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Mechanisms, terminology and State-of-the-Art

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DOI
10.1016/j.ijggc.2025.104385

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Publication date
2025

Document Version
Final published version

Published in
International Journal of Greenhouse Gas Control

International Journal of Greenhouse Gas Control 144 (2025) 104385

Contents lists available at ScienceDirect

International Journal of Greenhouse Gas Control

journal homepage: www.elsevier.com/locate/ijggc

Capillary pinning in sedimentary rocks for CO_2 storage: Mechanisms, terminology and State-of-the-Art

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ARTICLE INFO

Keywords:
Residual Trapping
Capillary trapping
Geologic CO_2 storage
Subsurface heterogeneity
Upscaling

ABSTRACT

Capillary pinning refers to the immobilization of CO_2 at capillary barriers when the uprising CO_2 pressure is lower than the capillary entry pressure of the overlaying pore throats. Also known as local capillary trapping, it has been proposed as a fifth geologic CO_2 storage mechanism, alongside structural, solubility, residual, and mineral trapping. Despite extensive research, the fragmented terminology surrounding capillary pinning has led to confusion, making it challenging to synthesize findings effectively. Often conflated with mechanisms such as residual and hysteresis trapping, capillary pinning is commonly underestimated or completely overlooked in reservoir-scale models. Furthermore, difficulties in characterizing and upscaling small-scale geologic heterogeneities that influence capillary pinning contribute to significant uncertainties, with estimates of CO_2 trapped via this mechanism ranging from 3 % to 100 % of total CO_2 trapped via capillary actions. This review explores the fundamental mechanisms, experimental findings, and modeling approaches for assessing CO_2 capillary pinning in carbon capture and storage (CCS). It seeks to bridge the gap between the reservoir engineering community, with its extensive expertise in hydrocarbon recovery but that needs adjustments for CCS applications, and the subsurface storage community, which stands to benefit from this knowledge but often lacks access to relevant literature. Additionally, the study identifies key research opportunities to advance the understanding of capillary pinning in sedimentary rocks, ultimately enhancing the efficacy and reliability of CCS operations.

1. Background

Carbon capture and storage (CCS) is an essential climate mitigation strategy for keeping human-induced global warming within 2 °C (IPCC, 2022). CCS operations typically capture CO_2 from point sources and inject it into deep underground rock formations for long-term storage (Bachu, 2008; Kelemen et al., 2019). Achieving this climate goal requires net-zero emissions along with large-scale CO_2 removal from the atmosphere, with models suggesting tens of gigatons of CO_2 (1 Gt = 1 billion metric tons) need to be removed annually by 2050 (NASEM, 2019). This demands a more than 100-fold increase in the current annual storage capacity (40 $MtCO_2$; Mt = million tons) (Clark et al., 2020). However, challenges such as CO_2 transportation costs (Selosse and Ricci, 2017) and limited geographic availability of storage sites remain (Bui et al., 2018; McQueen et al., 2021; Smith et al., 2024). Additionally, there are discrepancies between "theoretical" storage capacity (i.e., volumetric estimates based on pore space) and "realistic'' capacity, which accounts for the petrophysical properties of the reservoirs (e.g., pressurization and induced seismicity) (De Simone and Krevor, 2021). Therefore, improving our understanding of existing storage sites to optimize CO_2 storage strategies is crucial, especially when it comes to large storage sites where the subsurface flow dynamics become complicated.

Geologic formations offer long-term CO_2 storage through four main trapping mechanisms: structural, residual, solubility, and mineral trapping (Bickle et al., 2013). Structural trapping relies on an impermeable cap rock to confine CO_2 in subsurface formations. Residual trapping occurs when CO_2 becomes immobilized in the pore spaces of the rock as disconnected ganglia, held in place by capillary forces. Solubility trapping occurs when CO_2 dissolves into formation fluids, reducing its buoyancy and minimizing leakage risk. Mineral trapping involves chemical reactions between CO_2 and minerals, forming stable carbonate

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https://doi.org/10.1016/j.ijggc.2025.104385
Received 23 December 2024; Received in revised form 17 April 2025; Accepted 17 April 2025
Available online 28 April 2025

minerals that ensure long-term sequestration. These processes are complex and interconnected, collectively enhancing the safety and effectiveness of CO_2 storage. In practice, the first-order constraint on CCS capacity is pressure—the maximum amount of CO_2 that can be stored without exceeding the critical overpressure (De Simone and Krevor, 2021). Once this criterion is satisfied, the storage capacity is determined by the effectiveness of the trapping mechanisms, which are influenced by subsurface flow dynamics. Injecting CO_2 into geologic formations involves the flow of different phases—gas, liquid, or supercritical fluid—through porous media (Kuo and Benson, 2015). This multiphase flow is governed by factors such as reservoir conditions (e.g., pressure, temperature) and the presence of existing fluids (e.g., brine and/or hydrocarbons) (Christie, 2001; Golparvar et al., 2018). Differences in material properties such as density and viscosity between CO_2 and the reservoir fluids affect the flow dynamics, as CO_2 flow in the subsurface is primarily driven by pressure gradients, buoyancy, gravity, capillary, and viscous forces (Bachu, 2008). As a result, the heterogeneous nature of the porous media leads to spatial variations in fluid behavior within the geologic formations (Singh et al., 2021).

While structural, solubility, and mineral trapping are well-defined, residual (herein referred to as capillary) trapping can be further classified into two distinct processes: snap-off trapping and capillary pinning, both controlled by capillary forces. Snap-off trapping occurs when the advancing CO_2 displaces brine in the pore spaces, leaving behind disconnected blobs of CO_2 as the brine re-enters. Capillary pinning refers to the immobilization of CO_2 at pore throats due to its pressure being lower than the capillary entry pressure of the pore throats, preventing its further migration. This work will explore the nuances of these processes, examining their significance in enhancing CO_2 storage in sedimentary rocks and reviewing the state-of-the-art research in this field.

1.1. Capillary actions and the two types of capillary trapping

For immiscible fluids within porous media, capillary pressure (P_C) refers to the pressure difference between the two fluid phases—the wetting phase (P_W) and the non-wetting phase (P_{NW}) —occupying the same pore space (Leverett, 1941). This pressure differential arises from the interfacial tension between the fluids, which is equivalent to the force that must be overcome to initiate and sustain the flow of one fluid displacing the other. With the Young-Laplace equation (Finn, 1981; Young, 1805), P_C can be related to the principal radii of curvature R_1 and R_2 of the shared interface and the interfacial tension γ. Assuming a pore throat with a circular cross-section, P_C can be written as a function of γ, wetting angle (θ), and pore throat diameter (d) (for units, see Table 1):

$$P_C \equiv P_{NW} - P_W = \gamma\left(\frac{1}{R_1}+\frac{1}{R_2}\right) = \frac{\gamma\cos\theta}{d} \ . \quad (1)$$

Capillary pressure affects relative permeability hysteresis, thereby controlling fluid flow and distribution in porous media (e.g., Juanes et al., 2006). At the microscopic (pore) scale, since $P_C \propto \frac{1}{d}$, larger P_C occurs in smaller pore throats, where the wetting phase is more likely to displace the non-wetting phase. The non-wetting phase can be trapped if the wetting phase channels through connected pores and isolates larger pores, turning the non-wetting phase into disconnected, i.e. isolated, bubbles or ganglia (Lenormand et al., 1983). For this discussion, we consider a simplified scenario where brine is the wetting phase, while CO_2 is the non-wetting phase; more detailed investigations about mineral wettability can be found in literature (e.g., Chiquet et al., 2007; Hu et al., 2017; Huang et al., 1996; Iglauer et al., 2015; Tokunaga and Wan, 2013). This fluid displacement mechanisms causes "snap-off" of CO_2 (Fig. 1a), thus immobilizing it. At the reservoir scale, snap-off trapping of CO_2 is known as residual trapping or capillary trapping, which has been identified as one of the four long-term geologic CO_2 trapping mechanisms outlined above (Al-Futaisi et al., 2003; Bachu, 2008; Juanes et al., 2006; Valvatne and Blunt, 2004).

