multi-scale architecture spanning from pores to basins; to summarize the controlling effects and evolutionary patterns of the main potential leakage pathways (faults, caprocks, and wellbores) on CO<sub>2</sub> migration and sealing; and, based on this, to further propose a taxonomy of typical leakage modes categorized by pathway characteristics, leakage rate, and duration; (2) to propose a multi-scale definitional framework for leakage and sealing based on system boundaries, and to clarify the interaction mechanisms among driving forces, resistances, and pathways during leakage processes; and (3) to establish and synthesize a closed-loop framework centered on pressure management for “monitoring–prediction–regulation–intervention”, thereby providing a systematic conceptual basis and an integrated analytical perspective for risk assessment and engineering control in CO<sub>2</sub> storage.

## 2 Multi-scale characteristics of storage - transport spaces and entities

The migration of CO<sub>2</sub> within subsurface reservoirs exhibits characteristic multi-scale behavior. The scope of study encompasses both geological entities (e.g., reservoirs and caprocks) and the CO<sub>2</sub> fluid under varying temperature and pressure conditions. At different scales, the flow mechanisms, sealing processes, and potential leakage risks of CO<sub>2</sub> exhibit distinct characteristics. Therefore, establishing a cross-scale conceptual framework is essential for understanding the overall storage and leakage behaviors of CO<sub>2</sub>.

### 2.1 Multi-scale nature of storage systems and their components

Storage systems are inherently multi-scale, with their structural and behavioral characteristics varying significantly across scales. The scope of investigation extends across multiple

**Tab. 1** Comparison of pore-scale numerical methods

Methods	Description	Applicability	Advantages	Disadvantages	References
Lattice Boltzmann Method (LBM)	Represents the fluid as a collection of particles and simulates multiphase flow through the interactions of particles in pore spaces.	Suitable for simulating the displacement behavior of CO <sub>2</sub> -brine in porous media, taking into account factors such as wettability, viscosity ratio, and interfacial tension.	Simple to operate, computationally efficient, and capable of handling complex pore structures.	Limited applicability to CO <sub>2</sub> -brine systems with realistic density and viscosity ratios in heterogeneous pore structures.	Liu et al., 2014; Jing and Tsuji, 2016; Fakhari et al., 2018; Guo et al., 2020; Sun et al., 2023
Pore Network (PN) Model	Simplifies pores into a lattice network of randomly shaped elements connected by throats, representing a simplified model of porous media.	Used to study CO <sub>2</sub> capillary trapping and the impact of mineral dissolution/precipitation on pore structure.	Computationally efficient, highly scalable, capable of simulating fluid flow in complex pore structures.	Ignores microscopic details, strongly parameter-dependent, lower accuracy, struggles to capture microscopic flow details.	Blunt et al., 2013; Bensinger and Beckingham, 2020; Campos et al., 2015; Benali et al., 2022; Liu et al., 2020
Smooth Particle Hydrodynamics (SPH)	A mesh-free method used to simulate the behavior of multiphase fluids at the pore scale.	Can be used for simulating CO <sub>2</sub> flow in porous media.	Relatively easy to implement.	Requires calibration of model parameters.	Hu et al., 2017
Computational Fluid Dynamics (CFD)	Simulates fluid flow based on the Navier-Stokes equations, effectively capturing interfaces.	Suitable for pore-scale multiphase flow simulation.	Capable of accurately capturing interface behavior.	Interfacial tension may cause numerical instability.	Ferrari et al., 2013
Phase-field LBM	A variant of LBM that describes multiphase flow based on phase-field theory.	Used to simulate multiphase flow characteristics in heterogeneous porous media.	Capable of handling complex interface behavior.	Numerical stability is limited for systems with high density/viscosity ratios.	Fakhari et al., 2018;
Shan-Chen LBM	Uses a pseudo-potential to describe interactions between different fluid phases.	Investigates relative permeability changes during CO <sub>2</sub> -brine displacement processes.	Improved numerical stability and accuracy, particularly performing well under conditions of low resolution and low numerical viscosity.	Applicability to complex pore structures remains limited.	Shan et al., 1993; Sun et al., 2023

levels, from microscopic pores ( $\mu\text{m}$ – $\text{mm}$ ) and core fractures ( $\text{cm}$ – $\text{m}$ ) to fault zones ( $\text{m}$ – $\text{km}$ ) and regional basins ( $>\text{km}$ ) (Fig. 2). Faults, as key structural elements within these systems, possess composite architectures typically composed of low-permeability fault gouge, high-permeability breccia, and surrounding fracture damage zones (Ducellier et al., 2011; Guglielmi et al., 2017). Research methodologies correspondingly vary with scale: laboratory studies typically use centimeter-scale core samples to simulate the seepage behavior of fault cores (Zhang et al., 2019a; Shen et al., 2021), whereas physical

simulations and field tests are employed to investigate the controlling mechanisms of faults in realistic geological settings (Fernø et al., 2024; Michael et al., 2021).

The physicochemical properties of storage systems also exhibit pronounced multi-scale heterogeneity. Variations in mineral composition, stratigraphic architecture, fracture distribution, and pore morphology exert significant control on fluid migration and geochemical processes across scales—from pore to reservoir levels (Noiriel & Daval, 2017; Zhao et al., 2019).

The migration mechanisms of CO<sub>2</sub> likewise exhibit scale-

**Tab. 2** Multiscale Processes, Controlling Factors, and Modeling Approaches in CO<sub>2</sub> Geological Storage

Scale	Spatial range	Dominant mechanisms	Key controlling factors/risks	Typical modeling approaches	Main applications
Pore scale (10 nm – 1 cm)	Pores, throats, micro-fractures	Capillary trapping, dissolution, mineralization, precipitation	Pore-throat size, geometry, roughness, wettability (contact angle), capillary entry pressure	Lattice Boltzmann (LBM), Pore-network (PN), CFD, SPH	Mechanistic understanding; constitutive parameters (e.g., permeability, relative permeability)
Core scale (1 cm – 10 cm)	Laboratory core samples, representative elementary volume (REV)	Multi-phase flow, fines migration, mineral dissolution/precipitation, capillary heterogeneity	Heterogeneity distribution, mineral reactivity, injection rate, wettability alteration, fines migration & clogging risk	CT-scanning, core-flooding experiments, pore-network upscaling, discrete element method (DEM)	Determination of REV, calibration of constitutive models, parameterization for reservoir-scale simulation
Reservoir scale (10 cm – 10 <sup>2</sup> m)	Stratigraphic layers, lithological interfaces	CO <sub>2</sub> -brine two-phase flow, viscous fingering, capillary barrier effect	Relative permeability, heterogeneity (lamination, mudstone interlayers), capillary pressure contrasts	H, HM, THM, THMC coupled models	Plume evolution, storage capacity, leakage assessment
Site scale (10 <sup>2</sup> m – 10 km)	Traps, fault blocks, storage complexes	Plume migration, multi-well interference, fault reactivation	Geological structure, injection strategy, pressure build-up, stress perturbation	3D HMC coupled models; stochastic simulations	Risk evaluation, monitoring design, pressure management
Basin / regional scale (>10 km)	Sedimentary basins, clusters of storage sites	Source-sink matching, cumulative pressure effects, regional stress changes	Storage capacity, transport infrastructure, regional hydrodynamics, inter-site interference	System-level coupling models; techno-economic & policy scenario analysis	Regional deployment, strategic planning, policy support

dependent characteristics. The diffusion coefficient of CO<sub>2</sub> in porous media typically increases with the observation scale, with longitudinal dispersion capacity strengthening alongside scale and flow velocity gradients (Klotz et al., 1980; Appelo & Postma, 2004), whereas transverse dispersion remains relatively limited. At the field scale (km), the diffusion coefficient is generally 2–3 orders of magnitude higher than laboratory values and commonly increases with the measurement scale (Reimus & Callahan, 2007). Simultaneously, CO<sub>2</sub> migration in groundwater is strongly retarded by adsorption, leading to actual migration rates lower than average groundwater flow velocities (Dai et al., 2020). Adsorption behavior is highly sensitive to reservoir heterogeneity (Limousin et al., 2007), thereby increasing predictive uncertainties from the pore-throat scale to the field scale.

## 2.2 Multi-scale migration models and characteristics

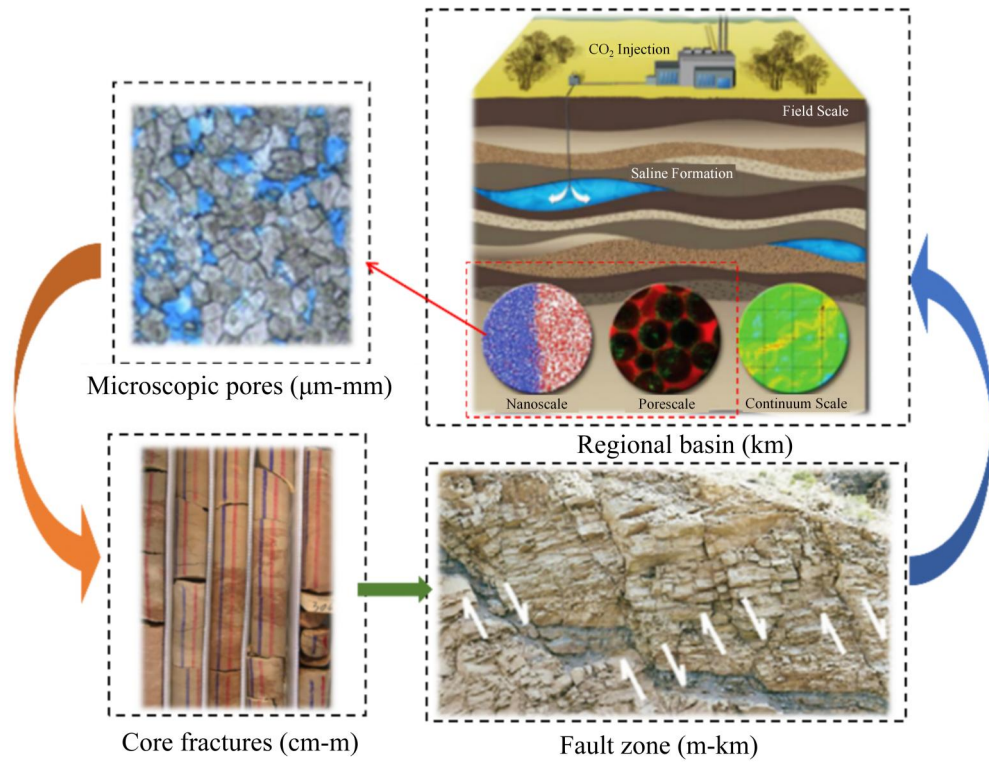
Studies have shown that CO<sub>2</sub> migration exhibits distinct physical mechanisms and characteristics across different observational and characterization scales (Middleton et al. (2012)). The commonly adopted multi-scale models include the pore scale, core scale, reservoir scale, site scale, and basin or regional scale.

### (1) Pore Scale (10 nm – 1 cm)

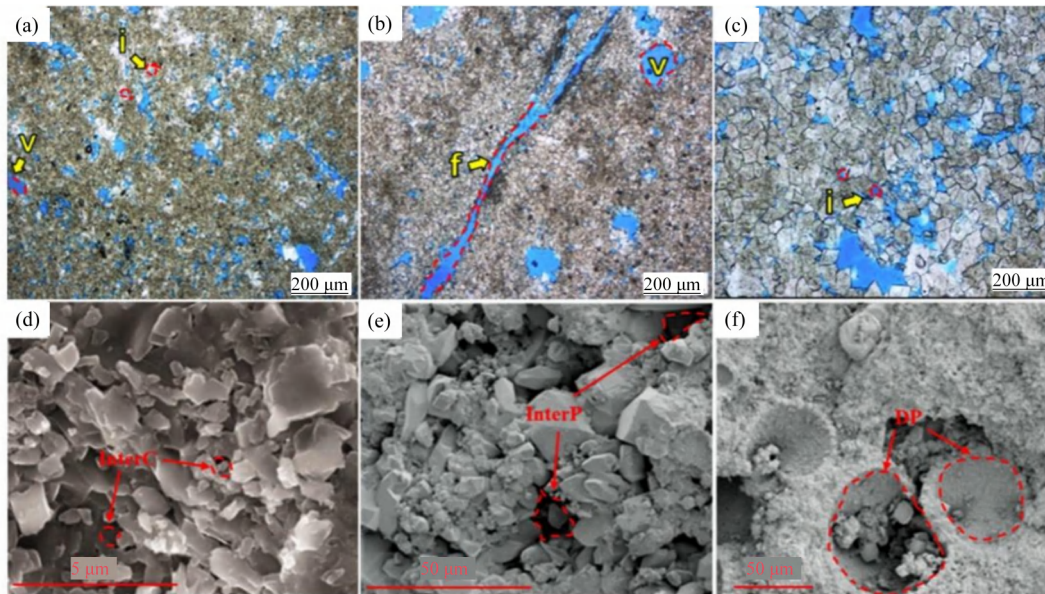
The pore system consists of diverse types, including inter-crystalline pores, intergranular pores, dissolution pores (vugs),

and fractures (Fig. 3), spanning scales from nanometers to centimeters (Al Haddad & Mancini, 2013; Gundogar et al., 2016). Nanopores constitute the primary spaces for CO<sub>2</sub> capillary trapping, whereas micron- to millimeter-scale dissolution pores and fractures form the dominant preferential flow pathways (Mitiku et al., 2013; Kang et al., 2015). At this scale, CO<sub>2</sub> migration is governed by multiple coupled physicochemical processes, including immiscible displacement, dissolution, capillary trapping, mineralization, and precipitation. The heterogeneity of pore structure (pore-throat diameter  $d$ , shape, roughness) and mineral surface wettability (contact angle  $\theta$ ) collectively determine the capillary entry pressure  $P_c$ , thereby controlling whether an individual pore-throat acts as a capillary barrier (Zhou et al., 2017; Ellis & Bazylak, 2012).

Pore-scale models typically allow a clear distinction between solid and pore phases, enabling accurate descriptions of coupled hydrodynamic and geochemical processes at solid–fluid interfaces. To elucidate pore-scale mechanisms, various numerical methods have recently been developed, including the lattice Boltzmann method (LBM), pore-network modeling (PNM), smoothed particle hydrodynamics (SPH), and computational fluid dynamics (CFD). Although CFD can accurately capture phase interfaces, it is often prone to numerical instabilities induced by surface tension. SPH is relatively straightforward to implement but requires parameter calibration. In contrast, LBM and PNM are widely adopted owing to their high efficiency and



**Fig. 2** Nanoscale to basin scale schematic diagram (modified after Evans and Bense (Evans, 2013; Bense et al., 2013))



**Fig. 3** Pore types in carbonate reservoirs: (a–c) Cast thin-section photomicrographs from northwest Iraq (Mohammed Sajed & Glover, 2020); (d–e) Scanning Electron Microscope (SEM) images from northern Iraq (Rashid et al., 2015). Labels: i and InterC: Intercrystalline pore; V: Vug; f: Fracture; InterP: Interparticle pore; DP: Dissolution pore (Tan et al., 2025)

broad applicability (Ferrari & Lunati, 2013; Hu et al., 2017) (Table 1).

