

SIMULATION INVESTIGATION OF VERTICAL HETEROGENEITY ON CO₂ TRAPPING IN DEEP SALINE AQUIFERS

by

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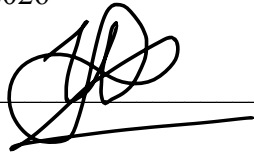
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Signed on 24.04.2026

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ABSTRACT

Geological storage of CO₂ in deep saline aquifers has been widely proposed as a long-term mitigation option. However, the influence of vertical reservoir heterogeneity on CO₂ trapping mechanisms remains insufficiently studied, representing a critical gap. This study uses high-resolution reservoir simulations to systematically quantify how vertical permeability trends influence CO₂ trapping in deep saline aquifers. A vertical cross-section model with a 5-year CO₂ injection followed by 195 years of monitoring, with heterogeneity levels from homogeneous to highly heterogeneous, explicitly comparing upward-decreasing vs upward-increasing permeability profiles, was developed using CMG software. The results show that permeability architecture ultimately affects trapping outcomes. Upward-decrease profiles create partial barriers that slow vertical migration, compartmentalize the CO₂ plume, and increase residual trapping and dissolution, especially at high heterogeneity. In contrast, models with upward-increase permeability preserve vertical connectivity, which leads to a continuous plume with greater structural trapping but less long-term immobilization of CO₂. Under high heterogeneity ($V_{DP}=0.93$), the upward-decreased case immobilizes a large fraction of the injected CO₂ (as residual and dissolved), whereas the upward-increased case retains a large connected gas cap. Permeability trends also affect injectivity: low-permeability layers near the well (coarsening-upward) raise the injection pressure, whereas a high-permeability base (fining-upward) maintains lower pressure. These findings provide practical guidance for site selection: in moderately heterogeneous sandstones ($V_{DP} \approx 0.3-0.5$), upward-increase trends favor efficient injection and enhanced CO₂ dissolution within ~50 years; in highly heterogeneous reservoirs ($V_{DP}>0.5$), upward-decrease trends support long-term (century-scale) CO₂ trapping, though potentially at the cost of higher injection pressure.

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1. INTRODUCTION

1.1 Background

Global warming has been recognized as a major problem affecting humanity over the past few decades. The Intergovernmental Panel on Climate Change (IPCC) reported that the global average surface temperature increased by approximately 0.85°C between 1880 and 2012, with further warming expected over the coming decades, leading to serious environmental consequences such as glacier melting, sea-level rise, rainfall intensity, increased atmospheric water vapor, more frequent heat waves, unexpected droughts and floods, also declining groundwater levels (IPCC, 2014). More recently, the highest level of global average temperature rise observed between 2015 and 2022 as reported by the World Meteorological Organization (WMO) (AL-Khulaidi et al., 2025). Among the main drivers of climate change, carbon dioxide (CO_2) emissions from fossil fuel combustion, industrial processes, and deforestation remain the most significant. Approximately 40 billion tons of CO_2 are released each year from global energy use, of which nearly 5 billion tons come directly from oil and gas operations (International Energy Agency, 2023). This major contribution highlights the urgent need for action. The Paris Agreement of 2015 strengthened international commitments to limit global warming, setting ambitious goals to limit global warming. The rise should remain below 2°C above pre-industrial levels, with efforts to keep it within 1.5°C (The Paris Agreement | UNFCCC, 2015). The average yearly CO_2 concentration reached its highest level in 2021, which indicate the continued accumulation of the main greenhouse gas in the atmosphere. For these reasons, CO_2 emission reduction and sequestration have become major priorities for governments worldwide (Rahman et al., 2022; W. Wang et al., 2022).

Considerable research has examined CO_2 sequestration leads to several storage strategies, some of which have already been implemented in practice. Among the main large-scale options are geological (Baines & Worden, 2004) and ocean (Orr et al., 2001) sequestration. One of the earliest ocean-based proposals, introduced in 1977, which involved transporting CO_2 to deep ocean waters for long-term isolation (Azin et al., 2022). Other marine-based methods, such as ocean fertilization, aim to stimulate phytoplankton growth and increase CO_2 uptake through photosynthesis. After the biomass decomposition, part of the absorbed carbon may be transferred to deeper waters. (Zhao & Itakura, 2023). However, direct CO_2 disposal in the ocean may also lead to acidification and poses risks to marine ecosystems. (Caldeira & Wickett, 2005) showed that continued CO_2 emissions could significantly alter ocean chemistry presents the ecological

uncertainty associated with this option. This approach faces with several important limitations, which include limited long-term storage security, high operational and transportation costs, environmental problems such as ocean acidification (Drange et al., 2001).