Table 1
Symbols and units.

Symbol	Parameter	Unit
P_C	Capillary pressure	Pa
P_{NW}	Pressure of the non-wetting phase	Pa
P_W	Pressure of the wetting phase	Pa
R	Radius of the curvature	m
γ	Interfacial tension	N/m
θ	Wetting angle	radians
d	Pore throat diameter	m
ρ	Density	kg/m^3
g	Gravitational acceleration	m/s^2
h	Column height	m

Capillary actions offer a different means of trapping when CO_2 cannot enter a capillary barrier filled with brine, i.e., $P_{CO2} - P_{brine} < P_C$. This mechanism of CO_2 trapping occurs in heterogeneous domains where the influence of heterogeneity of capillary entry pressure on buoyant displacement can override the influence of heterogeneity on relative permeability (Saadatpoor et al., 2009). The capillary heterogeneity results in a phenomenon where CO_2 gets "pinned" at locations where the entry pressure of the overlying rock exceeds the buoyant pressure of the rising CO_2 (Fig. 1b). This process is called local capillary trapping (Saadatpoor et al., 2009) or capillary pinning (Gershenzon et al., 2016). It is widely recognized that small-scale heterogeneities can strongly influence reservoir flow behavior, leading to highly uneven drainage patterns due to capillary heterogeneity, as indicated by previous studies in oil fields (e.g., Corbett et al., 1992; Honarpour et al., 1994, 1995; Huang et al., 1996; Saad et al., 1995). The observation that this mechanism also applies to CO_2 storage was initially made by Bryant et al. (2008), and in a following study, it was proposed as a fifth geologic CO_2 trapping mechanism (Saadatpoor et al., 2009). Both experimental (Krishnamurthy et al., 2022) and modelling (Gershenzon et al., 2014) results indicate that capillary barriers can form when there is capillary heterogeneity, meaning that variations in grain size and fabric structure—not just permeability—govern the degree of capillary pinning. This is especially important because it suggests that CO_2 trapping could be more reliable in heterogeneous reservoirs compared to homogeneous ones, regardless of the availability of impermeable rock layers, thus creating additional storage security (Cui et al., 2023; Ren et al., 2014), especially in marine sediments (Dai et al., 2018) and some saline aquifers (Woods and Farcas, 2009) where natural caprocks may be absent.

Capillary pinning plays a key role in subsurface gas storage by enhancing gas retention and creating capillary barriers even in rocks with high permeability. When positioned above a rock with lower entry pressure, these barriers can trap the gas or slow its vertical rise, especially in heterogeneous formations that might not have been previously considered as gas traps. This mechanism, in turn, can encourage lateral plume expansion, which is highly relevant for CO_2 storage where the horizontal plume migration must be monitored (Hesse et al., 2008; Krevor et al., 2011; Ren, 2015, 2018; Woods and Farcas, 2009). Such dynamics are also central to hydrogen (H_2) storage, where identifying these "permeable traps" becomes critical—not only for site selection but also for predicting plume behavior and ensuring gas recoverability. Studies suggest that with significant capillary heterogeneity, over 95 % of H_2 could be affected by capillary pinning, underscoring its importance in H_2 storage assessments (Krevor et al., 2023; Shahriar et al., 2024; Zivar et al., 2021).

1.2. Capillary entry pressure and storage security

When it comes to capillary barriers, P_C is typically characterized as a function of threshold or critical capillary entry pressure, also called breakthrough pressure, and displacement pressure (Vespo et al., 2024). It is the minimum pressure required for the non-wetting (CO_2) phase pressure (P_{CO2}) to overcome the forces of interfacial tension and thus displace the wetting phase (brine) from the pores of the overlying rock

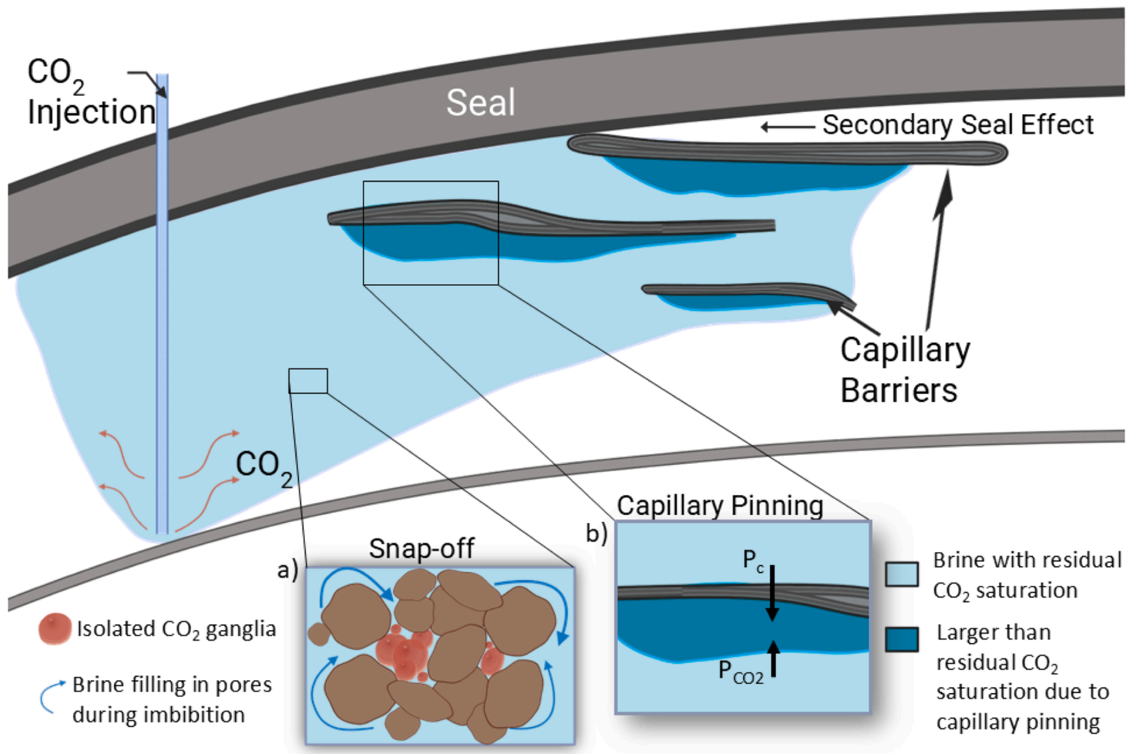

Fig. 1. Schematic illustration of the two capillary trapping mechanisms of CO_2 in the subsurface (a) snap-off and (b) capillary pinning (modified after Gershenzon et al., 2017; Juanes et al., 2006). Capillary pinning leads to a higher trapped CO_2 saturation than that achievable by snap-off alone (i.e., > residual saturation). The color-coded regions represent CO_2 saturation, but the sizes and shapes of the darker blue plumes are not to scale (details in Sect. 8).

formation (Busch and Müller, 2011). Assuming hydrostatic equilibrium, the maximum amount of CO_2 trapped under a capillary barrier can be estimated via:

$$h_{max} = \frac{P_C}{(\rho_{\mathrm{brine}} - \rho_{\mathrm{CO2}})\cdot g} = \frac{\gamma \cos\theta}{d\cdot(\rho_{\mathrm{brine}} - \rho_{\mathrm{CO2}})\cdot g}, \quad (2)$$

where h_{max} is the maximum CO_2 column height that can be stored underneath a capillary barrier before CO_2 enters the barrier, ρ_{brine} and ρ_{CO2} are the densities of brine and CO_2, respectively, and g is the acceleration due to gravity. By rearranging this equation and Eq. (1), it becomes evident that h_{max} is directly proportional to $\cos\theta$. This aligns with physical intuition: when $0^\circ < \theta < 90^\circ$, CO_2 is the non-wetting phase and the wetting fluid (brine) adheres more strongly to the solid surface. A smaller contact angle (or stronger contrast between the wetting and nonwetting behaviors) leads to a higher CO_2 column to be supported before capillary breakthrough occurs.