A primary objective of studying CO<sub>2</sub> migration mechanisms and characteristics at the pore scale is to elucidate the emergent phenomena observed at macroscopic scales and to identify key

controlling parameters, such as the capillary number—the ratio of viscous to capillary forces (Zhang et al., 2011). A second objective is to derive representative values of constitutive parameters, such as the permeability and relative permeability of porous media (Bachu & Bennion, 2008), thereby enabling more

realistic simulations at larger scales. Consequently, pore-scale modeling is essential not only for understanding the interactions among CO<sub>2</sub>, reservoir rocks, and fluids but also for providing key parameters to calibrate reservoir-scale simulations (Sun et al., 2025). Furthermore, upscaling methods—such as volume averaging, homogenization theory, and fractal geometry—are applied to incorporate pore-scale processes into reservoir models (Zhang et al., 2021). However, the scale dependence of petrophysical parameters (e.g., permeability, diffusion coefficient) and reaction rates presents a major challenge for cross-scale prediction. For example, mineral dissolution rates at the field scale can be four to five orders of magnitude lower than those measured in the laboratory (White et al., 1996).

#### (2) Core Scale (1 cm – 10 cm)

The core scale serves as a critical bridge between pore-scale mechanisms and reservoir-scale behavior. Determining its Representative Elementary Volume (REV) requires comprehensive consideration of factors such as pore structure heterogeneity and multiphase fluid interactions. Experimental studies indicate that, following CO<sub>2</sub> injection, fine particles may migrate due to scouring at the CO<sub>2</sub>–water interface, whereas residual water rings can immobilize some particles, collectively resulting in reduced permeability (Nguyen et al., 2024). Concurrently, mineral reactions exhibit marked lithological dependence: calcite-cemented sandstones may experience a pore volume increase of approximately 26.25%, whereas clay-cemented rocks show only about an 11.58% increase, underscoring the strong control of mineral reactivity on pore evolution (Wang et al., 2024). Furthermore, spatial heterogeneity in capillary forces can locally trap migrating CO<sub>2</sub>, thereby enhancing lateral dispersion and reducing the risk of upward migration (Cui et al., 2024). Imbibition experiments further demonstrate that water flooding in CO<sub>2</sub>-saturated cores can increase residual CO<sub>2</sub> saturation by 26–30%, primarily due to alterations in wettability and interfacial tension (Ge et al., 2022).

Migration patterns at the core scale are governed by the interaction between lithology and injection conditions. In calcite-cemented formations, pore enlargement and flow velocity can create a positive feedback loop, leading to unstable fingering phenomena. In contrast, clay-rich formations exhibit stable but constrained migration pathways due to strong capillary forces (Wang et al., 2025). Within nanopores of shale reservoirs, CO<sub>2</sub> displacement typically proceeds in three stages: pressure-driven flow, concurrent matrix–fracture production, and matrix release (Pan et al., 2025). CT imaging results reveal that pore heterogeneity strongly influences migration paths at low injection rates (0.1 cm<sup>3</sup>/min), whereas this effect diminishes at higher injection rates (3 cm<sup>3</sup>/min). This finding suggests that REV-scale parameters require dynamic adjustment during upscaling to account for specific injection conditions (Shi et al., 2010).

For upscaling, core-scale results can be transferred to the reservoir scale using methods such as pore-network modeling, volume averaging, and homogenization. For instance, pore-network models based on a truncated Weibull distribution indicate that miscible displacement efficiency is about 15% higher than that of immiscible displacement (Meng et al., 2014). At the same time, the effects of multi-field coupling must also be

considered. Thermal–hydraulic–mechanical–chemical (THM–C) processes triggered by CO<sub>2</sub> injection may cause fault reactivation, necessitating reduced-order models for computational simplification (Li et al., 2025). In addition, discrete-element fluid–solid coupling models elucidate the microscopic mechanisms of particle migration and accumulation, with particle morphology and size distribution exerting a strong influence on parameterization outcomes (Yang et al., 2023).

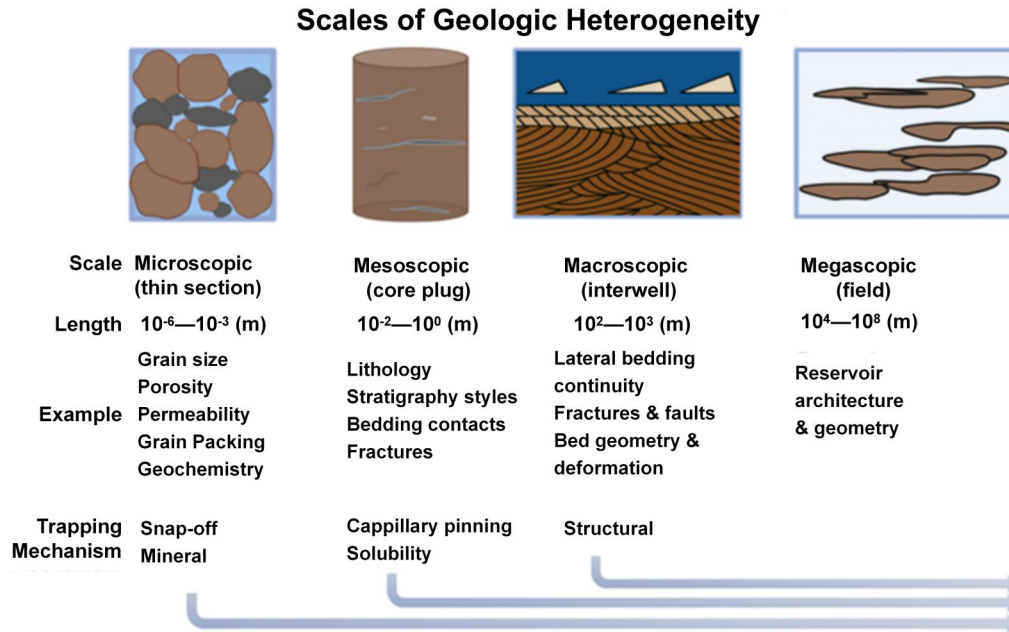
#### (3) Reservoir Scale (10cm – 10<sup>2</sup> m)

Models at this scale are predominantly grounded in continuum mechanics principles, with the study domain typically extending from tens of centimeters to several hundred meters, depending on research objectives and computational resources. The primary focus lies in investigating the spatiotemporal evolution of the CO<sub>2</sub> plume within the reservoir. The resulting data are directly applicable to assessing reservoir capacity, injectivity, and potential leakage, and can also inform site-scale simulations. At this scale, capillary trapping plays a major role. Geological heterogeneities—such as cross-bedding, mudstone interlayers, and lithological interfaces—generate continuous zones of capillary pressure contrast. Even in the absence of absolute sealing layers, these heterogeneities can form “permeable traps,” forcing buoyant CO<sub>2</sub> plumes to spread laterally and become immobilized beneath high-permeability units (Krevor et al., 2011; Krishnamurthy et al., 2022; Mishra & Haese, 2020)(Fig. 4).

Fig. 5. A conceptual sketch of the different scales of geologic heterogeneity and the CO<sub>2</sub> trapping mechanisms that can be observed at each scale. For example, capillary pinning is typically unobservable at microscopic scale, but it makes a systematic difference starting at the mesoscopic scale (Zhang et al., 2025).

Numerous studies have investigated this scale using a variety of multiphysics coupling models, including hydrological (H), hydrological–mechanical (H–M), thermal–hydrological–mechanical (THM), and thermal–hydrological–mechanical–chemical (THMC) models, among others (Fig. 5) (Bai et al., 2017; Cappa & Rutqvist, 2011; Carrillo & Bourg, 2021; Celia et al., 2015; Nordbotten et al., 2005; Rutqvist & Tsang, 2002; Rutqvist et al., 2007, 2008; Vilarrasa et al., 2011; Wu et al., 2016, 2018, 2021). The most fundamental characteristic of CO<sub>2</sub> migration at this scale is CO<sub>2</sub>–water two-phase flow, which exhibits a spatiotemporal distribution characterized by viscous fingering. This phenomenon arises from the low density and viscosity of CO<sub>2</sub> relative to water (Nordbotten et al., 2005; Wu et al., 2016, 2018). Relative permeability is the most critical parameter governing this two-phase flow. At present, the relative permeability models most widely used in reservoir simulation software—primarily based on experimental data—are the Van Genuchten model and the generalized power-law model (Olivella et al., 1994; Rutqvist et al., 2002). In recent decades, pore-scale theoretical research has also led to the development of models that calculate relative permeability directly from interfacial tension, thereby establishing a direct link between pore-scale and reservoir-scale models (Bachu, 2008; Middleton et al., 2012).

#### (4) Site Scale (10<sup>2</sup> m – 10 km)



**Fig. 4** A conceptual sketch of the different scales of geologic heterogeneity and the CO<sub>2</sub> trapping mechanisms that can be observed at each scale. For example, capillary pinning is typically unobservable at microscopic scale, but it makes a systematic difference starting at the mesoscopic scale (Zhang et al., 2025)

The site scale represents the core decision-making level that bridges reservoir characteristics with engineering practice. The study domain typically encompasses the entire storage complex (e.g., a complete anticlinal trap or fault block) and adjacent regions that may be affected. At this scale, factors such as formation dip and the spatial configuration of large-scale sedimentary units (e.g., bedsets) exert a strong influence. Dipping formations can divert vertically migrating CO<sub>2</sub> into long-distance lateral pathways, substantially increasing both the rock–fluid contact area and the residence time of CO<sub>2</sub> (Bryant et al., 2008; Ren et al., 2014). Models at this scale are designed to simulate and predict the spatiotemporal evolution of the entire CO<sub>2</sub> plume over decades of injection and centuries of post-injection monitoring, thereby supporting well placement optimization, risk management, and monitoring system design.

In addition to drilling engineering, pipeline layout, and groundwater systems, a central focus of site-scale analysis is the evaluation of synergistic and interference effects from multi-well injection. The simultaneous operation of multiple wells generates a superimposed pressure field that extends far beyond that of a single-well scenario. This elevated pressure field may activate far-field faults or induce microseismic events (Rutqvist, 2012). Consequently, site-scale simulations require highly refined 3D geological models and the integration of coupled processes—such as hydro-mechanical (HM) and thermo-hydro-mechanical-chemical (THMC) interactions—to assess the long-term integrity of the reservoir–caprock system under sustained injection (Celia et al., 2015).

Geological uncertainty constitutes the most critical challenge at this scale. To address it, stochastic modeling approaches

(e.g., geostatistical simulation, Monte Carlo simulation) are frequently employed to generate multiple equiprobable geological realizations. These enable evaluation of confidence intervals for CO<sub>2</sub> migration pathways, storage efficiency, and leakage risk (Sun et al., 2023). Furthermore, inverse modeling techniques assimilate real-time monitoring data (e.g., pressure, temperature, geochemistry) from injection and observation wells to continuously update and calibrate models, thereby enabling dynamic optimization of predictions and establishing a closed-loop “simulate–monitor–update” management strategy (Li et al., 2023).

Ultimately, the outputs of site-scale research quantify leakage probabilities, define pressure management thresholds, optimize monitoring network configurations (e.g., well placement, seismic arrays, surface gas detection sites), and provide the scientific basis for safe injection protocols. This scale is thus pivotal for ensuring project safety and compliance within regulatory frameworks (Fig. 6).

#### (5) Basin/Regional Scale (>10 km)

Research at the basin scale bridges the transition from project-level safety management to regional energy system planning and climate policy formulation. This scale encompasses the entire system within a large sedimentary basin, including multiple storage sites, numerous CO<sub>2</sub> emission sources, and the associated transportation infrastructure (e.g., pipeline networks) that connects them. The core objectives are source–sink matching optimization and system-level risk management. On the one hand, this involves assessing the basin’s total storage capacity and, by comprehensively considering reservoir properties, capacity, costs, and source–sink distances, planning

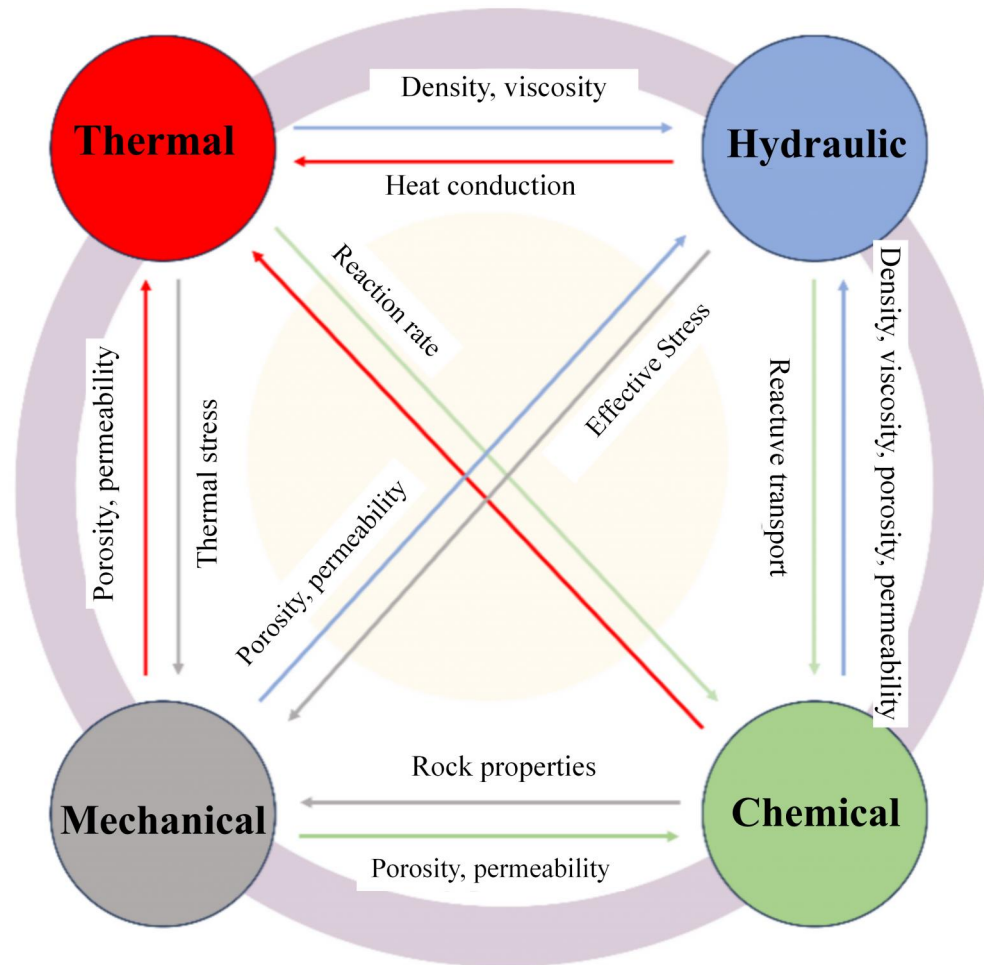


Fig. 5 THMC coupling of CO<sub>2</sub> geological storage (modified after (Sun et al., 2025))

optimal pipeline routing and storage deployment sequences to maximize the cost-effectiveness of CCUS clusters (GCCSI, 2023). On the other hand, the simultaneous large-scale development of multiple sites may produce cumulative regional effects. Injection operations at one site can elevate pore pressure, with the resulting pressure front propagating over tens of kilometers. Such effects may inadvertently influence neighboring storage sites or subsurface resources (e.g., geothermal reservoirs, freshwater aquifers) and could even induce regional modifications to the in-situ stress field (Birkholzer et al., 2009). Accordingly, basin-scale investigations commonly employ multi-site coupled models or system assessment frameworks that simplify detailed fluid-flow processes. These models must integrate economic cost functions, policy incentive schemes, infrastructure planning modules, and simplified porous media flow representations to conduct long-term (decadal to centennial) scenario analyses and sensitivity assessments. CO<sub>2</sub> storage and transport processes inherently span multiple scales—from pore and reservoir to site and basin—each dominated by distinct mechanisms, controlling parameters, and key risk factors (Tab. 2). The pore scale governs interfacial interactions and trapping mechanisms; the core scale, through experiments and detailed simulations, reveals the averaged effects and macroscopic expression of pore networks; the reservoir scale elucidates plume dynamics; the