1.2 Geological carbon storage

One of the most practical and effective ways to manage CO₂ is to capture and store into deep underground in geological formations such as sedimentary basins, depleted oil and gas reservoirs, deep unmineable coal seams, and deep saline aquifers (Gale, 2004). Of these, deep saline aquifers are widely considered as one of the most promising options because of their large storage capacity, wide distribution, and geological stability (Izadpanahi et al., 2024; Lackner, 2003). Previous studies have shown that saline aquifers may store up in range from 400 to 10,000 Gt, while some broader reviews suggest significantly larger total storage amount (Nazemi et al., 2025). In addition to their large capacity, saline aquifers are often located near major CO₂ capture sources, which can reduce transportation requirements and make sequestration process more economically feasible (Nazemi et al., 2025). Another important advantage is that these formations typically contain highly saline water unsuitable for drinking, which minimize conflicts with freshwater resources. In addition, deep saline aquifers are supported by favorable reservoir properties, especially adequate porosity and permeability, which enable injected CO₂ to displace formation fluids and occupy pore space effectively (Celia et al., 2015; X. Li & Yue, 2025).

The effectiveness of CO₂ storage in saline aquifers should be overlain by a low-permeability caprock, which acts as a seal and prevents injected CO₂ from migrating upward through faults or fractures (Ali et al., 2022; Haq et al., 2023). This sealing layer is essential for safe long-term storage. As depth increases, both temperature and pressure in saline aquifers rise, which strongly affects their suitability for CO₂ storage. The geothermal gradient is typically reported to range from about 25 to 35 °C/km, although it can vary across sedimentary basins (Nooraiepour et al., 2025). As a result, deep saline aquifers are generally much warmer than shallow subsurface formations. Pressure also increases with depth, and in hydraulically connected, water-saturated sedimentary rocks it often remains close to hydrostatic conditions. These depth-related changes are particularly important for CO₂ storage, because CO₂ density increases markedly at depths of approximately 500-1000 m, where temperature and pressure approach or exceed critical conditions (Celia et al., 2015). Current understanding suggest that the most suitable saline aquifers for CO₂ sequestration are typically found at depths of about 800-3000 m, where subsurface conditions are more favorable for safe storage. Within this depth range, CO₂ density can increase from approximately 200 to 900 kg/m³ before becoming relatively stable (Celia et al.,

2015). As shown in **Figure 1**, when CO₂ is injected into formations deeper than about 800 m, it enters as a supercritical state (ScCO₂), where the critical temperature and pressure are 31.1 °C and 7.38 MPa, respectively (Witkowski et al., 2014)). In this state, CO₂ has liquid-like density and gas-like compressibility, allowing it to occupy less subsurface volume while maintaining relatively low viscosity. This improves storage efficiency by reducing buoyancy effects and increasing the amount of CO₂ that can be stored in pore space (Al-Khdheawi et al., 2017b; Khanal et al., 2024)