CO_2 migrates into the overlying rocks when $P_{CO2} - P_{brine} > P_C$. When the brine is displaced sufficiently to exceed the percolation threshold, a continuous flow path for CO_2 is established across the pore system. Initially, this flow occurs through the largest interconnected pores. As pressure continues to increase, flow also passes through smaller pores, enhancing the effective permeability. Ultimately, the dominant flow paths are determined by both the fluid's flow properties and the geometric properties of the connected pore spaces in the sample (Shukla et al., 2010). The petrophysical properties of capillary barriers, including those of overlying rocks and rocks within the storage units, limit the amount of CO_2 that can be safely stored in potential sites. Once the risk of structural failure for these barriers, such as legacy wells (Gasda et al., 2009), reactivation of faults, induced shear failures, or hydraulic fracturing, is minimized, the sealing capacity is limited by the capillary pressure (or column height, Eq. (2)) at which the trapped fluid begins to migrate into the seal (Busch and Müller, 2011). Since capillary pinning reduces a portion of the buoyancy force exerted on the sealing layer (i.e., P_{CO2} exerted by h_{max} is dispersed by different capillary barriers in the storage unit, due to the secondary-seal effect, see Fig. 1), it enhances the storage unit's integrity. As such, P_C is likely one of the most critical parameters in determining a CO_2 storage project's long-term security.

2. Experimental proof of concept

Capillary pinning has also been investigated via experimental studies (Jackson et al., 2020; Krevor et al., 2011; Krishnamurthy et al., 2022; Ni et al., 2019). Based on their core flood experiments, Krevor et al. (2011) demonstrated that CO_2 plumes can be immobilized by capillary pinning as a continuous phase at saturations 2 to 5 times higher than would be achievable by snap-off. They also observed that cross-stratified bedsets in the sandstone, rather than small mudrock lenses, were responsible for the capillary heterogeneity causing the CO_2 pinning, resulting in more prevalent CO_2 pinning than previously expected based on the distribution of mudrocks. Jackson et al. (2020) observed a similar trend in their core flood experiments, and their coupled simulation results reveal that boundary conditions during imbibition are crucial for accurately recreating experimental observations. However, Jackson et al. (2020) cautioned that it is challenging to estimate these boundary conditions from experiments, making it difficult to match simulation data with experimental results. In their work, the end effects — specifically, the trailing edge of the non-wetting phase toward the outlet — are reduced or inverted during imbibition. Properly including these impacts in the models is essential for achieving an accurate match. Ni et al. (2019) conducted core flood experiments on nine sandstone samples with varying degrees of heterogeneity to study the petrophysical properties that maximize capillary heterogeneity trapping. Their findings revealed that capillary pinning accounts for 3 to 54 % of the total CO_2 trapped. Krishnamurthy et al. (2022) used cross-stratified bedsets constructed from bead packs to demonstrate that capillary heterogeneity—resulting from changes in fabric geometry and grain size contrast—significantly affects CO_2 migration times and trapped volumes, with variations of up to two orders of magnitude. In their study, approximately 80 % of trapped CO_2 resulted from capillary pinning, in the absence of any impermeable layers. Although capillary pinning was not the primary focus of the study by Fernø et al. (2023), it was observed during their room-scale CO_2 injection experiments conducted in unpressurized, unconsolidated sands (3 m length × 2 m height). The stratified sedimentary layers in the model acted as capillary barriers, temporarily trapping buoyant CO_2 and causing the gas to spread laterally along these interfaces. This lateral migration occurred as the gas was held back by capillary forces at layer boundaries. Synthesizing these experimental results, it is clear that, regardless of variations in the proportion of total CO_2 trapped by this mechanism, the degree of capillary pinning is primarily governed by capillary heterogeneities, which emerge from the combined influence of intrinsic material properties such as mineralogy, porosity, and pore connectivity.

3. Challenges in understanding capillary pinning

3.1. Setting the terminology straight

It has been shown that the amount of CO_2 trapped by capillary pinning may be comparable with the amount trapped by snap-off (Gershenzon et al., 2014, 2016, 2017), and that capillary pinning might even prevail as the primary trapping mechanism in cases of pronounced differences in capillary pressure among rock formations (Ren et al., 2014). Given the prevalence and reliability of CO_2 storage via capillary pinning, we suggest that the term "local capillary trapping" may be misrepresenting the significance of this CO_2 trapping mechanism (i.e., “local” indicates restricted location or small area). In alignment with Gershenzon et al. (2014), we adopt the terms "snap-off" and "capillary pinning" to denote the two CO_2 trapping processes in the following discussion. Other less commonly used terms for capillary pinning include heterogeneity-assisted and heterogeneity-induced trapping (Dai et al., 2018), capillary heterogeneity trapping (Kuo and Benson, 2015; Li and Benson, 2015), capillary barriers (Krevor et al., 2011; Mishra and Haese, 2020), capillary pressure effects (Ide et al., 2007), capillary pressure barriers (Bryant et al., 2008), intraformational baffles effects (Mishra and Haese, 2020; Yu et al., 2017), heterogeneity effects (Frykman et al., 2009) and CO_2 migration under heterogeneous capillary pressure (Cui et al., 2023). For clarity, we replace these terms with "capillary pinning" when discussing these studies (Table 2) on CO_2 trapping caused by capillary heterogeneity.

On a separate note, there is a substantial body of well-known literature on relative permeability hysteresis trapping effects, which are inherently related to capillary actions (e.g., Agada et al., 2016; Akbarabadi and Piri, 2013; Doster et al., 2013; Juanes et al., 2006; Spiteri et al., 2008). Hysteresis is the dependence of the relative permeability and capillary pressure on the saturation history (Elhaj et al., 2021). Hysteresis trapping occurs due to the different wetting behaviors of CO_2 and brine as they move through porous media, leading to one phase displacing the other. This phenomenon is, by definition, snap-off trapping. In the context of this study, we classify hysteresis trapping as snap-off trapping and will not showcase individual studies focused solely on it. In the later part of the text, "hysteresis" will be mentioned, but it refers to its original definition: the phenomenon where capillary pressure in porous materials depends on the history of fluid distribution, not snap-off trapping.

From the perspective of force balance (Eqs. (1) & (2)), capillary pinning is fundamentally equivalent to capillary sealing (Iglauer et al., 2015). However, the term "capillary sealing" is often associated with caprocks, which can be misleading in the context of this study, as we focus on capillary phenomena occurring within the storage unit itself. To avoid this confusion, we distinguish capillary pinning from the sealing effects typically attributed to caprocks. Structural trapping refers to the

Table 2
List of published studies on capillary pinning and the terms used to describe it.

References	Terms Used
Saadatpoor et al., 2008, 2009, 2010; Singh et al., 2021; Ren et al., 2014; Ren, 2015, 2018; Ren and Hoonyoung, 2018; Cui et al., 2023; Krishnamurthy and Prasanna, 2020; Krishnamurthy et al., 2022; Ellis and Bazylak, 2012; Ubillus et al., 2025; Zhang et al., 2011	local capillary trapping (LCL) / local capillary effects / local trapping structures
Gershenzon et al., 2014, 2016, 2017; this study	capillary pinning
Dai et al., 2018	heterogeneity-assisted / heterogeneity-induced trapping
Mishra and Haese, 2020; Krevor et al., 2011; Kuo and Benson, 2015; Debbabi et al., 2017; Jackson and Krevor, 2020; Harris et al., 2021; Ni et al., 2019; Li and Benson, 2015	capillary heterogeneity (trapping)
Ide et al., 2007; Li and Benson, 2015	capillary pressure effects
Bryant et al., 2008; Krevor et al., 2011; Mishra and Haese, 2020; Fernø, 2024; Flemisch, 2024	(gas accumulation under) capillary (pressure) barriers
Mishra and Haese, 2020; Yu et al., 2017; Jackson et al., 2022Jackson et al., 2022	intraformational baffles (effects), stratigraphic baffling / trapping
Frykman et al., 2009	heterogeneity effects
Cui et al., 2023	CO_2 migration under heterogeneous capillary pressure
Krishnamurthy and Prasanna, 2020, Krishnamurthy et al., 2022	geologic heterogeneity controls

accumulation of CO_2 beneath impermeable or low-permeability caprock layers, where buoyancy forces are counteracted by a continuous seal. This process operates at larger, typically reservoir, scales and is controlled primarily by the geometric configuration of the reservoir-seal boundary and the integrity of the seal (Fig. 2). In contrast, capillary pinning is a mesoscale mechanism driven by contrasts in capillary entry pressure across facies boundaries and similar heterogeneities. These contrasts can immobilize the CO_2 even without a continuous structural seal, through a local balance of capillary and buoyancy forces. While both mechanisms restrict CO_2 migration, they differ in terms of scale of operation, spatial context, and implications for storage security.