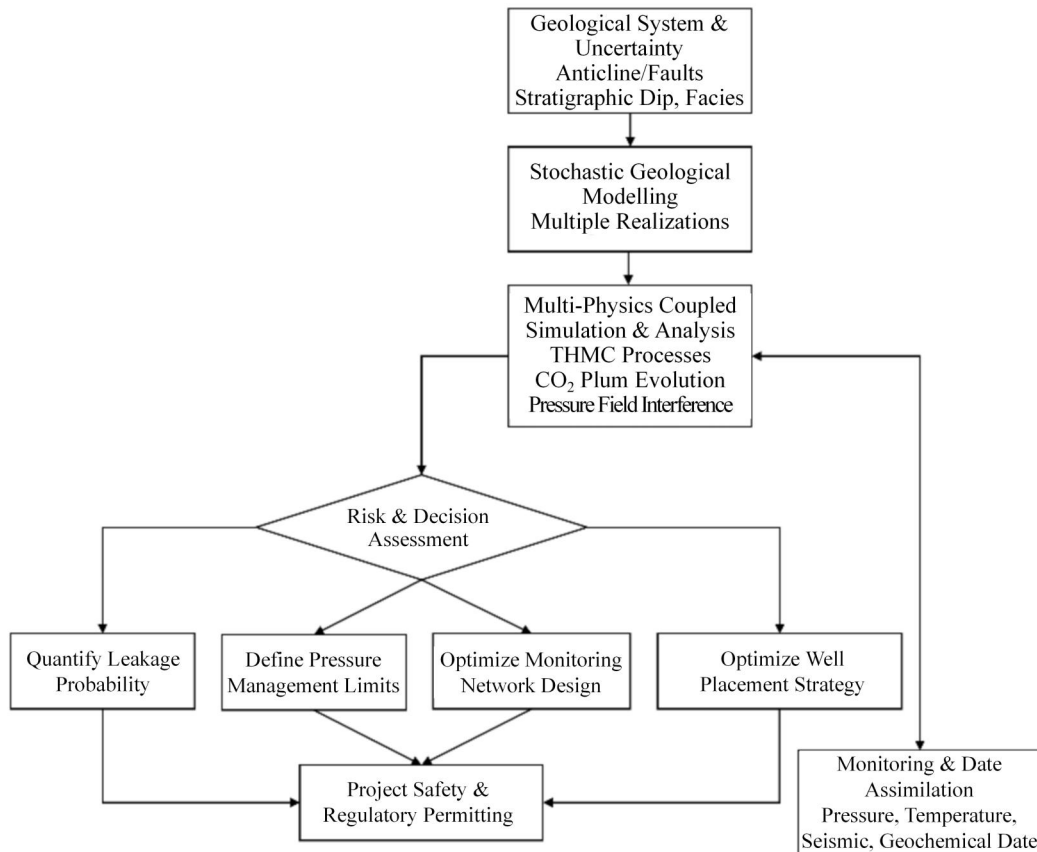
site scale emphasizes pressure-field coupling and monitoring requirements; and the basin scale addresses regional deployment and strategic security. Multiscale coupling is thus not only a fundamental scientific challenge but also a prerequisite for establishing a robust framework for leakage assessment and sealing evaluation.

### 3 Carbon Storage Systems and Potential Leakage Pathways & Modes

#### 3.1 System Components and Leakage Pathways: An Overview

An ideal carbon storage system consists of a reservoir and an overlying caprock. The sealing capacity of the system determines the ultimate fate of CO<sub>2</sub>, whereas inherent geological heterogeneities and engineering interventions govern the formation of potential leakage pathways. Essentially, leakage is not an independent process separate from storage but a specific manifestation of CO<sub>2</sub> migration. Within a typical reservoir, CO<sub>2</sub> migration is governed by the interplay between driving and resisting forces. When the resisting forces are insufficient to counteract the driving forces, CO<sub>2</sub> can breach sealing barriers, resulting in leakage events across multiple scales.

Common potential leakage pathways comprise engineered pathways (e.g., poorly sealed or abandoned wellbores), natural



**Fig. 6** The core logic of site scale research

pathways (e.g., faults, fractures, localized high-permeability zones), and hybrid pathways. According to the RISCs project, CO<sub>2</sub> leakage modes are classified into three types:

(1) localized point-source leakage (e.g., from wells experiencing seal failure),

(2) localized multi-point leakage distributed linearly along faults or fractures,

(3) diffuse, large-area leakage (commonly occurring in sediments or soils) (Pearce et al., 2014) (Fig. 7). Among these, the first two types are most prevalent, as CO<sub>2</sub> preferentially migrates along high-permeability pathways. Diffuse leakage is generally less likely; however, if it occurs, it poses a risk at a regional scale. Consequently, the primary potential leakage pathways in carbon storage systems are mainly associated with faults, the caprock, and wellbores (Adamu et al., 2019; Chen et al., 2024a).

## 3.2 Potential Leakage Pathways and Modes

### 3.2.1 Leakage Mechanisms and Dynamic Behavior of Faults

Faults constitute one of the most critical potential leakage pathways in geological storage systems. Their permeability characteristics directly influence storage security and are governed by the combined effects of multiple factors, including fault zone architecture, lithology, and in-situ stress conditions. A typical fault zone comprises a low-permeability fault core (gouge), a high-permeability damage zone (breccia and frac-

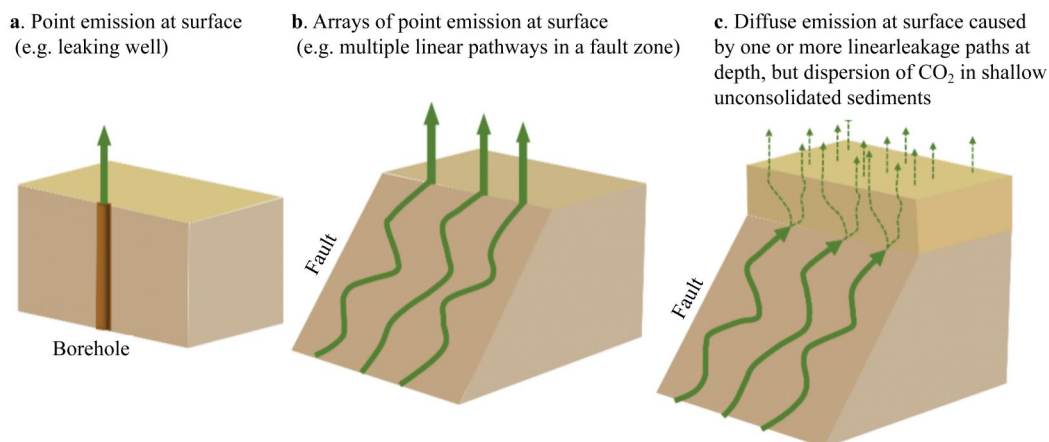
tures), and a peripheral fracture damage zone, collectively forming a structurally complex migration conduit (Ducellier et al., 2011)(Fig. 8). Fault reactivation can potentially induce seismic events and simultaneously create pathways for the leakage of CO<sub>2</sub> and brine, thereby threatening the safety of nearby potable aquifers. During their evolution, faults exhibit diverse structural configurations, ranging from a single slip surface or sealed pores to complex permeable networks comprising a fault core and damage zone; their geometric characteristics determine their capacity and behavior as potential leakage conduits (Sun et al., 2025). Numerical simulations suggest that the heterogeneous distribution of faults may act as a “double-edged sword”: while it can disperse CO<sub>2</sub> into multiple caprock regions, enhancing storage efficiency, it may also, if faults extend through the caprock, directly result in leakage (Zhang et al., 2024b).

The kinematic behavior of faults, particularly shear slip, dynamically modifies leakage pathways. Fault activation and slip can significantly alter their internal architecture (e.g., generating fault gouge, creating new fractures), resulting in substantial changes in permeability (Zhu et al., 2020; Shen et al., 2021). Injection-induced increases in pore pressure effectively reduce the normal stress acting on the fault plane, thereby triggering fault slip according to the slip criterion. This coupled process, known as hydro-mechanical coupling, represents a key kinematic mechanism controlling the potential of a fault to act as a leakage conduit (Guglielmi et al., 2021).

The mechanical and hydraulic behavior of faults is typically

**Tab. 3** Summary of Caprock Integrity Research.

Aspect	Key Findings & Conclusions	Corresponding References
Geometrical Features	<ol style="list-style-type: none"> <li>1. Caprock Thickness: A key physical barrier against vertical fracture penetration. Plastic strain can propagate through the entire thickness.</li> <li>2. Fracture/Fault Geometry: Includes orientation, dip, frequency, and spatial distribution. These features, controlled by in-situ stress fields and fluid pressures, are potential leakage pathways.</li> <li>3. Interface Geometry: The boundary between the caprock and reservoir (e.g., caprock-aquifer interface) is a zone of stress and strain concentration, prone to failure.</li> <li>4. Reservoir Geometry: The lateral extent and depth of the reservoir influence the extent of pressure propagation and buildup, thereby affecting the stress imposed on the caprock.</li> </ol>	Peacock and Mann, 2005; Raziperchikolae and Pasumarti, 2020
Sealing Mechanism	The caprock should be dense, intact, and have low permeability to maintain a supercritical CO <sub>2</sub> state and prevent leakage.	Watson and Gibson-Poole, 2005; Shukla et al., 2010
Failure Modes	<ol style="list-style-type: none"> <li>1. Fracture Formation &amp; Reactivation: Pore pressure changes from injection can alter effective stress, potentially initiating new fractures or reactivating existing faults.</li> <li>2. Plastic Strain Propagation: Plastic strain can spread through the caprock's thickness when vertical stress exceeds horizontal stress, facilitating CO<sub>2</sub> migration.</li> <li>3. Capillary Barrier Breakdown: High-stress conditions can potentially breach the caprock's capillary barrier.</li> <li>4. Chemical Degradation: High-salinity fluids can lead to mineral evaporation and crystallization (e.g., carnallite, halite), reducing pore connectivity.</li> </ol>	Song and Zhang, 2013; Vilarrasa et al., 2011; Orlic et al., 2011; Jayasekara et al., 2020
Influencing Factors	<ul style="list-style-type: none"> <li>- Stress State: Initial stress state, ratio of horizontal to vertical stress.</li> <li>- Injection Pressure &amp; Temperature: High-pressure injection may exceed fracture pressure; cold CO<sub>2</sub> injection can promote horizontal fracture propagation.</li> <li>- Fluid Properties: Salinity, CO<sub>2</sub> saturation, capillary entry pressure.</li> <li>- Rock Properties: Young's modulus, permeability, porosity, hysteresis coefficient.</li> <li>- Geological Structure: Fault orientation, fracture distribution, bedding heterogeneity.</li> </ul>	Raziperchikolae and Pasumarti, 2020; Martinez et al., 2013; Pan et al., 2013; Raziperchikolae et al., 2019; Khan et al., 2024
Research Methods	<ul style="list-style-type: none"> <li>- Numerical Simulation (coupled flow-geomechanical models)</li> <li>- Experimental Studies (triaxial tests, breakthrough pressure tests)</li> <li>- Probabilistic Modeling (Monte Carlo simulation, response surface methodology)</li> <li>- Field Monitoring (microseismic, pressure monitoring)</li> <li>- Imaging Techniques (3D Digital Image Correlation - 3D-DIC)</li> </ul>	Rutqvist, 2012; Raziperchikolae et al., 2013b; Adisornsupawat et al., 2024; Lee et al., 2023; Nath et al., 2024
Protection/ Mitigation Measures	<ul style="list-style-type: none"> <li>- Control injection pressure to avoid exceeding fracture pressure.</li> <li>- Prefer high-salinity formations to enhance caprock sealing.</li> <li>- Use nanoparticles or surfactants to improve caprock wettability and enhance sealing capacity.</li> <li>- Implement monitoring and early warning systems (pressure, microseismic, geochemical monitoring).</li> <li>- Conduct integrity assessments and re-plug wells (reopen and re-plug high-risk wells).</li> </ul>	Bai et al., 2015; Jayasekara et al., 2020; Khan et al., 2024; Yang et al., 2019

**Fig. 7** Three types of CO<sub>2</sub> leakage modes classified by the RISCS project (Pearce, J. et al., 2014)

**Tab. 4** Potential Leakage Paths, Mechanisms, and Kinetic Behavior in CO<sub>2</sub> Geological Sequestration.

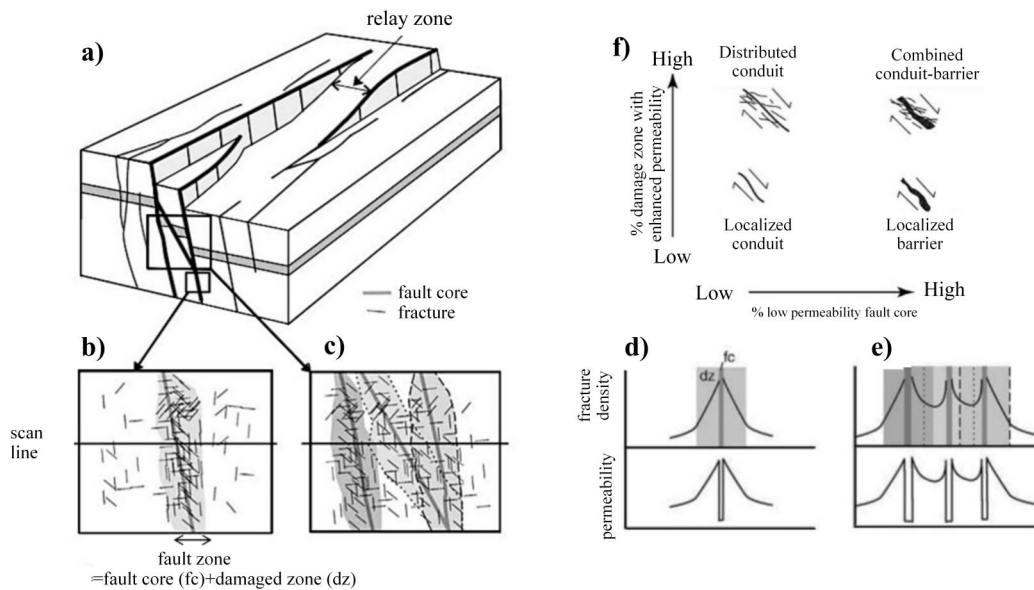
Aspect	Fault	Caprock	Wellbore	Multiphysics-Chemical Coupling
Leakage Pathway	Fault	Caprock	Wellbore	Multiphysics-Chemical Coupling
Structure/Composition Characteristics	Fault gouge (low permeability), fractured rock (high permeability), fracture damage zone	Mudstone, evaporites, carbonate rocks	Casing–cement–formation interfaces; artificial construction defects	Pore–mineral–fluid interface reactions; micro-to-reservoir scale effects
Controlling Factors	Geometric characteristics, heterogeneity, stress field, pore pressure disturbance	Pore pressure, fracture orientation and stress field alignment, heterogeneity	Cement quality, material properties, temperature–pressure cycling, construction defects	Temperature–pressure conditions, salinity, mineral composition
Main Leakage Mechanisms	Shear slip modification, permeability change; fault reactivation; channeling effect	Hydraulic fracturing; shear-induced rupture; dissolution expansion; overpressure	Interface debonding; cement cracking; casing corrosion; screw thread leakage	CO <sub>2</sub> dissolution–acid–mineral reaction/precipitation; permeability evolution coupled with porosity
Mechanical Behavior	Shear stress increase → fault slip; injection pore pressure increase → effective stress decrease; fault structure rearrangement	Injection rate and stress state controlled fracture propagation; vertical stress dominates normal fracture opening; horizontal stress dominates oblique shear	Injection–sealing period affected by stress distribution; thermal–chemical–mechanical coupling leads to weak sealing; micro-leakage aggravation	Cumulative micro-reaction → permeability nonlinear evolution; mineral reaction alters mechanical strength; THMC coupling → flow field restructuring
Typical Mode	Layer-permeated leakage vs. dispersed injection	Hydraulic fracture; shear failure leakage	Annular flow; cement channel leakage	Pore-scale reaction → reservoir weakening → leakage channel formation
Research Methods	Core experiments, physical modeling, numerical modeling, discrete element/finite element modeling, Mohr-Coulomb criterion	Fracture pressure tests, caprock mechanics experiments, numerical modeling (THM coupling)	Engineering diagnosis, monitoring, finite element simulation (FEM, THM coupling)	Reactive transport modeling (pore scale/continuum), cross-scale modeling (THMC coupling)