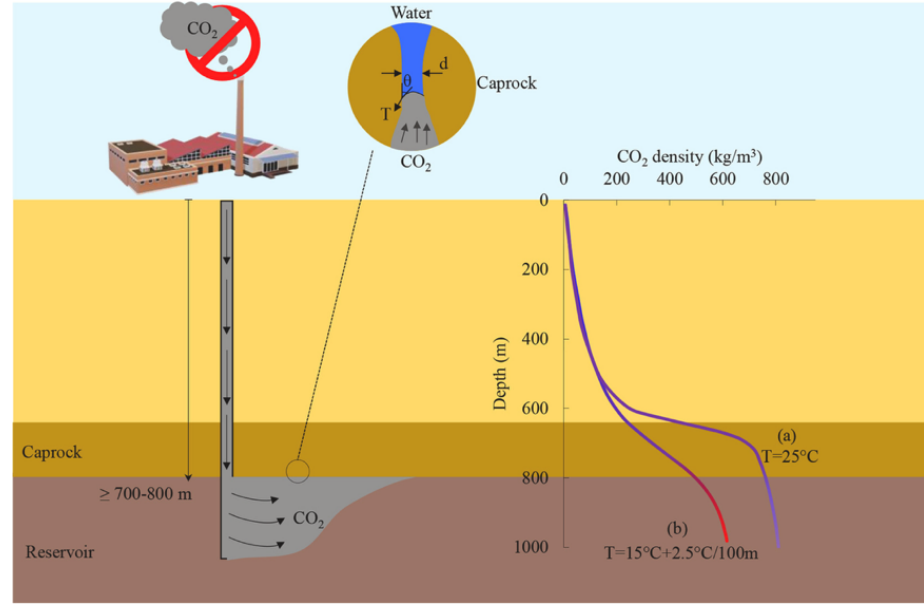


Figure 1. Schematic of the CO₂ subsurface sequestration concept, alongside CO₂ density (kg/m³) curves (Massarweh & Abushaikh, 2024).

In saline aquifers, site selection is a key factor because storage performance is strongly influenced by depth, pressure regime, and the physical and chemical characteristics of the reservoir. In caprock-sealed formations, pore pressure can be higher than hydrostatic pressure because of the stress from the overlying rock, and this effect usually increases with the depth. (Rutqvist, 2012). As a result, CO₂ injection into very deep saline aquifers may require higher injection pressures. This suggests that suitable storage formations should be identified with an optimal depth range rather than at extremely shallow or very deep conditions.

Injected supercritical CO₂ displaces brine and acts as a non-wetting phase. Under typical reservoir conditions, CO₂ and brine are not miscible, so CO₂ remains mobile and is affected by gravity. Therefore, CO₂ plume movement is determined by the combined effect of pressure gradients and gravity (Ernestos et al., 2014; C.-W. Kuo et al., 2010). As more CO₂ is injected, it spreads in the pore space, where it can be disconnected by brine imbibition, resulting in capillary-trapped CO₂ (Krevor et al., 2015a).

1.3 Trapping mechanisms

CO₂ trapping mechanisms are generally classified into physical and chemical types. When CO₂ is injected into an aquifer, it can be stored by four main mechanisms: structural, residual, solubility, and mineral trapping, as illustrated in **Figure 2** (Han, McPherson, et al., 2010; Kim et al., 2023a). Structural and residual trapping are considered physical trapping mechanisms, whereas solubility and mineral trapping are classified as chemical forms.

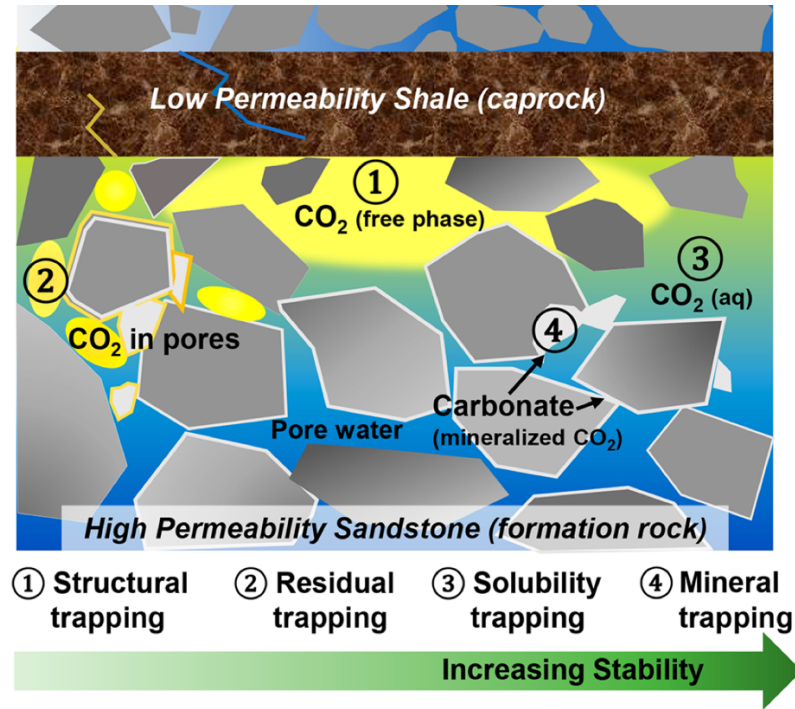


Figure 2. Main CO₂ trapping mechanisms in deep saline aquifers and their relative storage stability (Jun et al., 2017).