3.2. Scales and uncertainties

Sedimentary heterogeneities comprise a wide range of variations in physical and chemical properties across different scales (Figs. 2, 3), from microscopic to field levels (e.g., Haldorsen, 1986; Jordan and Pryor, 1992; Koltermann and Gorelick, 1996; Miall, 1988; Weber, 1982). At the microscale, heterogeneities include variability of minerology, pore fluid chemistry, pore sizes, pore shapes, and pore connectivity, which affect fluid flow and capillary actions (Boggs, 2006; Zhang and Tutolo, 2021). At the mesoscale to macroscale, larger features like grain packing, layering, faults, stratigraphic changes, and facies variations become prominent, determining the overall flow and storage characteristics of entire reservoirs (Boggs, 2006; Friedman et al., 1992). Finally, heterogeneities can span entire sedimentary basins, where tectonic structures, regional stratigraphy, and large-scale hydrodynamic conditions play important roles. These interconnected scales of heterogeneities collectively shape the flow dynamics in subsurface porous media, making it essential to consider the effects of small-scale heterogeneities in reservoir modelling (i.e., upscaling; Christie, 2001; Honarpour et al., 1995; Pickup and Stephen, 2000; Ringrose and Bentley, 2021; Yang et al., 2013). However, accounting for all small-scale heterogeneities in numerical models is computationally expensive. Therefore, the concept of the Representative Elementary Volume (REV) is commonly employed (Fig. 3). An REV (Bear, 1972) represents a volume at which the parameter of interest is both homogeneous and statistically stationary, ensuring the effective modelling of subsurface flow dynamics without

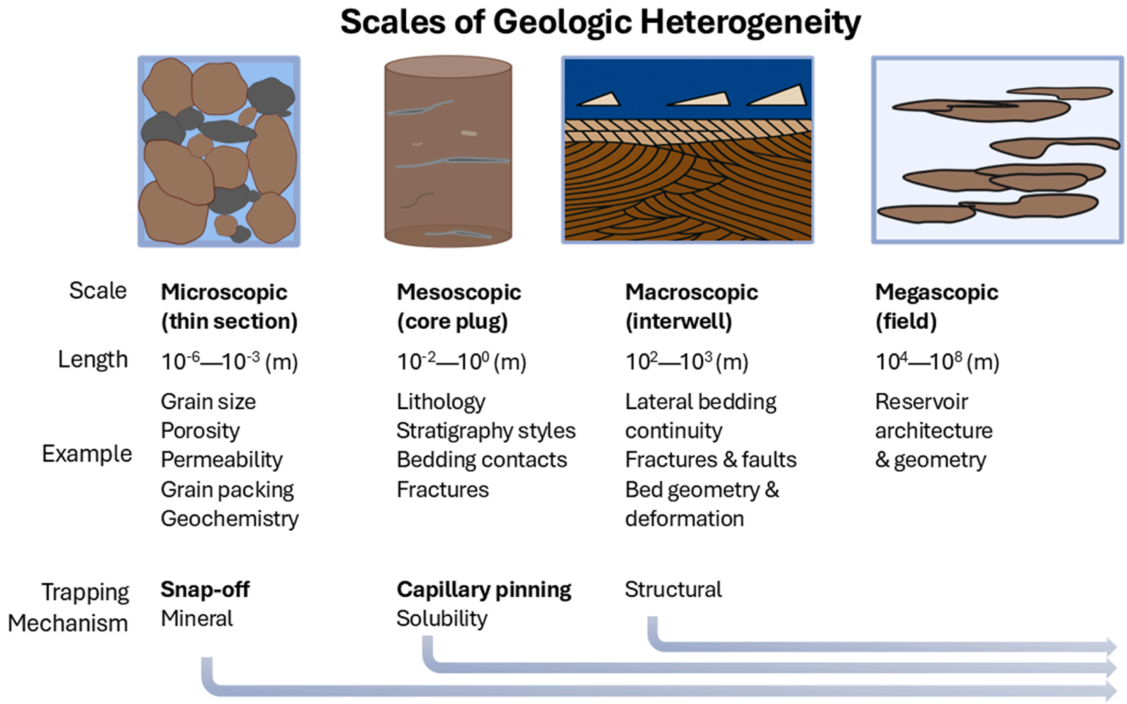

Fig. 2. A conceptual sketch of the different scales of geologic heterogeneity (modified after Keogh et al., 2007) and the CO_2 trapping mechanisms that can be observed at each scale. For example, capillary pinning is typically unobservable at microscopic scale, but it makes a systematic difference starting at the mesoscopic scale.