**Tab. 5** Unified definitions of migration, leakage, and sealing across multiple scales.

Scale	Migration	Leakage	Sealing	Measurable Sealing Metric
Pore scale ( $m - mm$ )	CO <sub>2</sub> movement or phase transformation within pores and throats	Breakthrough of pore throat into adjacent fractures or matrix	Capillary trapping, residual trapping, mineral transformation	Capillary Entry Pressure ( $P_{ce}$ ), Residual CO <sub>2</sub> Saturation ( $S_{gr}$ ), Contact angle ( $\theta$ ).
Core/fracture scale ( $cm - m$ )	CO <sub>2</sub> migration within core samples or fracture networks	Penetration through fractures or damage zones	Fracture self-sealing, pore clogging, mineral precipitation	Breakthrough Pressure ( $P_b$ ), Relative permeability hysteresis, Fracture transmissivity reduction rate.
Reservoir scale ( $m - km$ )	CO <sub>2</sub> migration and accumulation beneath caprock within the reservoir	Breakthrough of caprock or upward migration along faults	Structural/lithologic trapping, caprock sealing, dissolution trapping	Maximum Sealing Pressure, Fault reactivation pressure, Seal Capacity.
Site scale ( $km - 10km$ )	CO <sub>2</sub> redistribution within storage site	Exceeding monitoring boundary or entering shallow aquifers	Pressure management, monitoring and control	Area of Review extent, Pressure interference threshold between wells.
Basin scale ( $10 - 100km$ )	Regional redistribution of CO <sub>2</sub>	CO <sub>2</sub> migration into shallow aquifers, atmosphere, or ecosystems	Regional sealing, structural traps, multi-site integrated management	Integrated basin-scale risk metric (e.g., Probability of Release < $10^{-6} yr^{-1}$ ).

**Tab. 6** Multi-scale and Dimensional Characteristics of Resistance and Driving Force Attenuation Effects in Geological CO<sub>2</sub> Storage.

Scale Level	Pore-Core Scale	Reservoir-Fault-Seal Scale	Regional-Basin Scale
Spatial Range	<i>m – cm</i>	m - km	km - 100+ km
Dominant Driving Forces	Buoyancy, Pressure gradient	Buoyancy, Pressure gradient, Flow induced by heterogeneity	Regional pressure regime, Basinal thermo-fluid field
Dominant Resistance Mechanisms	Capillary trapping, Mineral dissolution/precipitation	Fault/fracture sealing, Lithological heterogeneity, Seal breakthrough pressure	Macroscopic structural trapping (anticlines, synclines), Regional seal integrity
Effect Characteristics & Attenuation Laws	Strong attenuation. Resistance mechanisms significantly inhibit CO <sub>2</sub> migration at early stages, manifesting as residual trapping and permeability alteration.	Duality and abruptness. Resistance efficacy depends on structural sealing but can be rapidly overcome by highly connected fracture networks, leading to “conduit-flow” leakage.	Non-linearity and catastrophic potential. Resistance provides the ultimate sealing constraint. A critical pressure breach leads to large-scale, sudden release. Driving force attenuation is highly non-linear.
Dimensional Effects & Modeling Insights	Pore-network models (3D). Neglecting 3D pore structure overestimates permeability and migration rates.	3D simulation is crucial. 2D models severely underestimate lateral dispersion and leakage risk along faults. Fracture flow approximates 1D pipeline flow, drastically accelerating leakage.	3D geomechanical models. 2D models fail to capture the volume of complex traps and the overall stability of the seal. Upscaling is key for accurate prediction.



**Fig. 8** (a) 3D block diagram showing a normal fault zone (Childs et al., 2009). (b, c) Definitions of fault zone width for single-strand and multi-strand faults, respectively (Chester & Logan, 1986; Caine et al., 1996; Faulkner, 2004; Faulkner et al., 2010). (d, e) Conceptual fracture density and permeability profiles for crystalline bedrock in single and multi-strand fault zones (modified after (Faulkner et al., 2010; Bense et al., 2013)). (f) Fault classification based on the proportion of fault core to damage zone (Caine et al., 1996)

characterized using numerical modeling, which generally falls into two categories. The first approach employs continuum elements, enabling the assignment of various constitutive models (e.g., elastic, elasto-plastic, or visco-plastic) to the fault zone. This approach can represent internal heterogeneity within the fault zone and its interaction with the surrounding rock mass; however, it becomes computationally expensive when model-

ing large slip displacements and complex geometries (Cappa & Rutqvist, 2011; Morris et al., 2011). The second approach utilizes interface elements, treating the fault as a discrete surface characterized by parameters including friction, cohesion, and stiffness. This approach is well-suited for simulating fault reactivation across multiple scales and within complex fault networks (Li et al., 2006; Cappa & Rutqvist, 2011). Fault re-

activation generally follows the Mohr-Coulomb criterion (Fig. 9) and may occur when the shear stress acting on the fault plane exceeds the Mohr-Coulomb failure threshold (Jaeger et al., 2009), expressed as:

$$|\tau_s| \geq c + \sigma_n \tan \phi \quad (1)$$

Where  $\tau_s$  is the shear stress,  $\sigma_n$  is the normal stress,  $c$  is the cohesion, and  $\phi$  is the friction angle. The primary controlling parameters are the friction coefficient and cohesion. This framework can be extended through slip-weakening models or rate-and-state friction laws to distinguish between seismic and aseismic slip processes. These modeling frameworks not only elucidate the underlying mechanisms of fault kinematic behavior but also offer critical support for assessing leakage risks during CO<sub>2</sub> storage operations.

### 3.2.2 Caprock Integrity and Failure Modes

The caprock, acting as the primary barrier overlying the reservoir, relies on its low permeability and significant mechanical strength to prevent upward migration. Key sealing mechanisms of the caprock include capillary sealing, hydraulic sealing, overpressure sealing, and hydrocarbon concentration sealing (Rutqvist, 2012; Shukla et al., 2010). The effectiveness of a carbon storage system depends on the integrity of the caprock. However, in realistic geological settings, caprocks are rarely perfectly homogeneous and may contain fractures, weak planes, or heterogeneous zones, which serve as potential leakage pathways. Typical caprocks comprise argillaceous rocks (shale, claystone, mudstone), evaporites (salt, anhydrite), and, in certain cases, carbonate rocks (limestone, dolomite) (Griffith et al., 2011). These lithologies exhibit notable differences in fracture development, pore structure, and weak plane distribution; their geometric characteristics govern potential CO<sub>2</sub> migration modes

CO<sub>2</sub> leakage through the caprock may occur via multiple mechanisms, including hydraulic fracturing, induced shear failure, leakage along pre-existing faults, dissolved gas diffusion, pore pressure exceeding the breakthrough pressure, or leakage through wellbores. The primary geomechanical failure modes include hydraulic fracturing and induced shear failure (Fig. 10). Hydraulic fracturing is triggered by excessive injection pressure; however, this risk can be largely mitigated by maintaining injection pressure below 90% of the fracturing pressure (Lecampion et al., 2018; Chen et al., 2021). Induced shear failure occurs when the shear stress exceeds the shear strength, typically evaluated using the Mohr-Coulomb failure criterion (Zhang et al., 2015), analogous to fault reactivation. Key factors affecting caprock integrity include the orientation of fractures relative to the in-situ stress field, the magnitude of the minimum horizontal stress, injection rate, and the initial stress state (Peacock & Mann, 2005; Karimnezhad et al., 2014; Raziherchikolaee & Pasumarti, 2020).

Rutqvist et al. reported that shear failure generally occurs at lower injection pressures than hydraulic fracturing (Rutqvist et al., 2008). When horizontal stress exceeds vertical stress, shear failure preferentially occurs along low-angle fractures, which may not compromise the upper portions of the caprock.

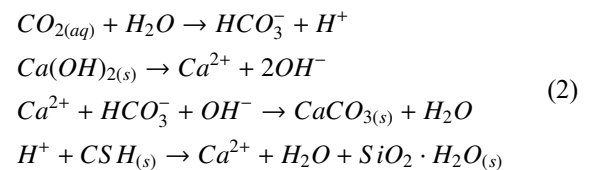
However, when vertical stress exceeds horizontal stress, fracture propagation is more likely to occur as steeply dipping fractures that may penetrate the entire caprock sequence. Numerical modeling indicates that the lower portion of the caprock is more susceptible to pore pressure changes, whereas the overall caprock generally remains stable under appropriate operational conditions (Rutqvist & Tsang, 2002; Sun et al., 2023).

Caprock breakthrough pressure represents the most direct and critical parameter for assessing its sealing capacity. If CO<sub>2</sub> pressure exceeds this threshold, preferential flow pathways may form within the caprock, potentially allowing CO<sub>2</sub> leakage. Moreover, CO<sub>2</sub> adsorption can reduce shale permeability but may also induce pressure buildup and decrease frictional strength (Birkholzer et al., 2009; Song & Zhang, 2013). Thermo-chemical-mechanical (TCM) coupling effects can generate local negative effective stresses and promote mineral precipitation, thereby modifying caprock sealing performance (Xiao et al., 2020; Thompson et al., 2021). Consequently, although the overall caprock typically maintains good sealing capacity, local instabilities and reactivation can still generate potential pathways for CO<sub>2</sub> leakage.

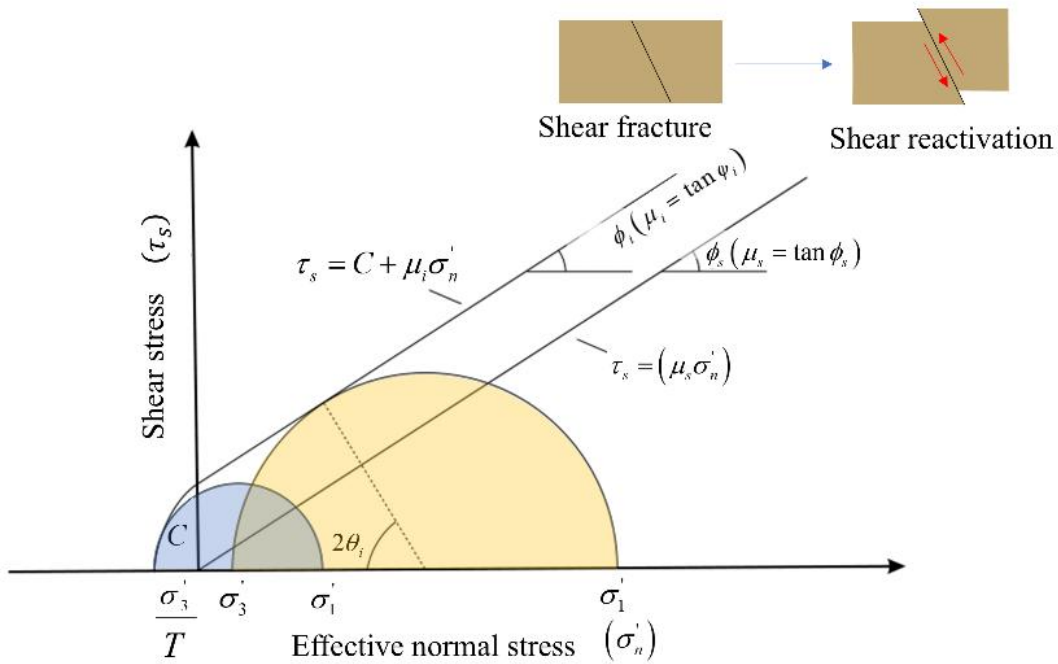
### 3.2.3 Wellbore Leakage: An Engineering Vulnerability

Wellbores, acting as the primary conduits connecting the surface to the subsurface, contain interfaces (casing-cement, cement-formation) that constitute potential weak points (Fig. 11). Wellbore integrity—defined as the capacity to maintain sealing and isolation functions during CO<sub>2</sub> storage—represents a critical factor for ensuring safe sealing. Compared with geological features (e.g., faults, fractures), wellbores are more susceptible to acting as potential leakage pathways due to their engineered nature (Bachu & Watson, 2009; Wigand et al., 2009). This aspect of integrity relates to the ability to maintain zonal isolation throughout the storage lifecycle, primarily encompassing internal mechanical integrity (sealing of tubing, casing, packers, etc.) and external integrity (sealing of the casing-cement-formation system).

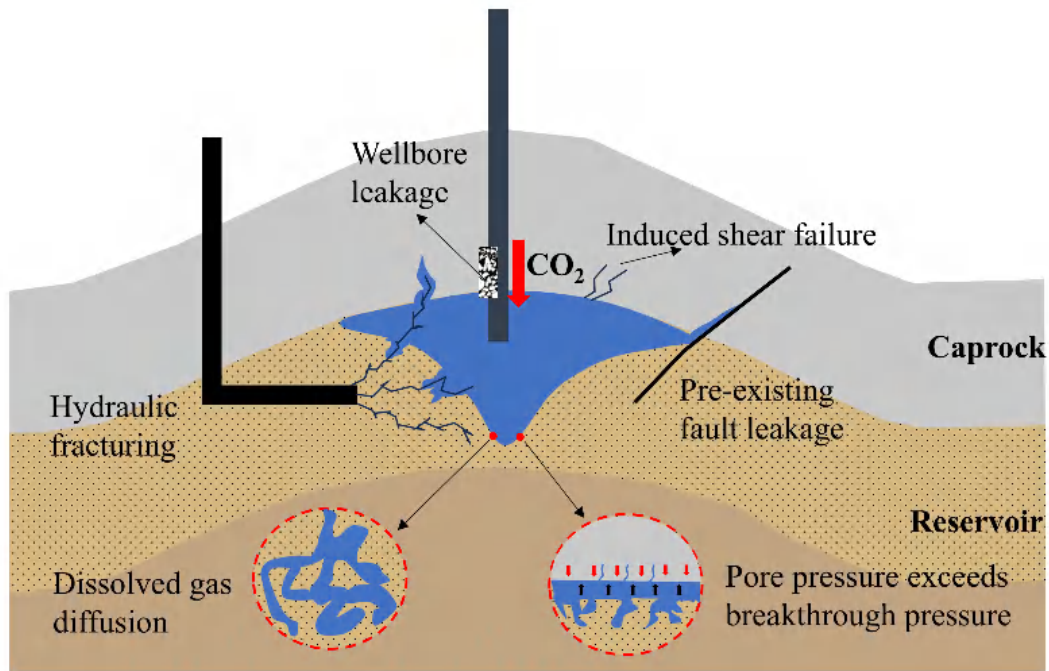
Existing studies indicate that wellbore failure can result from multiple factors, including chemical reactions (e.g., cement carbonation, Eq. (2)), thermo-mechanical loading, or construction defects, potentially leading to the formation of multiple leakage pathways. Typical leakage conduits include casing corrosion, incomplete cement placement, flow through micro-annuli or open-hole sections, casing thread leaks, interfacial debonding, poor cement consolidation, and fractures or channels within the cement sheath (Reinicke & Fichter, 2010; Carroll et al., 2016).