1.3.1 Structural Trapping

Structural trapping is the earliest storage mechanism for injected CO₂. In this type of trapping, CO₂ remains as a free phase trapped beneath an impermeable caprock. Due to its lower density than brine, it quickly rises to the top of the reservoir. This upward movement continues until it is blocked by geological barriers such as caprocks, sealing faults, anticlines, and domes (Y. J. Chen et al., 2011; He et al., 2016; C. C. Kuo et al., 2011; Szulczewski et al., 2013). Plume migration is influenced by reservoir heterogeneity, fluid viscosity, gravity, and capillary forces. As a result, analytical estimation of structurally trapped CO₂ mass is challenging. Therefore, numerical simulation is more often used to assess structural storage capacity.

The effectiveness of structural trapping depends strongly on the sealing capacity of the caprock. Although caprocks are porous, their very small pore throats and high capillary entry pressures prevent CO₂ invasion and reduce leakage risk (Nelson, 2009). The upward buoyancy pressure of the CO₂ plume, can be expressed in Equation (1):

$$P_b = \Delta\rho gh \quad (1)$$

where: $\Delta\rho$ is the density difference between brine and CO₂, g is gravitational acceleration, and h is the height of the CO₂ column.

The capillary pressure provided by the caprock, P_c , is given by Equation (2):

$$P_c = \frac{2\sigma\cos\theta}{r} \quad (2)$$

where: σ is the CO₂-brine interfacial tension, θ is the CO₂-brine-rock contact angle, and r is the average pore-throat radius of the caprock.

At the limit of secure containment, the buoyancy pressure is balanced by the capillary pressure, that is, $P_b = P_c$. By combining these two expressions, the maximum CO₂ column height can be expressed in Equation (3):

$$h = \frac{2\sigma\cos\theta}{\Delta\rho gr} \quad (3)$$

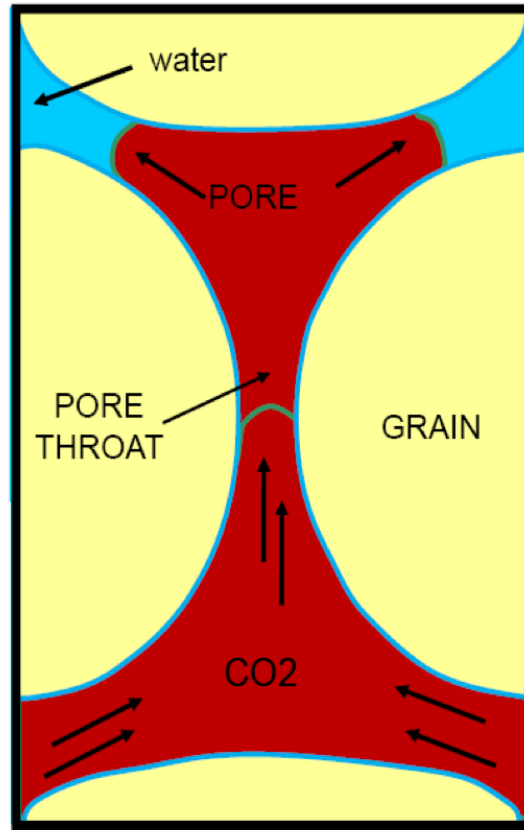
This relationship shows that the structurally trapped CO₂ column directly depends on interfacial tension, wettability, pore-throat size and the density difference between CO₂ and brine (Iglauer, 2018; Naylor et al., 2011). Higher interfacial tension, more favorable wetting conditions, and smaller pore throats increase capillary sealing efficiency. Whereas a larger buoyancy force associated with a greater density contrast which usually promote upward migration. If the buoyancy pressure exceeds the capillary resistance of the caprock, CO₂ may enter the sealing formation and, in severe cases, induce cracking or mechanical damage (Iglauer, 2018). Thus, structural trapping efficiency depends not only on structural closure, but also on caprock properties, including low permeability, strong capillary sealing capacity, and sufficient mechanical strength.