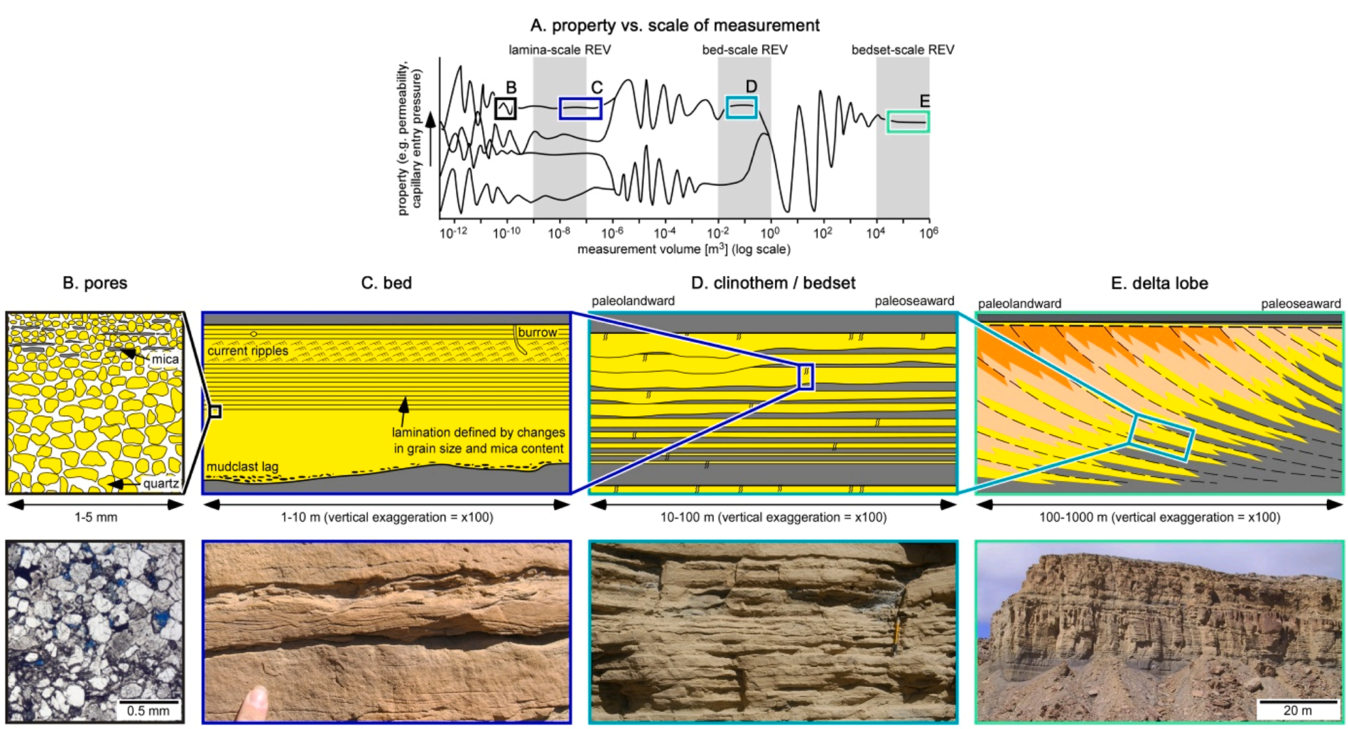

Fig. 3. (a) Conceptual sketch illustrating variations in a rock property related to length scales of measurement, highlighting Representative Elementary Volumes (REVs) specific to a particular scale of sedimentary geologic heterogeneity (after Nordahl and Ringrose, 2008). In this example there are four different lamina types that combine into two bed types which are combined in a bedset. (b-e) Sketch cross-sections (upper) and photographs (lower) of sedimentologic heterogeneities, which are arranged hierarchically across different length scales. The hierarchy of heterogeneity is illustrated for river-dominated deltas (after Graham et al., 2015) and, specifically, the Cretaceous Ferron Sandstone, Utah, USA: (b) grains arranged in laminae; (c) laminae arranged in bed; (d) beds arranged in bedset; (e) bedsets arranged in delta lobe. Photographs are from (a) thin section (after Braathen, 2018) and (b-e) outcrop.

the need to account for every minute detail at smaller scales (Nordahl and Ringrose, 2008).

Due to our current understanding of capillary pinning, existing methods of REV determination may not accurately account for the effects of capillary heterogeneities. For example, prior models applying a single drainage capillary pressure curve for each rock type may lack physical accuracy when it comes to capillary pinning (Saadatpoor et al., 2009). Upscaling models in the context of capillary heterogeneities requires a nuanced approach because capillary pinning is influenced by force balances rather than just permeability contrasts (Debbabi et al., 2017; Gasda and Celia, 2005), which requires additional considerations to represent the reservoir properties and to characterize the CO_2 plumes (Cavanagh and Haszeldine, 2014), as will be discussed below. It has been demonstrated that the conventional method of upscaling small-scale flow barriers by varying vertical permeability fails to capture the dispersion and trapping of the CO_2 plume by the flow barriers, because it combines the effects of different, undifferentiated processes (Hesse and Woods, 2010; Yang et al., 2013). As a result, upscaling heterogeneity in capillary pressure characteristics is more important for predicting local and upscaled flow behavior than heterogeneity in absolute or relative permeability (Singh et al., 2021).

Despite numerous modeling efforts that account for geological heterogeneities, quantitative investigations of capillary pinning at the reservoir scale remain limited. This is largely because many studies group capillary pinning with other mechanisms, such as snap-off, under the broad category of "residual trapping" (Bui et al., 2018). Others (Y. Zhang et al., 2011) have shown that significant uncertainties can persist in modeling residual trapping, even when multiple types of data are integrated. These uncertainties stem not only from the variability in model parameters and geologic heterogeneity, but also from the influence of capillary pinning, as an undefined mechanism in model formulation, that remains difficult to isolate and quantify. In the FluidFlower Validation Benchmark (Flemisch et al., 2023), which followed the physical CO_2 injection experiments by Fernø et al. (2023), participants implemented a range of modeling approaches to replicate the observed migration dynamics. While most employed Brooks–Corey relationships using experimentally measured capillary entry pressure (*Pc*) data, others adopted simplified formulations, such as linear relationships. This variation in constitutive models led to notable discrepancies in simulation results, emphasizing the sensitivity of CO_2 flow predictions to model parameterization and the importance of rigorous calibration when simulating complex, heterogeneous systems.

The lack of differentiation and understanding of the trapping mechanisms can lead to significant errors in predicted CO_2 migration path and leakage development, especially in the horizontal direction (Fig. 4). This uncertainty can, in turn, substantially impact the projected storage capacities (Hesse and Woods, 2010; Saadatpoor et al., 2009; Zhang et al., 2011). Moreover, when non-hysteretic capillary pressure curves are used in upscaled models, and viscous forces dominate the flow regime, simulation outcomes can even contradict those from more detailed, mechanism-based models (Bech and Frykman, 2018; Green and Ennis-King, 2010; Joodaki et al., 2020). In the following sections, we synthesize the current understanding of capillary pinning and identify knowledge gaps, aiming to enhance the quantification of CO_2 storage in heterogeneous geologic formations.

4. Characterization of heterogeneities

A significant challenge in simulating CCS is the impact of geologic heterogeneities on fluid migration and trapping across various length scales. These heterogeneities, formed through sedimentary depositional and diagenetic processes, manifest as structures such as cross-stratification and concretions, and tectonic processes, manifest as structures such as fractures (Boggs, 2006; Friedman et al., 1992). Although it is widely accepted that incorporating the effects of small-scale features (mm to m) in field-scale models is essential for

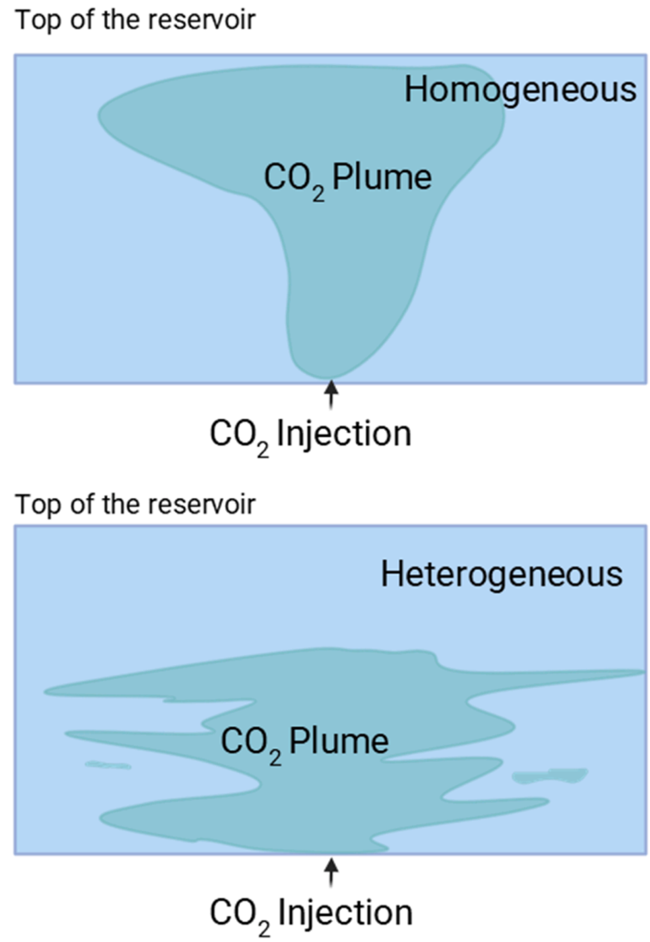

Fig. 4. Schematic illustration of CO_2 plume evolution in homogeneous (top) versus heterogeneous (bottom) reservoirs. Given the same injection rate, in the heterogeneous case, the plume does not reach the top boundary within the same time frame due to capillary pinning, but it exhibits greater lateral spreading (modified after the modelling results by Gershenzon et al., 2014).

accurately capturing CO_2 trapping processes (Krevor et al., 2023), characterizing reservoir heterogeneities at scales below the resolution of seismic imaging remains difficult. For instance, Krishnamurthy et al. (2022) demonstrated that 80 % of trapped CO_2 in their experiments was influenced by sub-seismic heterogeneities that are commonly overlooked in CCS simulation studies. While it is impractical to model every aspect of a reservoir, it is crucial to include the effects of heterogeneities that significantly impact the modelled process. So far, formation dip and cross-stratified bedsets have been studied as features controlling capillary pinning. We summarize the findings here and highlight the considerable potential for future research on the impact of capillary pinning by other types of geologic heterogeneities.