During drilling, casing, cementing, hardening, and injection operations, the wellbore and surrounding formation undergo stress redistribution and changes in material properties: drilling modifies the in-situ stress distribution; cement shrinkage during hardening may cause interfacial debonding; and temperature



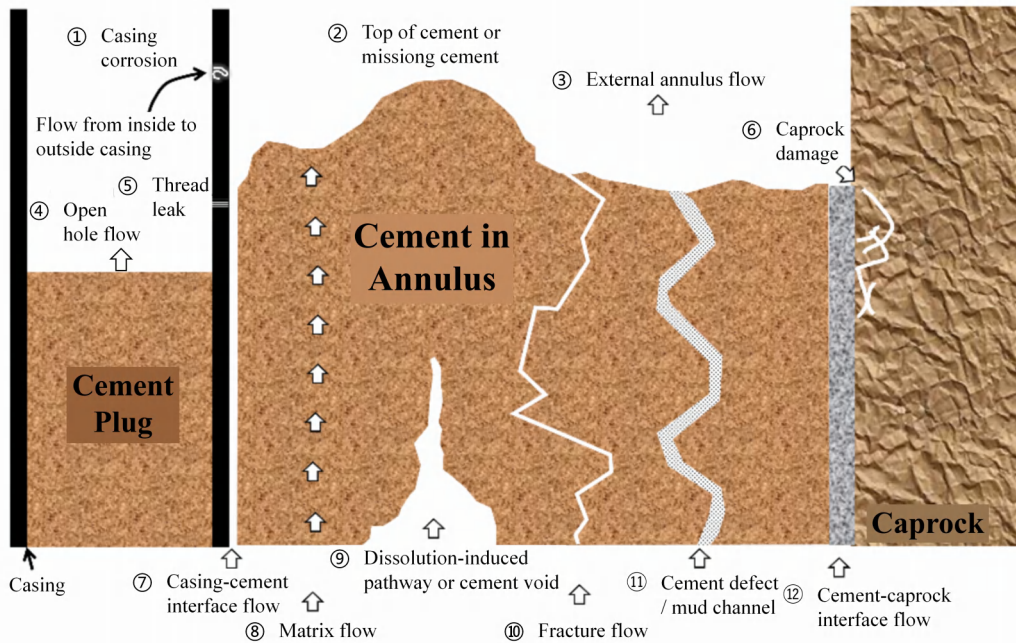
**Fig. 9** Schematic diagram of shear fracture and reactivation mechanism based on Mohr-Coulomb criterion (modified after Mildren et al., 2005)



**Fig. 10** The schematic diagram of the CO<sub>2</sub> leakage paths of the cap rock

differences induced by CO<sub>2</sub> injection generate thermal stresses, further promoting fracture formation or interface failure (Gray et al., 2009; Zhang, 2013; Nygaard et al., 2014). Simultaneously, increasing pore pressure can degrade cement integrity and may trigger caprock fracturing or the reopening of existing fractures. Moreover, acidic fluids and CO<sub>2</sub>-saturated formation water can corrode casing and cement, thereby reducing bond

strength and sealing capacity. During the migration and long-term storage phases, injection wells, abandoned wells, and unidentified faults or fractures may evolve into leakage points. Stress field changes induced by increasing pore pressure may also trigger microseismic events, further exacerbating integrity degradation in the wellbore and adjacent caprock. To address these risks, geomechanical numerical modeling has emerged as



**Fig. 11** Potential leak pathways through an abandoned well (modified after (Carroll et al., 2016))

a critical tool for predicting the stress-deformation response and potential failure modes of the wellbore and adjacent formations throughout the injection and storage lifecycle (Li et al., 2023; Sun et al., 2024). The Finite Element Method (FEM), renowned for its capability to handle complex geometries and material nonlinearity, is extensively employed in wellbore integrity analysis, often integrated with coupled thermal-hydrological-mechanical (THM) processes. For example, simulations for the Northern Lights CCUS project in the North Sea indicated that the temperature difference between injected CO<sub>2</sub> and the formation could generate significant thermal stresses at the cement-casing interface; however, the deep in-situ stress field partially mitigated the risk of interfacial debonding (Thompson et al., 2021).

Consequently, wellbore leakage constitutes one of the most significant engineering risks in CO<sub>2</sub> geological storage systems, with underlying mechanisms characterized by complex multi-factor coupling. Future efforts should focus on continuously strengthening well abandonment protocols, developing corrosion-resistant materials, improving cementing quality, and advancing multi-physical numerical modeling to enhance the long-term sealing reliability of wellbores.

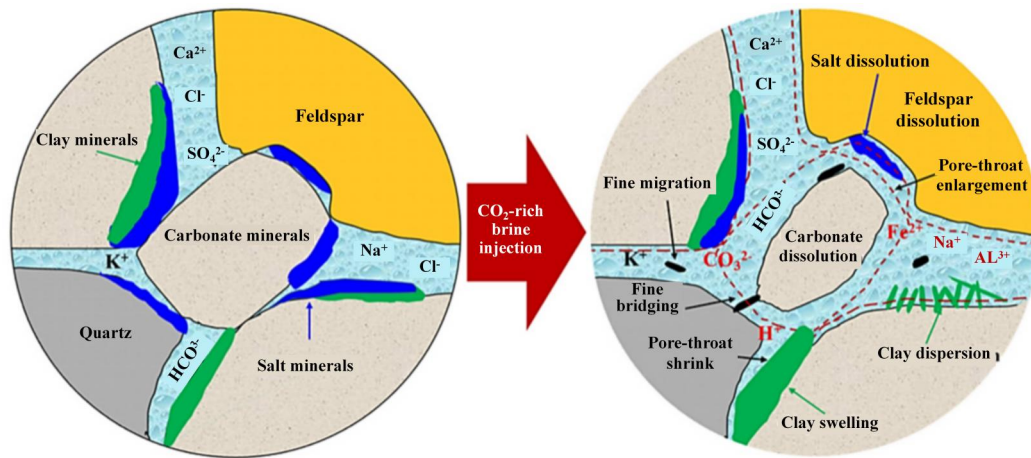
### 3.2.4 Coupling of Multi-Physicochemical Processes and Leakage Evolution

Interfacial phenomena at the pore scale constitute the fundamental reactive unit in CO<sub>2</sub> geological storage systems. Injected CO<sub>2</sub> initially dissolves into the pore fluid, inducing acidification, and subsequently reacts with mineral surfaces, triggering dissolution-precipitation processes that modify key parameters such as porosity, permeability, and tortuosity. The evolution of these microstructures governs not only CO<sub>2</sub> migration and trapping efficiency within the reservoir but also directly affects the integrity of the caprock and wellbores. When pore-scale

reactions propagate temporally and amplify spatially to the reservoir and site scales, they can manifest as characteristic leakage pathways and modes. Examples include diffuse leakage caused by caprock weakening, channelized leakage along reactivated faults, and vertical leakage following cement carbonation in wellbores. Therefore, understanding and characterizing water- CO<sub>2</sub>-rock interactions at the pore scale is fundamental to elucidating the long-term stability of carbon storage systems and their potential leakage mechanisms (White et al., 2005; Gaus et al., 2005; Gaus, 2010; Molins et al., 2014).

In deep saline aquifers, CO<sub>2</sub> solubility is primarily governed by temperature, pressure, and salinity. The resulting acidification induces dissolution followed by reprecipitation of carbonate, sulfate, and aluminosilicate minerals. These reactions buffer or enhance acidity, thereby modifying pore structures and solute transport properties. Carbonate minerals react relatively rapidly, influencing system behavior during early injection stages, whereas feldspars and clays react more slowly, typically requiring geological timescales to produce significant effects (White et al., 2005). Such water- CO<sub>2</sub>-rock reaction processes ultimately govern the long-term sealing capacity of both the reservoir and the caprock (Fig. 12).

CO<sub>2</sub>-water-rock interactions are commonly represented using reactive transport models (RTMs). These models are generally classified into two categories: continuum-scale and pore-scale models. Continuum-scale models are primarily employed for site-scale risk assessment and long-term prediction, whereas pore-scale models focus on microscopic dissolution-precipitation mechanisms. Combining these approaches enables cross-scale characterization: pore-scale models reveal fundamental mechanisms, whereas continuum-scale models are employed for risk prediction. However, key parameters, including reactive surface area and kinetic constants, carry substantial uncertainties, directly influencing predictions of leakage modes



**Fig. 12** Process of CO<sub>2</sub>-water-rock reaction (Tan et al., 2025)

(Lasaga et al., 1994; Palandri & Kharaka, 2005; Zheng et al., 2009). If mineral reactions modify the pore network within the caprock, even slow diffusion processes may evolve into CO<sub>2</sub> leakage pathways.

Geological CO<sub>2</sub> storage represents a classical Thermo-Hydro-Mechanical-Chemical (THMC) coupled process. CO<sub>2</sub> injection induces increased pore pressure and reduced effective stress, accompanied by temperature gradients and mineral reactions. These processes modify porosity, permeability, and rock mechanical properties, thereby influencing CO<sub>2</sub> migration and storage integrity. Simulations indicate that mineral dissolution may reduce the shear modulus of the caprock, increasing fracture risk, while fluid pressure buildup can propagate along faults or the wellbore-caprock interface, forming leakage conduits. Consequently, potential leakage modes in a storage system should be analyzed using an integrated multi-physical framework (Li et al., 2016; Gan et al., 2021; Fan et al., 2023).

### 3.3 Leakage Mode Classification and Summary of Characteristics

Based on the preceding analysis, leakage modes can be categorized according to pathway characteristics, leakage rate, and duration. These categories primarily include pore-type versus fracture-type, slow versus abrupt, continuous versus intermittent, and localized versus global leakage (Fig. 13).

Pore-type leakage refers to the slow, diffusive migration of CO<sub>2</sub> through microscopic pores within the rock matrix. It is commonly observed in deep saline aquifers or low-permeability reservoirs and is primarily controlled by porosity, permeability, and capillary pressure. This mode exhibits a low leakage rate but may persist over extended durations. In contrast, fracture-type leakage occurs along high-permeability conduits, such as faults and fractures, where CO<sub>2</sub> migrates rapidly under pressure gradients. This mode is typically associated with fault-developed zones or high-pressure injection scenarios and can result in significant CO<sub>2</sub> leakage over short periods.

From a dynamic perspective, slow leakage manifests as long-term, low-rate seepage, commonly associated with pore-type pathways. Although the instantaneous leakage rate is small, the long-term cumulative effect may be substantial. Abrupt

leakage, however, is typically triggered by events such as fault reactivation, wellbore failure, or caprock fracturing. It is characterized by a sudden onset and high flow velocity, posing an immediate environmental risk. Continuous leakage refers to a stable, sustained release of CO<sub>2</sub> along a leakage pathway, commonly associated with pore-type or slow leakage modes. Intermittent leakage exhibits a periodic or conditionally triggered pattern, often associated with fractures or pressure fluctuations, resulting in significant variations in leakage rate.

Regarding spatial scale, localized leakage is confined to a single or a few point sources (e.g., a wellbore, a localized fault), with a limited area of impact but potentially high local concentrations. Global leakage involves extensive networks formed through multiple faults or fracture systems, posing a substantial threat to the overall sealing integrity of the storage system.

The characteristics delineated by this classification suggest distinct priorities for monitoring design and imply different risk profiles. Pore-type, slow, and diffuse leakage presents significant monitoring challenges due to its low signal strength; it requires long-term, high-sensitivity geochemical (e.g., groundwater composition) and pressure monitoring in overburden aquifers. Fracture-type, abrupt, and localized leakage (e.g., from a wellbore), while high-risk, often yields clearer signals such as rapid pressure changes, microseismic activity, or focused soil gas anomalies, enabling detection with wellhead instruments, seismic arrays, and targeted surface surveys.

In summary, the features most prone to CO<sub>2</sub> leakage are concentrated in wellbores (e.g., seal failure) and faults or fractures (e.g., fracture propagation induced by natural or triggered seismicity, or interactions between the reservoir/caprock and pre-existing faults). In contrast, molecular diffusion through intact rock matrices is an extremely slow process and typically becomes a practical leakage concern only if the diffused CO<sub>2</sub> subsequently enters higher-permeability pathways, such as fractures. It is crucial to emphasize that CO<sub>2</sub> leakage rarely occurs via a single mode and often involves multiple mechanisms:

- (1) supercritical CO<sub>2</sub> may undergo viscous fingering or channeling along high-permeability pathways;
- (2) driven by buoyancy, CO<sub>2</sub> may ascend rapidly through fractured conduits;