1.3.2 Residual trapping

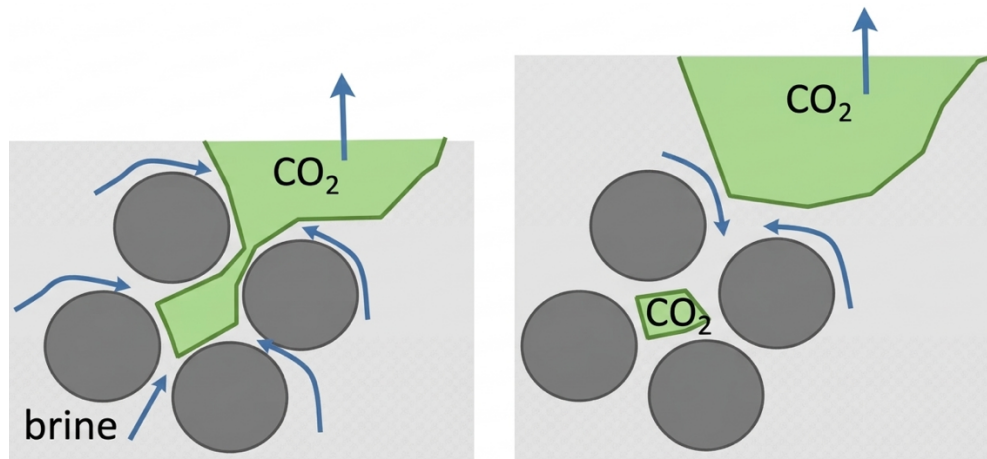
Residual, or capillary, trapping is a key CO₂ storage mechanism in which CO₂ becomes immobilized within the pore space as disconnected ganglia or droplets when buoyancy is no longer sufficient to overcome the capillary entry pressure of pore throats, as shown in **Figure 3** (a) buoyancy-driven migration, (b) snap-off effect. Unlike structural trapping, which mainly depends

on the sealing capacity of the caprock, residual trapping is governed by pore-scale interactions between CO₂ and brine within the reservoir rock (Hermanrud et al., 2009; Krevor et al., 2015b; Saadatpoor et al., 2010a). This process occurs during drainage and imbibition cycles. In drainage process, injected CO₂ enters the pore network as the non-wetting phase and preferably fills the larger pores, while brine remains in the smaller pores, pore corners, and surface roughness. During imbibition, brine re-enters the pore space and displaces part of the CO₂ and causes some of it to become disconnected from the main flow pathways and remain trapped within the rock (Li et al., 2017a).

The effectiveness of this trapping mechanism strongly depends on the pore-scale displacement mechanism. Piston-like advance generally produces a more uniform displacement and, as a result, leads to relatively limited trapping. In contrast, snap-off caused by wetting-layer flow isolates CO₂ more efficiently and substantially increases trapping, especially in water-wet (Krevor et al., 2015c; Massarweh & Abushaikha, 2024). With continued imbibition, brine continues to displace CO₂ until the relative permeability of the trapped CO₂ is reduced to zero, thereby immobilizing it within the pore network and enhancing long-term storage security (Li et al., 2017a). Residual trapping is commonly characterized by the relationship between initial CO₂ saturation and residual CO₂ saturation. It is expressed through trapping curves, by which capillary pressure and relative permeability hysteresis are used to represent this behavior in multiphase-flow and reservoir simulation models. The extent of residual trapping is influenced by a range of reservoir and fluid properties, including heterogeneity, pore-throat size ratio, connectivity, flow rate, wettability, rock type, porosity, and interfacial properties. In general, more water-wet conditions and stronger heterogeneity tend to enhance trapping, whereas higher porosity may reduce the amount of residually trapped CO₂ (Jerauld & Salter, 1990; Y. Li et al., 2017a; Raza et al., 2015a; Valvatne & Blunt, 2004). Studies have shown that heterogeneity enhances trapping, whereas high porosity tends to reduce it (Ni et al., 2019; Raza et al., 2015b). Therefore, residual trapping is not only a consequence of drainage-imbibition history, but also a function of the physical characteristics of the reservoir system that control how CO₂ and brine redistribute within the pore space.



(a)



(b)

Figure 3. Schematic illustration of pore-scale CO₂ displacement and trapping processes: (a) upward buoyancy-driven migration of CO₂ through pore throats (Caprock systems for CO₂ geological storage 2 GEOLOGICAL STORAGE, 2011); (b) snap-off leading to residual CO₂ trapping (Gershenzon et al., 2017).