4.1. Formation dip

The effect of capillary pinning was noted by Bryant et al. (2008) during their investigation of heterogeneity, formation dip, and capillary pressure on rising CO_2 fronts in aquifers. They observed that the lateral diversion of CO_2 by P_C barriers was significant in a dipping aquifer comprising layered beds with varying average permeability. A bed with lower permeability situated above a bed with higher permeability could act as a seal, causing CO_2 to move laterally up the stratal dip instead of vertically. Importantly, this sealing effect could occur even if the permeability difference between the beds was relatively minor, provided the dip angle is sufficiently large.

Following an investigation using a 2D aquifer model into the effects of injection rate, anisotropy, formation dip, aquifer types, and residual gas saturation on capillary pinning, where capillary pinning was defined as the mass of CO_2 trapped with saturation ranging from maximum residual gas saturation (0.286) to 1, Ren et al. (2014) also discovered that the formation dip angle was the most influential parameter on the location and mass fraction of injected CO_2 held in capillary pinning. This finding aligns with the observed linear relationship between the seal formation dip and drainage length noted by Woods and Farcas (2009).

4.2. Cross-stratified bedsets

Cross-stratified bedsets (Fig. 5) are amongst the most common heterogeneities in reservoir rocks, leading to capillary heterogeneity that can be crucial for CO_2 storage. Previous research on oil recovery (Huang et al., 1996; Saad et al., 1995) has demonstrated that cross-stratified strata can greatly enhance capillary pinning. Additionally, the lens-like and dipping geometry of laminae that characterize cross-stratification have been shown to be advantageous for trapping CO_2 (Mishra and Haese, 2020). In their models of capillary-limited flow regime, when CO_2 was injected beneath a cross-stratified bedset, it rose due to buoyancy during the drainage phase and reached the interface (bounding surface) between the foresets and the overlying lamina. The lamina with higher P_C hindered the upward migration of CO_2, causing it to accumulate below the bounding surface, thereby increasing CO_2 saturation here. The dipping laminae surrounding the foreset also restricted lateral CO_2 migration, resulting in a further increase in CO_2 saturation within the foreset. In their modeling investigation, Mishra and Haese (2020) demonstrated that alongside capillary forces, the most influential factor was the anisotropy in rock properties across the bounding surface. This could lead to up to 69 % difference in trapped CO_2 saturation. These results reinforce the notion that capillary heterogeneity caused by bed geometry, rather than relative permeability, plays a vital role in capillary pinning.

5. Pore-scale determination of capillary entry pressure

There is extensive knowledge on CO_2 capillary trapping from pore network characterization and modeling studies in the context of both CCS and hydrocarbon recovery (e.g., Akbarabadi and Piri, 2013; Andrew et al., 2013, 2014; Chalbaud et al., 2007; Hu et al., 2017; Tokunaga and Wan, 2013; Valvatne and Blunt, 2004; Wang et al., 2013). However, most of these studies focus on snap-off (Singh et al. 2017) or wettability effects (Silin et al., 2011; Turner et al., 2004; Van Dijke et al., 2007), while largely overlooking capillary pinning (Ellis and Bazylak, 2012). This is likely because, although capillary pinning arises from pore-scale capillary effects, it remains unobservable without first characterizing the heterogeneity of pore throats that cause capillary variation (Xu et al., 1997). Due to limitations in X-ray microtomography and the computational intensity of pore network simulations, many pore network studies have focused on small numbers of pore throats (e.g., Singh et al., 2017), opted not to investigate capillary heterogeneity effects (Hu et al., 2017), or represented porous media as a network of discrete pores connected by uniform throats (Bromhal, 2001; L. Li et al., 2006).

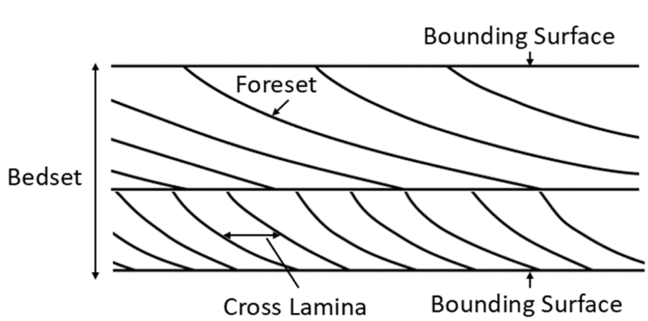

Fig. 5. A conceptual illustration of a cross-stratified bedset. Here, we adapted the definition presented by Friedman et al. (1992): cross laminae refer to laminae that were deposited at an angle to the bounding surfaces of a bedset. The term cross-stratified bedset only refers to the geometry of the rock formation and has no implication of any specific lamina thickness or length scale. Accordingly, no scale is included in the figure.

Because P_C is fundamentally determined by molecular interactions between fluids and solids, quantifying the absolute value of it requires time-consuming experimental measurements (e.g., in-situ measurements on cores summarized by Busch and Müller, 2011; Vespo et al., 2024) or molecular dynamic modeling (Iglauer et al., 2012), which are difficult to scale up due to the requirement of specified boundary conditions (Vespo et al., 2024). As a result, researchers have aimed to establish a dependency of capillary entry pressure with reservoir properties, such as depth and mineralogy. This knowledge allows future models to establish threshold conditions that can predict whether modelled reservoir volumes (e.g. grid blocks) act as flow barriers or paths.

For instance, Zhou et al. (2017) investigated the relationship between P_C and formation depth, since the key parameters that determine P_C for a given pore size and geometry are interfacial tension (γ) and wetting conditions, which are both depth-dependent. Generally, P_C for a given pore geometry decreases with storage depth for two reasons: 1) CO_2 pressure increases with burial depth, resulting in a decrease in CO_2-brine γ; and 2) the system becomes less water-wet with burial depth, lowering P_C. Using scanning electron microscopy (SEM) 2D rock imaging, pore spaces were estimated as straight capillary tubes, and the CO_2-brine γ was obtained as a function of the density difference between the two phases. Their results showed that pore roughness and shape played a crucial role in predicting P_C as a function of hydraulic radius, particularly for storage depths shallower than 1000 m, where CO_2 was not in a supercritical state. However, these effects became less significant at depths exceeding 1200 m, where CO_2 becomes supercritical. This observation aligns with the conclusion of Mouallem et al. (2024), who, based on a compilation of 14 CO_2-brine interfacial tension datasets, found that γ becomes pressure-independent above approximately 30 MPa.

Nevertheless, inconsistencies persist in the literature regarding the dependence of P_C on salinity and temperature, with most studies showing that increasing temperature and salinity results in higher γ (Mouallem et al., 2024). This suggests that using depth as a proxy for P_C may be overly generalized —while temperature typically increases with burial depth, it also tends to increase γ. While the method employed by Zhou et al. (2017) may not comprehensively capture all aspects of P_C estimation, it provides a semi-analytical method for estimating CO_2 capillary entry pressure using simple imaging data inputs and offers valuable insights into injection depth considerations, particularly in scenarios where CO_2 mineralization or secondary mineral precipitation may occur and alter pore throat geometry (Li et al., 2006).

In addition to pore geometry, heterogeneity of wettability caused by the distribution of various mineral surfaces is another known factor causing heterogeneities in P_C (Ellis and Bazylak, 2012). To assess the effects of contact angle heterogeneity and its impact on flow networks, Ellis and Bazylak (2012) performed a series of calculations on model networks composed of randomly distributed quartz and mica, with each mineral having a unique and well-characterized contact angle. Their results showed an increase in trapped saturation by 3.5 % for the heterogeneous wettability network over the homogeneous ones when modeled in capillary-dominated flow regimes. Mineral surface heterogeneity had almost no impact on the amount of trapped CO_2 when the flow was viscous-dominated. On the other hand, heterogeneous mineral surfaces led to thicker fingering patterns and increased lateral migration regardless of the flow regime. Consequently, the authors noted that pore-scale heterogeneities resulting from mineralogical differences, variations in pore and pore throat shapes, or geochemically-induced changes in pore structure need to be evaluated before the outputs of pore network models are upscaled as bulk transport properties.