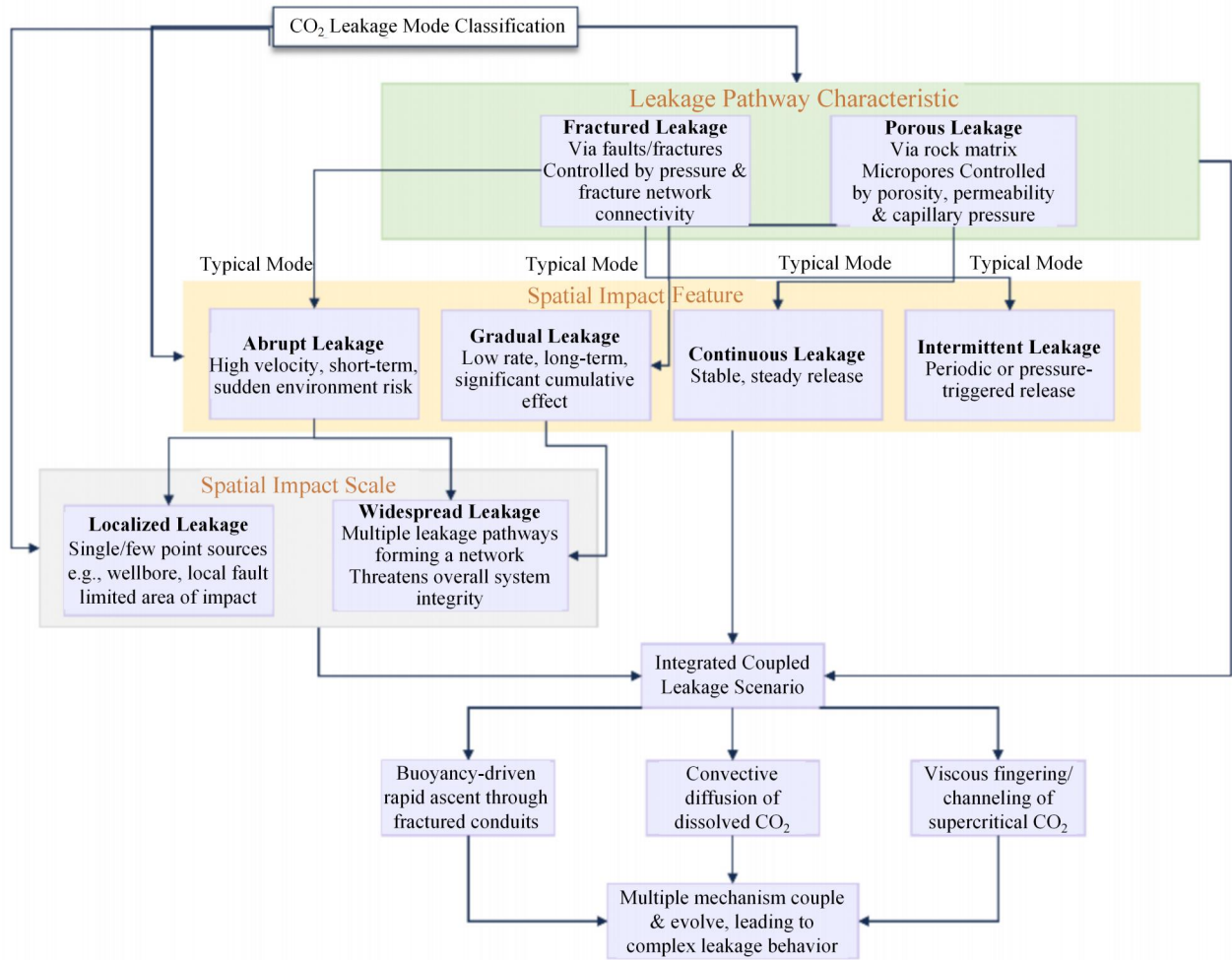


Fig. 13 Classification and Characteristics of CO<sub>2</sub> Geological Sequestration Leakage Models

(3) a portion of CO<sub>2</sub> dissolved in formation water may migrate gradually through convective mixing and diffusion. These mechanisms may interact and evolve over time, resulting in complex leakage behaviors.

#### 4 Leakage and Sealing: Multiscale Definitions and Dynamics

##### 4.1 Definitions of Leakage and Sealing

Leakage and sealing are fundamental concepts in evaluating the safety of storage systems in geological CO<sub>2</sub> storage research. Existing definitions primarily derive from general dictionaries or regulatory documents. For instance, the Encyclopædia Britannica defines leakage as “the accidental escape of a substance through a crack or hole”; the Contemporary Chinese Dictionary describes it as “the flow of liquids, gases, etc., through gaps or holes, typically referring to physical leakage”; and the EU Directive on the Geological Storage of Carbon Dioxide (2009/31/EC) defines it as “any release of CO<sub>2</sub> from the storage complex”, in which the storage complex encompasses not only the reservoir but also the caprock and surrounding formations that affect overall storage integrity (Fig. 14). This broader definition extends beyond the notion of a simple “escape through holes”, yet it fails to distinguish internal

migration within the reservoir from leakage occurring after breaching the system boundary. While they possess a degree of universality, these definitions are hindered by three critical operational limitations:

- (1) lack of pore-to-basin scalability,
- (2) ambiguity between internal migration and boundary-breach failure,
- (3) absence of measurable metrics to support engineering and regulatory decisions.

As a result, they may inadequately represent the multiscale nature of CO<sub>2</sub> storage and can risk conflating the distinct processes of migration, transformation, and leakage.

From the perspective of geological CO<sub>2</sub> storage, defining leakage merely as “escape” is insufficient. The behavior of CO<sub>2</sub> in the subsurface is primarily characterized by migration—namely, its movement and redistribution within the reservoir driven by pressure gradients, buoyancy, and permeability. This migration can induce changes in phase state or distribution, thereby resulting in different trapping modes, that is, transformation processes such as the transition from a free phase to a dissolved or mineral phase. Leakage occurs when CO<sub>2</sub> breaches the boundary of the storage unit and subsequently enters non-target zones. Correspondingly, sealing denotes the long-term capacity of the reservoir, caprock, and associated geological

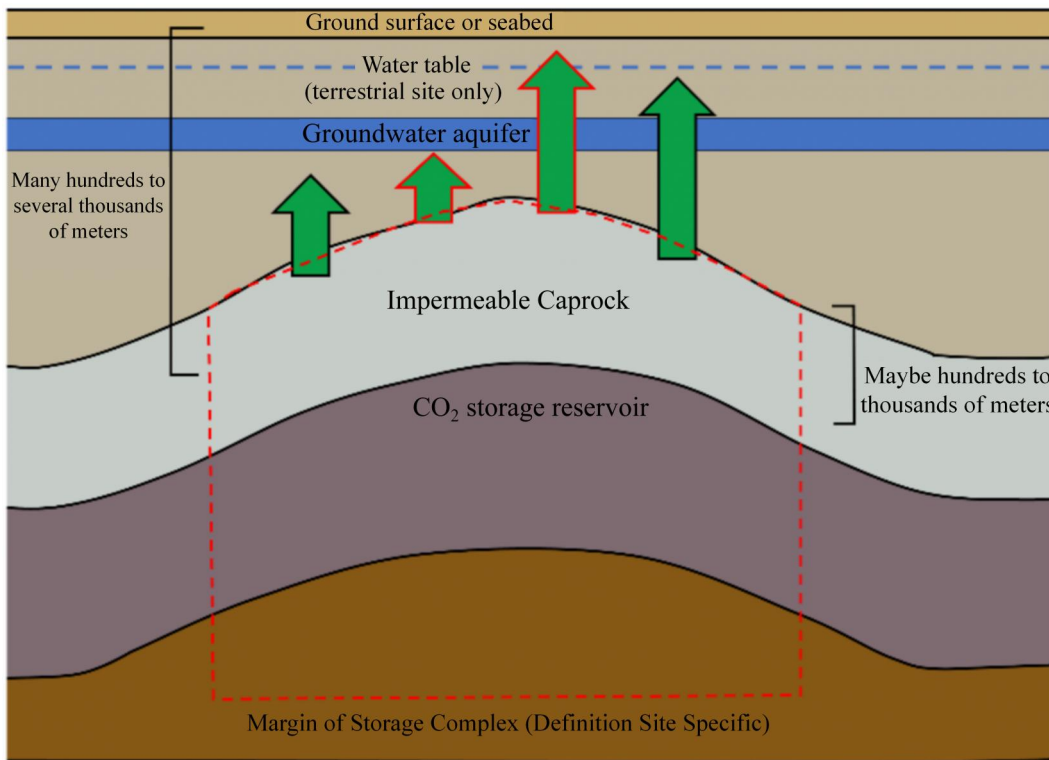


Fig. 14 Schematic illustration of a CO<sub>2</sub> storage complex and the meaning of leakage in accordance with the EC Storage Directive (EC, 2009)

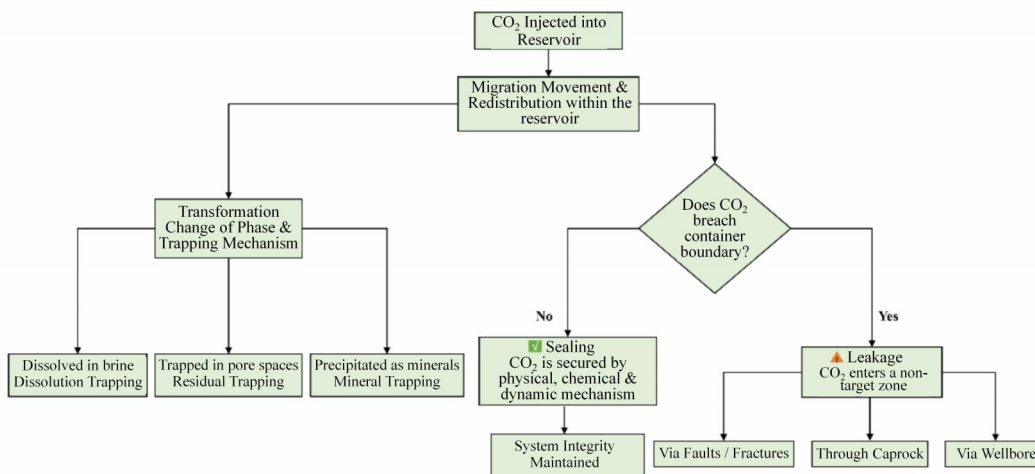


Fig. 15 Migration, Transformation, and Boundary Breakthrough in Geological CO<sub>2</sub> Storage

formations to confine and impede CO<sub>2</sub> through physical, chemical, or dynamic mechanisms, with its primary function being the maintenance of storage system integrity (Bryant et al., 2008; Rutqvist, 2012)(Fig. 15).

To establish a precise and operational multiscale definitional framework, this study proposes an analytical approach centered on the Object-Process-Boundary (OPB) concept, emphasizing that the determination of leakage and sealing at different scales must be grounded in the boundaries of the corresponding system (Fig. 16). This framework emphasizes the following principles: Migration denotes the internal movement and redistribution of CO<sub>2</sub> within a defined scale, without breaching

the system boundary of that scale. Leakage denotes the process by which stored CO<sub>2</sub> breaches the system boundary of its sealing unit. Critically, “breach” is defined by a quantifiable condition where the driving forces (e.g., pressure, buoyancy) exceed the resistance forces (e.g., capillary entry pressure, fracture strength) at the boundary. Sealing denotes the capacity of physical, chemical, or mechanical mechanisms to prevent this breach. It is crucial to underscore that leakage adopts “boundary breach under defined force thresholds” as its unified criterion, sealing embodies “boundary maintenance quantified by maximum resistance metrics” as its core function, and migration represents a dynamic process confined within the boundary.

To operationalize these principles, a clear boundary selection protocol and corresponding measurable engineering metrics are required for each scale. Boundaries are selected based on their primary function:

- (1) Structural boundaries (e.g., caprock geometry) for physical confinement;
- (2) Dynamic boundaries (e.g., pressure front, monitored plume extent) based on system behavior and monitoring capability; and
- (3) Regulatory/Protective boundaries (e.g., base of underground sources of drinking water) defined by safety regulations.

The selection dictates the relevant leakage indicators and sealing metrics. This unified criterion can be systematically applied across hierarchical levels—pore, core, reservoir, site, and basin (Table 5).

To be specific, at the pore scale, the movement of CO<sub>2</sub> within the pore network constitutes migration; breaching a pore-throat boundary occurs when the local capillary pressure exceeds the capillary entry pressure ( $P_c > P_{ce}$ ), representing leakage; and immobilization by capillary threshold pressure constitutes sealing, quantified by  $P_{ce}$  and residual saturation. At the core scale, migration occurs within the REV; leakage is indicated by a sustained CO<sub>2</sub> flux across the REV boundary, measurable in core-flood experiments. At the reservoir scale, migration occurs beneath the caprock; leakage is signaled by CO<sub>2</sub> saturation at the caprock interface (via seismic) or when formation pressure exceeds the fracture gradient (e.g.,  $> 0.85$  of the minimum principal stress,  $\sigma_3$ ). At the site scale, migration is within the monitored domain; leakage is confirmed by detecting CO<sub>2</sub> (e.g., via tracers) outside the monitored boundary or above regulatory concentration limits in protected aquifers. At the basin scale, leakage constitutes a surface flux exceeding natural baselines or groundwater chemistry anomalies beyond designated zones (Fig. 17). In summary, this operational OPB framework transforms qualitative concepts into a decision-support tool. It provides the essential logical link within the “Monitoring-Prediction-Regulation-Intervention” closed-loop management system: monitoring data are evaluated against the scale-specific boundaries and metrics defined here to classify system state, which in turn triggers predictive modeling and, if necessary, regulatory or intervention actions.

Multiscale sealing processes act in opposition to leakage. Sealing can be understood as the set of restriction mechanisms acting on CO<sub>2</sub> prior to its breaching a boundary. These mechanisms are commonly categorized into four types: (i) Structural and capillary sealing, controlled by impermeable caprocks and capillary threshold pressures, which prevent further upward migration of CO<sub>2</sub> (Shukla et al., 2010); (ii) Residual sealing, in which CO<sub>2</sub> is trapped as disconnected ganglia by capillary forces within pore spaces (Bachu, 2003); (iii) Solubility sealing, whereby CO<sub>2</sub> dissolves into the formation water and the resulting denser brine may sink (Ennis-King & Paterson, 2002); and (iv) Mineral sealing, in which CO<sub>2</sub> reacts with host rock minerals to form stable carbonate solids, thereby enabling long-term storage (Egermann et al., 2005). Additionally, other mechanisms, such as pressure sealing and concentration sealing, have been proposed in various studies, often acting in superposition

with capillary sealing to collectively form resistance barriers. It is important to note that “trapping mechanisms” describe the long-term fate of CO<sub>2</sub>, whereas “sealing capacity” emphasizes the immediate effectiveness in preventing boundary breaches; the two are complementary but conceptually distinct. Furthermore, the characterization of sealing capacity should be based on quantifiable indicators with clear physical significance, such as breakthrough pressure and maximum sealing pressure. This approach not only facilitates the unification of a cross-scale sealing evaluation framework but also provides a robust basis for risk prediction and engineering design.

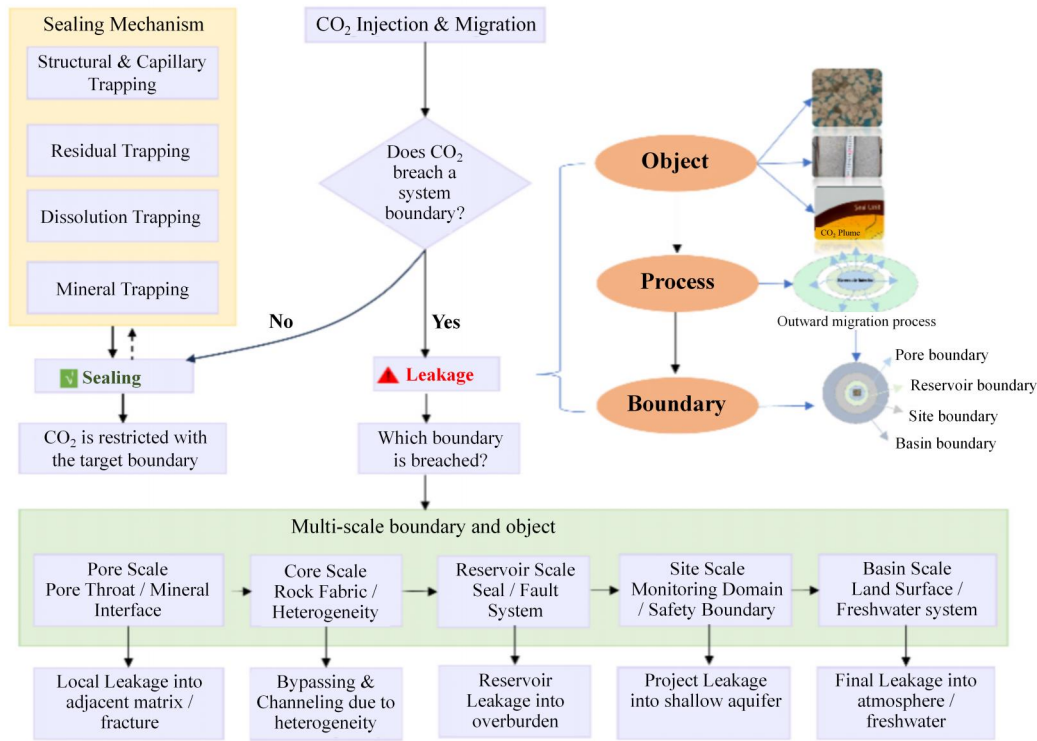
To transition from a conceptual schema to an actionable tool, this OPB framework is designed to integrate directly with the “Monitoring–Prediction–Regulation–Intervention” management cycle (Section 5). It provides the critical decision logic by establishing scale-specific, measurable criteria for a “boundary breach”. For instance, at the reservoir scale, leakage is operationally defined by monitoring data satisfying criteria such as CO<sub>2</sub> saturation at the caprock interface (from seismic) or formation pressure exceeding a defined fraction of the fracture gradient. This creates a direct mapping from monitoring variables (e.g., pressure anomalies, tracer presence, geochemical shifts) to the binary classification of system state (migration vs. leakage). When such criteria are met, it triggers a state reclassification within the management system, activating the subsequent “prediction” (model updating and forecasting) and “regulation/intervention” modules. Thus, the OPB framework furnishes the essential, quantifiable thresholds that enable the closed-loop system to function not merely as a conceptual diagram but as a responsive control logic.