6. Modelling CCS systems with capillary pinning

To predict the behavior of CO_2 in the subsurface, several commonly used modeling approaches are available, such as full-physics, invasion-percolation, and vertical-equilibrium methods. A full-physics simulation involves solving equations that represent various physical phenomena, including solid and fluid dynamics, thermodynamics, mechanics, and fluid properties such as density and viscosity (Nordbotten and Celia, 2011). As a result, a full-physics simulation offers the most detailed information about the modelled system but is the most computationally expensive method (Ringrose and Bentley, 2021). The invasion-percolation method is commonly applied for slow-moving immiscible fluids in geologic flow systems, and it assumes that viscous forces have a negligible effect on fluid displacement. Because the balance between buoyancy and capillary forces is the key factor in this method for predicting plume migration (e.g., Cavanagh and Ringrose, 2011; Ioannidis et al., 1996; Mehana et al., 2020; V. Singh et al., 2010), it is a common method of modelling capillary pinning. The vertical equilibrium method assumes that the strong buoyancy forces in the system cause rapid vertical segregation of the injected CO_2 and resident brine, occurring much faster than the overall simulation time scale (Celia and Nordbotten, 2011; Nordbotten et al., 2012). This results in a scenario in which each fluid exhibits a pressure distribution that is nearly hydrostatic, referred to as vertical equilibrium (e.g., Celia and Nordbotten, 2011; Court et al., 2012; Gasda at al. 2009; Nordbotten and Celia, 2011).

Simulations of CCS are computationally expensive due to the complex multiscale flows involved and the large spatial and temporal scales, so approximate solutions by simplifying the domain and the equation parameters (i.e., upscaling) offer a way to reduce computational costs while approximately preserving important aspects of the fine-scale flow solution (Nordbotten and Celia 2011; Rabinovich et al. 2015). Because capillary action plays a major role in CCS systems, prior upscaling techniques designed for oil-water simulations (Huang et al., 1996; Saad et al., 1995), in which viscous forces dominate the force balances of the system, are not directly applicable (Hassan and Jiang, 2012). As mentioned earlier, many upscaling methods failed to differentiate between snap-off and capillary pinning due to a lack of awareness of the latter. In some cases, even when the effects of capillary pinning were acknowledged, they were not incorporated into the upscaling process. This omission assumed that only capillary heterogeneities of considerable thickness would significantly contribute to CO_2 pinning (Gasda et al., 2011), an assumption that may be oversimplified given that cm-scale heterogeneities have been shown to cause significant capillary pinning (Debbabi et al., 2017; Krevor, et al., 2011). As a result, only a few upscaling studies captured the importance of capillary pinning. Here, we highlight two examples of upscaling methods, the Geologic Criteria Algorithm (Ren et al. 2015) for fast evaluations of post-injection buoyant flows, and dynamic upscaling (Rabinovich et al., 2015) for more detailed insights into modelled CCS operations.

In their upscaling effort, Ren et al. (2015) decoupled the simulation into two parts: the first is the prediction of CO_2 plume behavior based on permeability through connectivity analysis, and the second is the identification of capillary pinning distribution influenced by P_C heterogeneity, determined using the Geologic Criteria Algorithm. Here, we focus on the later part.

Upon determining the P_C, a Geologic Criteria Algorithm (Ren et al. 2015) can be established to quantify capillary pinning in the CO_2 storage domain via the following steps:

1) Identify all grid cells in the domain that have entry pressures exceeding the P_C; these cells are recognized as barriers.
2) Determine all the connected clusters of barriers among the cells identified in Step 1.
3) Locate the non-barrier clusters surrounded by the set of barrier clusters from Step 2; these cells represent where capillary pinning occurs.

By establishing a threshold P_C, this approach provides a fast algorithm for predicting capillary pinning distribution based on geologic models. The primary uncertainties in this method that cause discrepancies with full-physics simulations lie in 1) selecting P_C values, as they directly influence the quantification of capillary pinning; and 2) characterizing CO_2 plumes, which determines whether CO_2 sweeps certain grid cells and whether the upward forces can breach the capillary barriers (detailed in Sect. 7). Importantly, while the Geologic Criteria Algorithm method provides important insights about CO_2 entry into rock layers, it needs to be coupled with a CO_2 flow model (i.e., the first part of Ren et al. (2015)'s approach) to predict the time it takes for CO_2 to pass through them.

The dynamic upscaling technique introduced by Rabinovich et al. (2015) also effectively addresses scenarios with significant capillary heterogeneity. This method uses global upscaling procedures, demanding a complete fine-scale simulation to determine the relevant properties. The coarse-scale governing equations are then derived by averaging the fine-scale equations over the regions corresponding to the coarse grid blocks. For instance, the capillary pressure curve for a coarse grid block is obtained by averaging the capillary pressure curves of all the underlying fine-scale grid blocks. By comparing their results with traditional upscaling techniques (Pickup and Sorbie, 1996), Rabinovich et al. (2015) demonstrated that their dynamic upscaling is particularly robust in regions where flow rate dependency is important, while the results were comparable to conventional upscaling methods in both high (viscous limit, VL) and low flow (capillary limit, CL) regions. Although more computationally demanding, this technique captures rate-dependency effects, making it applicable to the injection phase of a CCS operation.

7. Characterization of CO_2 plume

Many of the upscaling methods and techniques developed in hydrocarbon reservoir modeling can be applied for CO_2 storage purposes. However, in petroleum engineering applications, gravity is frequently overlooked, especially in oil-water systems, where viscous forces are the primary factor at the reservoir scale (Pickup and Sorbie, 1996). Yet, when injected as a supercritical fluid, CO_2 is buoyant compared to formation pore water, thus making gravity a significant factor in CO_2 injection and migration (Hassan and Jiang, 2012).

To address this issue, Mouche et al. (2010) conducted upscaling of a buoyant flux in a one-dimensional vertical column filled with a periodically layered porous medium (Mouche et al., 2010). They investigated two scenarios: 1) a capillary-dominant case where capillarity drove flow in a layer, and 2) a capillary-free case where buoyancy was the sole driving force. In both cases, the buoyant flux exhibited a bell-shaped function of saturation, similar to a homogeneous porous medium. In the capillary-dominant case, the upscaled saturation was governed by capillary pressure continuity at the layer interfaces. They demonstrated that the upscaled buoyant flux was the harmonic mean of the fluxes in each layer, with the contribution from the high-permeability layer being dominant. In the capillary-free case, the upscaled buoyant flux and saturation were determined by flux continuity conditions at the interfaces.

Observations from the Sleipner storage site, offshore Norway, which exhibits extensive capillary heterogeneities (Cavanagh and Haszeldine, 2014), offered another example of the importance of capillary pinning in CO_2 plume migration. Seismic reflection surveys revealed that the injected CO_2 plume had breached eight shale barriers within the storage sandstone unit. Since no evidence of structural damage was observed in these shales, the authors investigated capillary breakthrough as the mechanism driving CO_2 ascent. The upward migration of CO_2 plumes was conceptualized using an invasion-percolation simulator based on the threshold breakthrough pressure (Eq. (1)): if the pressure from the trapped CO_2 column did not exceed the P_C, the CO_2 would accumulate beneath the shale and fill the structural relief of the underlying sandstone layer until reaching a spill-point. Upon breaching this pressure threshold, the CO_2 would migrate vertically until encountering the next shale layer, where it would be trapped again, creating a vertical sequence of pooled CO_2. Seismic surveys supported this pattern of capillary flow, pooling, breaching, and lateral migration as matching the observed plume distribution.