The multiscale definitional framework proposed in this section not only addresses the shortcomings of existing definitions but also establishes a more rigorous and operational conceptual system by clarifying the interrelationships among migration, transformation, leakage, and sealing. This framework emphasizes the boundary conditions of leakage, highlights the multiple mechanisms of sealing, and provides theoretical support for subsequent leakage risk modeling, monitoring technology development, and management strategies.

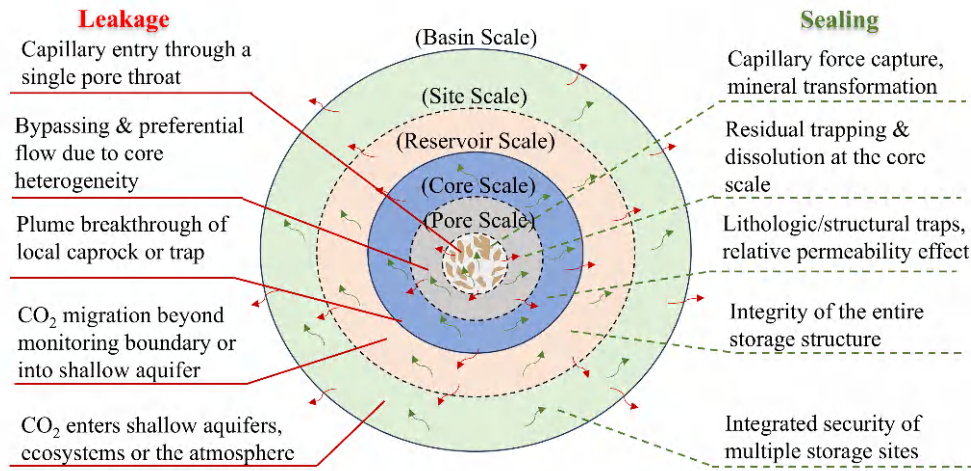
## 4.2 Driving and Resisting Forces in CO<sub>2</sub> Migration and Sealing

The migration and sealing of CO<sub>2</sub> in subsurface geological formations fundamentally represent a dynamic balance between driving forces that promote migration and resisting forces that ensure sealing across multiple scales (Bachu et al., 1994; Lindeberg & Wessel-Berg, 1997; Celia et al., 2005). To clarify the interaction, it is essential to distinguish the fundamental driving forces (e.g., buoyancy, pressure gradient), the physical-chemical processes they induce (e.g., two-phase flow, geochemical slip, dissolution), and the key properties or thresholds that govern the outcome of these processes (e.g., capillary entry pressure, fracture gradient, friction coefficient). Driving mechanisms constitute the primary sources of CO<sub>2</sub> mobility and include:

- (1) Buoyancy Drive: The density of supercritical CO<sub>2</sub> is 30–50% lower than that of brine, making buoyancy the dom-



**Fig. 16** A Multi-Scale Object-Process-Boundary (OPB) Framework for Defining CO<sub>2</sub> Leakage and Sealing



**Fig. 17** Conceptual Framework of Multi-scale CO<sub>2</sub> Leakage and Sealing

inant force for upward migration toward the caprock. The dominance of buoyancy over capillary trapping can be assessed by the dimensionless Bond number  $B_0 = \Delta\rho gk/(\gamma \cos \theta)$ . For typical storage conditions ( $P > 8$  MPa,  $T = 30-50^\circ\text{C}$ , salinity  $< 5$  mol/kg), the large density contrast ( $\Delta\rho$ ) ensures  $B_0 \gg 1$  in high-permeability zones, driving vertical migration. In contrast, in low-permeability caprocks,  $B_0 \ll 1$ , and capillary forces dominate, inhibiting flow.

(2) Pressure Gradient: The excess pressure generated during injection facilitates radial plume expansion and helps overcome local capillary entry resistance.

(3) Natural Hydraulic Gradient: Regional groundwater flow dictates the migration pathways and velocities of CO<sub>2</sub> plumes (Evans, 2013).

(4) Stress perturbations can reactivate faults or fractures, generating new leakage conduits.

(5) Although slow, diffusion along concentration gradients allows CO<sub>2</sub> to penetrate caprock micropores and dissolve into groundwater, influencing long-term storage security (Johnson et al., 2005).

Resisting mechanisms represent the constraints on CO<sub>2</sub> migration imposed by various physical and chemical processes,

primarily including capillary resistance, viscous effects, chemical reactions, and mineral precipitation (Geloni et al., 2011; Dashtian et al., 2019). The efficacy of each mechanism is quantified by specific, measurable parameters: capillary resistance by the capillary entry pressure, geomechanical resistance by the fault reactivation pressure derived from the Mohr-Coulomb criterion, and chemical resistance by reaction kinetics and thermodynamic equilibria. These parameters, whether measured in the lab or inferred from field tests, form the basis for defining sealing thresholds. A critical aspect for practical risk assessment and storage security is the characteristic time scale over which each resistance mechanism dominates, ranging from immediate (short-term) barriers to gradual (long-term) immobilization processes. Geological heterogeneities, such as low-permeability mudstone lenses and barriers, can also prevent the upward breakthrough of the plume, forcing it to spread laterally and become immobilized in structural or stratigraphic traps (Doughty et al., 2001; Flett et al., 2005). Specifically, the capillary entry pressure of a tight caprock is the first and most crucial barrier resisting CO<sub>2</sub> buoyancy and preventing its seepage into the caprock (Ajayi et al., 2019; Ding et al., 2023). This capillary resistance acts as the primary short-term (operational to decadal scale) sealing mechanism. When the CO<sub>2</sub> pressure ( $P_{CO_2}$ ) is lower than the capillary entry pressure ( $P_c$ ) of a pore throat, it becomes immobilized at the throat, preventing further migration. Similarly, in deep saline aquifers, when CO<sub>2</sub> cannot enter a brine-saturated capillary barrier—i.e.,  $P_{CO_2} - P_{brine} < P_c$ , where  $P_{brine}$  is the brine pressure—the resulting fluid displacement mechanism leads to “snap-off” trapping of CO<sub>2</sub> (Saadatpoor et al., 2009). Conversely, CO<sub>2</sub> will migrate into the overlying rock if the condition is not met. When sufficient brine is displaced to exceed the percolation threshold, a continuous flow path for CO<sub>2</sub> becomes established within the pore system.

Capillary effects are strongly coupled with viscous forces. The viscosity contrast between CO<sub>2</sub> and brine often induces unstable fingering during displacement, fragmenting the plume into smaller clusters. This enhances residual trapping by increasing the volume of immobilized CO<sub>2</sub>. Both capillary and viscous (hydrodynamic) resistances are dominant during the injection and early post-injection phases, providing essential short- to medium-term security. Additionally, CO<sub>2</sub> dissolution into formation brine produces weak carbonic acid, initiating mineral-fluid reactions (Brantley & Conrad, 2008; Gysi & Stefánsson, 2012; Kanakiya et al., 2017). Dissolution not only increases storage density but also provides the reactive basis for subsequent mineral trapping, where CO<sub>2</sub> precipitates as stable carbonate minerals (De Silva et al., 2015; Ma et al., 2020). Solubility trapping strengthens over decades to centuries, while mineralization represents the most secure long-term (centennial to millennial scale) sealing mechanism, although localized precipitation may clog pore throats, reducing permeability and impairing injectivity (Gunter et al., 1993; Liu et al., 2011; Sbai & Azaroual, 2011; Cho et al., 2019). Thus, the resistance system operates as a dynamic sequence: robust short-term physical barriers (capillary, viscous) are paramount for initial integrity, effectively “buying time” for the slower-acting chemical processes (dissolution, mineralization) to develop and ultimately

provide permanent storage security.

The relative dominance of driving and resisting forces varies across scales. At the pore scale, capillary entry pressures and surface chemical reactions control local CO<sub>2</sub> distribution. At the reservoir scale, buoyancy, injection pressure, and heterogeneity jointly determine plume migration and immobilization. At the site scale, well placement, injection strategies, and regional hydraulic conditions constrain plume evolution, making reservoir engineering measures (e.g., injection rate management, pressure control) essential for enhancing resistance and mitigating leakage risk.

#### 4.3 Multiscale and Multidimensional Variations in Driving and Resisting Force Attenuation

The preceding sections have discussed the processes of CO<sub>2</sub> leakage and sealing in geological reservoirs with respect to driving and resisting forces. However, these mechanisms vary significantly across spatial scales and modeling dimensions; their effects are not linearly additive but instead exhibit systematic attenuation or amplification as scale increases. This section examines the evolutionary characteristics of these forces across three primary scales—pore–core, reservoir–fault–caprock, and regional–basin—while also considering dimensional effects.

At the pore–core scale ( $\mu\text{m}$ – $\text{cm}$ ), CO<sub>2</sub> migration is primarily governed by capillary forces and mineral reactions. Capillary trapping results in residual fluid saturation, while mineral dissolution–precipitation occurs within pore throats and microfractures, potentially exerting both beneficial and detrimental effects on permeability. The size and distribution of pore structures determine the efficiency of capillary resistance, whereas reaction rates and precipitation sites control the persistence and stability of chemical trapping. At this scale, resisting mechanisms exert a strong attenuating effect on driving forces, significantly restricting CO<sub>2</sub> migration during the early stages.

At the reservoir–fault–caprock scale ( $\text{m}$ – $\text{km}$ ), the dominant factors controlling driving and resisting forces change. Stratigraphic heterogeneity, fracture network connectivity, and fault sealing capacity collectively determine CO<sub>2</sub> migration patterns within the reservoir. Faults and fractures may function either as sealing barriers or leakage conduits, with their dual role governed by breakthrough pressure and the presence of clay gouge. At this scale, attenuation of driving forces depends largely on resistance provided by structural trapping and lithological contrasts. However, once a highly connected fracture network forms, it can rapidly reduce the effectiveness of resistance, enabling CO<sub>2</sub> to breach reservoir sealing through a pipeline-flow mode.

At the regional–basin scale ( $\text{km}$ – $100\text{ km}$ ), macroscopic tectonic controls constitute the decisive factors for sealing and leakage. Tectonic features such as folds, anticlines, and rift basins frequently form large-scale traps, allowing CO<sub>2</sub> to accumulate beneath caprocks under buoyancy forces. At this scale, resisting mechanisms manifest as the macroscopic integrity of caprocks and the ultimate constraint imposed by their breakthrough pressure. Once a critical pressure threshold is exceeded, leakage may occur in a sudden and catastrophic manner. Conversely, driving forces at this scale are modulated by the

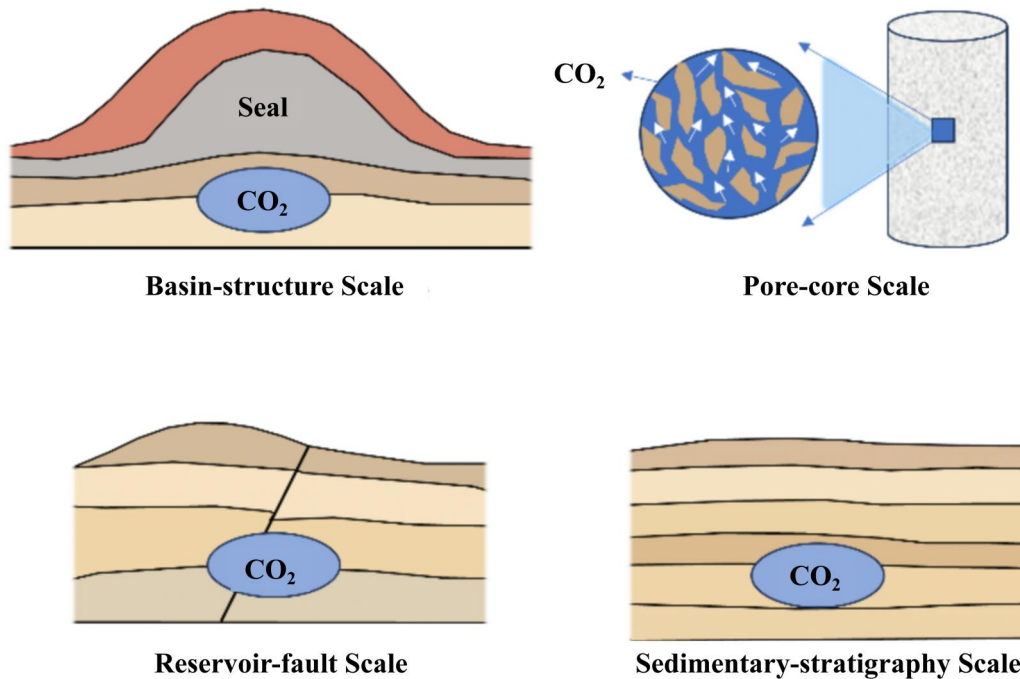


Fig. 18 Conceptual Diagram: Multi-Scale and Multi-Dimensional Differences in Geological CO<sub>2</sub> Storage

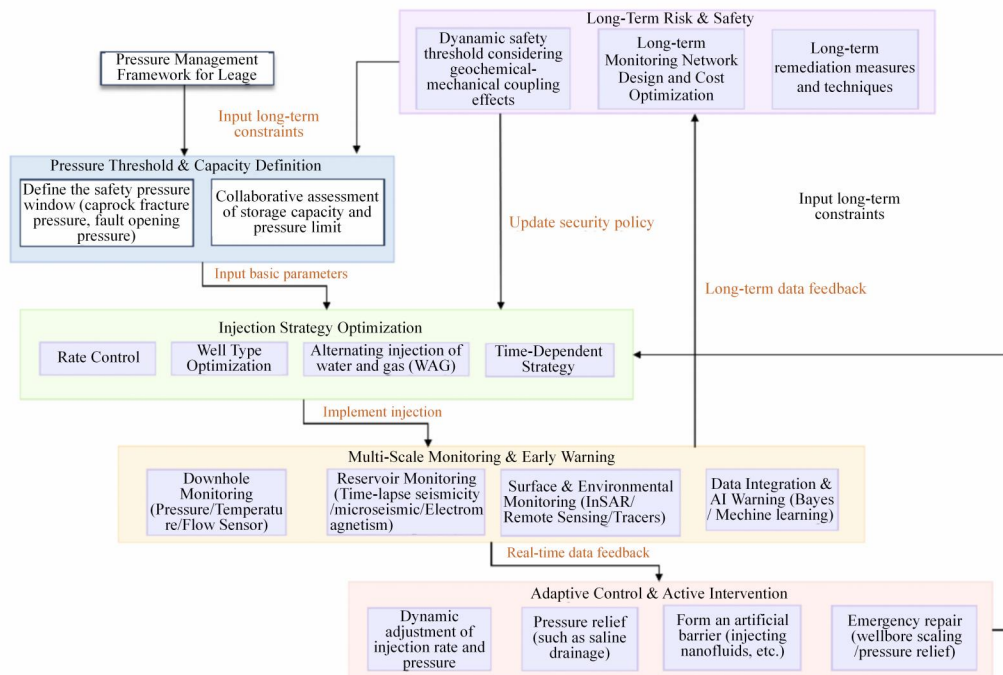


Fig. 19 A Framework for Leakage-Oriented Pressure Management in Geological CO<sub>2</sub> Storage

basin’s thermo-fluid environment, and their attenuation exhibits strongly nonlinear characteristics (Fig. 18).

It is important to note that the scale dependence of key parameters further complicates the behavior of resisting and driving forces. For instance, field-scale feldspar dissolution rates are frequently several orders of magnitude lower than laboratory measurements, whereas diffusion coefficients and hydraulic

conductivity generally increase with scale. This implies that direct application of laboratory data to field-scale predictions may lead to significant deviations, necessitating integration through upscaling methods (e.g., fractal geometry, method of moments). Furthermore, dimensionality is particularly critical in leakage simulations. Two-dimensional (2D) models frequently underestimate lateral dispersion and leakage risks, whereas three-

dimensional (3D) models offer a more realistic representation of CO<sub>2</sub> migration pathways within complex fault and anticline structures. The presence of fractures may transform dispersed flow into an approximately one-dimensional (1D), high-velocity channelized flow, substantially weakening resisting mechanisms and accelerating the dominance of driving forces. Neglecting the 3D structure of faults and fractures in simulations may result in over- or underestimation of sealing efficiency, thereby compromising the reliability of storage security assessments.

Therefore, attenuation of resisting and driving forces in geological CO<sub>2</sub> storage exhibits significant dependence on both scale and dimensionality: capillary forces and mineral precipitation provide the primary resistance at the pore–core scale; heterogeneity and fault sealing capacity control leakage risk at the reservoir–fault scale; and tectonic trapping and caprock integrity govern overall security at the regional–basin scale. Concurrently, systematic differences between 2D and 3D simulations highlight the need to enhance predictive accuracy through integrated multiscale and multidimensional approaches. This necessitates explicit guidance on model application: Two-dimensional simulations are generally inadequate for quantifying leakage risk, as they cannot capture the lateral connectivity and complex, channelized flow pathways (e.g., through fracture networks) that critically control leakage. A credible 3D assessment must, at minimum, incorporate the geometry of major faults and conceptualize fracture network connectivity based on site data. Neglecting 3D effects risks false-negative leakage predictions, while oversimplifying connectivity may lead to false-positive risk overestimates (Table 6). In CO<sub>2</sub> storage safety assessments and risk management, reliance on single-scale or simplified models should be avoided. Instead, a coupled methodology integrating multi-parameter upscaling with multidimensional numerical simulation should be adopted. This approach provides not only a more comprehensive understanding of the evolution of resisting and driving forces but also a theoretical foundation for future research on leakage control and remediation technologies.

## 5 A Pressure Management Framework for Leakage Mitigation

Building upon the preceding analysis of multiscale leakage and sealing dynamics, it is evident that pressure perturbation induced by injection is a core factor in triggering leakage risks. Excessively high reservoir pressure may lead to caprock fracturing or fault reactivation, thereby creating highly conductive leakage pathways. Consequently, establishing an active control framework focused on pressure management is crucial for ensuring the long-term safety of CO<sub>2</sub> storage (Rutqvist, 2012; Adisornsupawat et al., 2024). This section synthesizes existing research and proposes a closed-loop pressure management framework—“Monitoring–Prediction–Regulation–Intervention”—to achieve life-cycle risk control in CO<sub>2</sub> storage.

### (1) Defining Pressure Thresholds and Storage Capacity

Effective pressure management requires defining the safe operating window of the reservoir–caprock system. Its up-

per limit is typically governed by two critical pressures: the caprock breakthrough pressure, defined as the minimum capillary pressure required for the non-wetting phase to enter caprock pores (Ajayi et al., 2019), and the fault/fracture opening pressure, which depends on fault gouge properties and infill strength (Guglielmi et al., 2017). To translate these concepts into actionable engineering thresholds, explicit geomechanical criteria must be applied. The caprock integrity limit should be assessed against the minimum principal stress criterion to prevent hydraulic fracturing, while the fault reactivation limit must be evaluated using the Mohr-Coulomb failure criterion (or slip tendency analysis) to prevent shear slip. In practice, the maximum allowable injection pressure must be maintained below the lower of these two values (Adisornsupawat et al., 2024). Standard practice typically involves maintaining injection pressure below 90% of the fracturing pressure to prevent formation failure, which represents one form of incorporating an operational pressure margin. A comprehensive margin should also account for uncertainties in in-situ stress, rock properties, and model predictions. However, operational protocols must consider thermo-hydro-mechanical (THM) coupling effects induced by cold fluid injection, which can generate new fracture networks in the reservoir, effectively lowering the safe threshold. Furthermore, a coupling exists between injectivity and pressure thresholds: higher injection rates can increase short-term storage capacity but may also induce overpressure and elevate leakage risks (Calabrese et al., 2005). Therefore, capacity assessments should be performed in conjunction with pressure limits to ensure efficient reservoir utilization without breaching structural sealing thresholds.

### (2) Injection Strategy Optimization

The injection strategy constitutes the primary means of pressure management, aiming to enhance storage efficiency while preventing localized overpressure. Studies indicate that lower injection rates facilitate CO<sub>2</sub> accumulation at the reservoir base and its dissolution into formation water, thereby mitigating pressure buildup, whereas excessively high rates promote channeling through high-permeability pathways, reducing storage efficiency (Calabrese et al., 2005). Simulation results suggest that horizontal wells outperform vertical wells in reducing pressure concentration and mitigating fault reactivation risks (Zhang & Agarwal, 2012). Moreover, Water-Alternating-Gas (WAG) injection promotes CO<sub>2</sub> dispersion and fingering within the reservoir, enhancing residual trapping and attenuating continuous gas-phase migration (Chaturvedi et al., 2021). Recent time-dependent strategies emphasize immediate brine displacement after CO<sub>2</sub> injection to rapidly convert mobile CO<sub>2</sub> into the residual phase and accelerate solubility trapping, thereby significantly reducing leakage potential (Huber et al., 2016). These findings suggest that comprehensive pressure management—through rate control, well placement optimization, and alternate injection—can achieve controllable reservoir pressure and safe storage under varying conditions.

### (3) Multiscale Monitoring and Geomechanical Model-Based Prediction

The dynamic evolution of the pressure field and its influence on leakage must be monitored in real time. Wellbore monitoring

constitutes the first line of defense, encompassing wellhead pressure and flow meters, fiber-optic pressure/temperature sensors, and cement bond logs, which are employed to identify well integrity issues (Lippmann et al., 2007). At the reservoir scale, time-lapse seismic, microseismic, electromagnetic, and gravity monitoring are extensively utilized to observe CO<sub>2</sub> plume migration and pressure perturbations (Chadwick et al., 2009). At the surface and environmental level, InSAR and fiber-optic sensing detect surface deformation induced by pressure changes, whereas hyperspectral remote sensing and tracer detection can directly identify leakage signals (Ajayi et al., 2019).

The critical link between monitoring and actionable insight is provided by geomechanical models. Poroelastic and coupled THM models translate monitored data (e.g., pressure, deformation) into quantitative updates of the subsurface stress field and failure risk. For instance, semi-analytical workflows based on layered poroelasticity can efficiently compute stress changes induced by distributed pressure and temperature variations, accounting for caprock-reservoir contrasts and undrained conditions—a significant advantage for rapid assessment and screening (Zhai et al., 2024). For detailed near-well analysis, such as leakage through a compromised wellbore with material heterogeneities, full coupled finite element models are essential. The accuracy of such models depends critically on the selection of primary variables (e.g., the capillary pressure-gas pressure (PP) scheme versus the liquid pressure-gas saturation (PS) scheme) and coupling algorithms (monolithic vs. sequential), especially at interfaces between different materials like cement, steel, and rock (Islam et al., 2020). Integrated analysis increasingly utilizes these calibrated models with Bayesian inference and machine learning techniques to assimilate real-time data, reduce uncertainty, and enable dynamic risk forecasting (Jackson et al., 2024; Liu et al., 2024). Thus, monitoring coupled with robust geomechanical prediction forms the intelligent core of the management framework.

#### (4) Adaptive Regulation, Stress Management, and Active Intervention

Based on monitoring data, pressure management should incorporate capabilities for real-time regulation and active intervention. Dynamic adjustment of injection rates and pressures constitutes the most direct method to maintain reservoir pressure below the safe threshold (Gholami et al., 2021). For targeted mitigation of localized overpressure and stress perturbations, more specific strategies are employed. Pressure relief wells can be strategically deployed to extract formation brine in overpressured zones, directly reducing pore pressure and thereby increasing the effective stress on seals and faults to prevent their activation (Javadpour & Nicot, 2011); their placement and extraction rates are optimized using geomechanical models. Co-injection strategies, including Water-Alternating-Gas (WAG), serve a dual purpose: beyond managing macroscopic pressure buildup, they mitigate near-wellbore thermal stresses and promote a more uniform pressure distribution, actively stabilizing the stress field. Geomechanical models are crucial for optimizing the co-injection ratio and scheduling. Furthermore, controlled micro-fracturing, though primarily a diagnostic tool, can be engineered to create localized, conductive pathways

within the reservoir rock itself. This acts as a deliberate “stress buffer,” dissipating concentrated pressure that might otherwise load critical faults, but requires precise geomechanical design to ensure sealing. When monitoring and models indicate the development of potential leakage pathways, proactive measures such as injecting fluids that induce mineral precipitation or applying nanofluids to enhance sealing can be deployed to form artificial barriers (Vialle et al., 2016; Rathnaweera & Ranjith, 2020). In the event of a leakage incident, emergency measures include wellbore plugging (e.g., squeeze cementing, sidetracking), pressure relief, and the injection of sealing or repair materials. Consequently, the pressure management framework must incorporate dual functionalities: preventive regulation and emergency remediation.

#### (5) Long-term Risk Management and Security

CO<sub>2</sub> storage represents a long-term process spanning decades to millennia. Therefore, pressure management should not be confined to the injection phase but must extend throughout the entire lifecycle. Long-term risks primarily arise from geochemical-mechanical coupling effects; for instance, acidification may dissolve fracture fillings, reducing fault strength and dynamically lowering the safe pressure threshold (Raziperchikolaee et al., 2019). Consequently, the safe pressure window should be regarded as a dynamic parameter, necessitating continuous revision based on long-term monitoring. Simultaneously, the design of long-term monitoring networks must balance cost and accuracy, enabling rapid deployment of additional sensors upon detection of pressure anomalies. Regarding remediation, measures include both wellbore repair techniques and pressure dissipation or sealing technologies for fault or caprock leakage. Only through a continuous cycle of “Monitoring–Revision–Remediation” can the long-term security of geological CO<sub>2</sub> storage be ensured (Fig. 19).

In summary, the enhanced pressure and stress management framework for mitigating leakage incorporates five core, inter-linked components:

- (1) Defining pressure thresholds for caprock fracturing and fault activation based on geomechanical experiments and numerical modeling;
- (2) Implementing dynamic injection control through strategies such as rate control, well placement optimization, and alternating injection;
- (3) Establishing an integrated monitoring system coupled with geomechanical models for prediction;
- (4) Performing adaptive regulation, including specific stress control methods (e.g., relief wells, co-injection), and active intervention based on model forecasts;
- (5) Extending pressure management throughout the long-term lifecycle, integrating dynamic risk revision and cost optimization to ensure complete lifecycle security.

This framework integrates geomechanical understanding, multiscale monitoring technologies, and intelligent control methods, embodying the closed-loop philosophy of “Monitoring–Prediction–Regulation–Intervention”. It serves as a crucial safeguard for the long-term safe operation of large-scale geological CO<sub>2</sub> storage projects.

## 6 Conclusions

This paper reviews and synthesizes the current understanding of leakage and sealing in geological CO<sub>2</sub> storage from a multi-scale perspective, systematizing the conceptual framework and regulatory principles involved. The principal conclusions are summarized as follows:

(1) Clarification of Multi-Scale Definitions: Through a systematic analysis of storage and migration spaces across scales and of dominant leakage pathways, existing concepts are integrated within an “object–process–boundary” analytical framework. This framework serves to clarify the distinctions and relationships among migration, transformation, sealing, and leakage, and establishes consistent identification criteria across pore, reservoir, site, and basin scales. This synthesis addresses prevalent conceptual ambiguity and scale fragmentation in the literature. The operational application and validation of this unified analytical approach in specific field contexts remain a key direction for future research.

(2) Synthesis of Driving–Resisting Force Coupling: The interplay of forces governing CO<sub>2</sub> fate is analyzed and synthesized. Buoyancy, seepage forces, and pressure perturbations are identified as the primary drivers for upward migration, while capillary sealing, mineral reactions, residual trapping, and caprock integrity constitute the primary resisting mechanisms. The dynamic spatiotemporal balance between these forces is established as the fundamental determinant of permanent immobilization versus boundary breach and leakage.

(3) Elucidation of Multi-Scale Dependencies: The review elucidates the hierarchical dependencies across scales and dimensions. At the pore–core scale, capillary effects and chemical reactions are shown to govern residual and mineral trapping. At the reservoir–fault–caprock scale, heterogeneity, fracture connectivity, and fault sealing capacity emerge as the critical factors controlling migration pathways and leakage risks. At the basin–regional scale, macroscopic geological structures are recognized as the overarching controls on the spatial distribution of CO<sub>2</sub> and its long-term sealing.

(4) Integration of Pressure Management Principles: Injection-induced overpressure is highlighted as a critical risk factor. The review integrates key principles into a closed-loop “Monitoring–Prediction–Regulation–Intervention” concept centered on pressure management. This conceptual model underscores the importance of lifecycle risk control through threshold management, dynamic adjustment, and long-term monitoring, outlining a coherent pathway for risk management in large-scale storage projects.

The safety of geological CO<sub>2</sub> storage is contingent upon the dynamic balance between driving and resisting forces, the coherent understanding of multiscale sealing mechanisms, and the implementation of proactive pressure management strategies. Future research should prioritize the development of cross-scale multi-physics coupling models and the integration of intelligent monitoring with real-time control technologies. This evolution is essential to advance storage strategies from “passive response” towards “active prevention”, thereby ensuring the long-term security of large-scale geological CO<sub>2</sub> storage.

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## Conflict of interest

The authors declare no competing interest.

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