The invasion percolation simulation, similar to the Geologic Criteria Algorithm (Ren, 2015) described above, provides quick evaluations of whether CO_2 plumes will breach certain rock layers. However, these methods only conduct threshold checks which are independent of time; full-physics models are still necessary to investigate time-dependent factors.

8. Quantifying CO_2 trapped by capillary pinning

Using multi-scale models of fluvial channel-belt deposits, Gershenzon et al. (2017) showed that the amount of capillary pinning increased with increasing capillary pressure contrast and CO_2 plume volume, and the ratio of total snap-off to pinning ranged from 0.5 to 2. The impact of capillary pressure hysteresis also remained a major uncertainty in quantifying the amount of CO_2 stored via capillary pinning, for most previous studies omitted capillary pressure hysteresis due to long simulation run times (Bech and Frykman, 2018; Harris et al., 2021). Hysteresis in capillary pressure may diminish a layer's CO_2 pinning effectiveness. Consequently, omitting capillary pressure hysteresis in simulations might lead to significant overestimations of trapped CO_2 amounts. In the cases presented by Bech and Frykman (2018), the overpredictions were more than double.

Using the Captain Sandstone (UK North Sea) as an example, Harris et al. (2021) demonstrated that the proportion of capillary pinning decreased when capillary pressure hysteresis is considered. The amount of capillary pinning varied between 30 % and 100 % of the amount of CO_2 trapped without hysteresis, depending on the functional form of the imbibition capillary pressure curve used. These results suggested that simulations without hysteresis should be viewed as an upper bound for capillary pinning within a system, and Harris et al. (2021) recommended applying a correction factor between 0.3 and 1 (where 1 = no correction) to adjust for overestimations in systems that had not accounted for capillary pressure hysteresis. These studies suggested that capillary pinning was strongly dependent on the imbibition threshold pressure, and a decrease in this threshold pressure reduced the ratio of capillary forces in the system, leading to less CO_2 trapping in total. Harris et al. (2021) noted that the functional forms of the imbibition capillary pressure curve showed the same inverse trend with rate, indicating that this pattern is consistent across different capillary pressure relationships.

With a series of dimensionless models, Debbabi et al. (2017) showed the significant impacts of flow direction and wettability. When flow was directed across layers of alternating permeability, capillary pinning trapped the non-wetting phase, irrespective of whether it was the injected or displaced phase. Yet, capillary pinning became minimal when the injected phase was intermediate-wetting or when high-permeability layers contained a smaller moveable fluid volume than low-permeability layers. The authors showed that a dimensionless capillary-to-viscous number, defined using layer thickness instead of length, was most relevant for predicting capillary pinning in this case. They also demonstrated a special case in which flow was directed along layers. In this case, high-permeability layers contained less moveable fluid volume than low-permeability layers, and capillary pinning trapped the wetting phase, regardless of whether it was the injected or displaced phase.

9. Conclusions and future work

This review has examined the fundamental mechanisms and modeling approaches critical for estimating CO_2 capillary pinning in CCS operations. While significant progress has been made in understanding capillary pinning, the body of research remains fragmented, with varying terminologies and occasional inconsistencies even within individual studies. This lack of cohesion not only complicates effective literature searches but also makes it difficult for researchers to pinpoint the most relevant factors to investigate. Capillary pinning is frequently conflated with, or categorized alongside, other trapping mechanisms such as residual trapping, snap-off, or hysteresis trapping. This blending of concepts obscures the distinct characteristics of capillary pinning and contributes to ongoing confusion. Furthermore, because experimental evidence is predominantly limited to core-scale studies, due to the practical challenges of conducting large-scale pressurized experiments, there is a widespread misconception that capillary pinning is solely a core-scale phenomenon. Consequently, its role is often underestimated or entirely neglected in larger-scale models. These challenges are compounded by the inherent difficulty of characterizing and upscaling fine-scale heterogeneities and CO_2 plume dynamics, resulting in significant uncertainty around the quantification of capillary pinning. As a result, reported contributions of capillary pinning to CO_2 trapping vary widely (from as little as 3 % to nearly 100 %, depending on the methodology used).

We emphasize that incorporating capillary pinning into modeling is not intended to discredit previous approaches, but rather to provide a framework for deeper understanding. Modeling serves as a powerful tool for testing hypotheses, exploring scale effects, and bridging the gap between core-scale observations and field-scale predictions. By integrating modeling efforts with experimental insights, we can refine our interpretations and better capture the role of capillary pinning in CCS systems.

We highlight that capillary pinning becomes particularly important in the following scenarios:

1) Heterogeneous reservoirs with interbedded lithofacies (e.g., sandstones and mudstones) exhibiting strong contrasts in capillary entry pressures. In such settings, capillary barriers can significantly alter plume geometry and lead to early immobilization, which is not captured by models relying solely on structural trapping or simple relative permeability scaling.
2) Poorly sealed reservoirs lacking a continuous caprock or well-defined structural trap. In these cases, lateral migration control and plume stabilization may be dominated by capillary heterogeneity rather than structural closure.
3) Thin, dipping, or compartmentalized formations where vertical migration is restricted by multiple fine-grained layers, but traditional structural traps are absent or poorly developed.
4) Low injection-rate scenarios where the flow regime is more capillary-dominated, giving capillary pinning greater influence on plume evolution and residual trapping efficiency.

In order to improve our understanding of CCS processes and to maximize storage capacity and security, we suggest the following future research directions:

1) Enhance the quantitative understanding of capillary heterogeneity resulting from geologic heterogeneities. While existing studies have examined the effects of grain size contrasts and dipping rock layers, more complex heterogeneities remain unexplored. Understanding the significance of different types of heterogeneities will help reservoir geoscientists and engineers determine the level of detail required in their models.

2) Flow direction plays a crucial role in quantifying capillary pinning, yet most studies focus only on the upward migration of CO_2 plumes, neglecting the CO_2 injection phase and lateral plume development. Future research should address the lateral movement of CO_2 plumes influenced by various geologic heterogeneities coupled with injection rates to ensure more accurate predictions of CO_2 migration. This effort can lead to better matches between modeled CO_2 plumes and monitoring results.
3) Due to the lack of a well-defined concept for capillary pinning in the CCS community, there is no widely accepted numerical method for quantifying it at the reservoir scale. Establishing an optimal upscaling protocol for the dynamic simulation of capillary pinning is therefore crucial.
4) Since the impact of capillary pinning has been previously overlooked, there is a need to reevaluate the total CO_2 storage capacity with the influence of capillary pinning and its impact on the security of caprocks. This effort is also directly beneficial to H_2 storage operations.
5) Future research on dissolution trapping and in-situ carbon mineralization could leverage capillary pinning to extend the time available for mineral-water-CO_2 reactions.

CRediT authorship contribution statement

Qin Zhang: Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Data curation, Conceptualization. **Sebastian Geiger:** Writing – review & editing, Writing – original draft, Validation, Supervision, Investigation. **Joep E. A. Storms:** Validation, Supervision. **Denis V. Voskov:** Writing – review & editing, Supervision, Conceptualization. **Matthew D. Jackson:** Writing – review & editing, Writing – original draft, Validation, Investigation. **Gary J. Hampson:** Writing – review & editing, Writing – original draft, Project administration. **Carl Jacquemyn:** Writing – original draft. **Allard W. Martinius:** Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Investigation, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Qin Zhang reports financial support was provided by Equinor ASA. Qin Zhang reports financial support was provided by Exxon Mobil Corporation. Qin Zhang reports financial support was provided by TGS. Qin Zhang reports financial support was provided by Shell. Qin Zhang reports financial support was provided by ENI. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. Allard W. Martinius reports financial support was provided by Equinor ASA.

Acknowledgements

We thank the sponsors of the STOWCe consortium: ENI, Equinor, ExxonMobil Technology and Engineering Company, TGS, and Shell. Sebastian Geiger thanks Energi Simulation for supporting his Chair.

Data availability

Data will be made available on request.

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