1.3.3 Solubility trapping

Solubility trapping is an important CO₂ storage mechanism that begins once injected CO₂ is found in contact with formation brine. A portion of the injected gas dissolves in the aqueous phase and is transformed into dissolved and ionic species, including as CO₂ (aq), H₂CO₃, HCO₃⁻ and CO₃²⁻. It reduces the amount of CO₂ present as a separate buoyant phase and lowering its leakage potential (Balashov et al., 2013; Bert Metz et al., 2005). Equation (4) shows process of dissolution in brine, dissolved CO₂ first forms carbonic acid and then dissociates according to the reaction:



Because dissolved CO₂ no longer subject to the same buoyancy-driven migration as free-phase CO₂, solubility trapping contributes significantly to storage security, particularly over longer timescale (Bert Metz et al., 2005; Celia & Nordbotten, 2009). The extent and rate of dissolution depend strongly on reservoir conditions and transport processes. In general, CO₂ solubility increases with pressure but decreases with rising temperature and brine salinity.

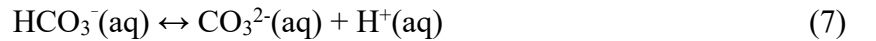
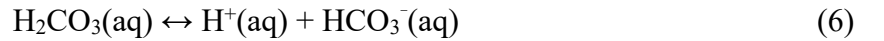
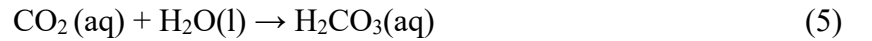
Dissolution is relatively fast during the initial stage of CO₂-brine contact, but as the brine approaches saturation, the rate gradually declines and becomes increasingly controlled by diffusion, dispersion, and convective mixing. The dissolution of CO₂ slightly increases brine density, typically by about 0.1-1% depending on temperature, pressure, and salinity. Increase of density may generate gravitational instability and initiate natural convection between CO₂-rich brine and the underlying CO₂-free brine (Y. Chen et al., 2023; Efika et al., 2016). This density-driven convection often produces finger-like flow patterns known as convective fingering, in which CO₂-enriched brine sinks while fresher brine rises. Fingering effect increases interfacial contact and preserves steep concentration gradients. As a result, CO₂ dissolves faster than it would by molecular diffusion alone, which improves trapping efficiency (D. Li et al., 2023).

Solubility trapping is affected by reservoir heterogeneity, especially variations in porosity, permeability, anisotropy, layering and inclined interfaces. Such heterogeneity can modify the onset, direction, and evolution of convective fingers and influences dissolution rates and overall storage behavior (Agartan et al., 2017; Q. Li et al., 2020; Taheri et al., 2021). Dissolved CO₂ reduces brine pH, which increases geochemical activity and later results in mineral precipitation. These reactions create favorable conditions for CO₂ mineralization. In this way, solubility trapping not only contributes to its own form, but also enhances the mineralization mechanism (Bert Metz et al., 2005).

1.3.4 Mineral trapping

Mineral trapping is related to solubility trapping, because dissolved CO₂ in brine forms carbonic acid and then dissociates into bicarbonate and carbonate ions. (Matter et al., 2016). Through this sequence, dissolved CO₂ becomes chemically available to react with reservoir minerals and dissolved cations in the brine, particularly Fe²⁺, Ca²⁺, Mg²⁺ and Fe²⁺ (Raza et al., 2022; S. Hurter et al., 2007). These reactions can lead to the precipitation of stable carbonate minerals such as calcite (CaCO₃), magnesite (MgCO₃), and siderite (FeCO₃), while silica-rich phases may remain as residual SiO₂. As a result, dissolved CO₂ is slowly becoming mineralized (F. Khan et al., 2024; Mat Razali et al., 2022). **Figure 4** illustrates two pore-scale scenarios of mineral trapping. In panel (a), CO₂ occurs as a more isolated phase surrounded by brine, which enhances dissolution, water-rock interaction, and the precipitation of carbonate minerals such as CaCO₃, MgCO₃, and FeCO₃. In panel (b), CO₂ occupies a larger and more connected pore region, preserving phase continuity and concentrating reactions near the CO₂-brine interface. This comparison shows that pore geometry and CO₂ connectivity strongly affects dissolution pathways (Sun et al., 2023).

The process begins with dissolution of CO₂ in brine, followed by acidification of the aqueous phase. After equilibrium is reached, dissolved CO₂ forms carbonic acid and dissociates according to the Equation (5-7):



Mineral trapping depends on reservoir and geochemical conditions such as temperature, pressure, pH, mineralogy, brine chemistry, porosity, permeability, and flow dynamics. Together, these factors control CO₂ dissolution, mineral reactions, and carbonate precipitation.

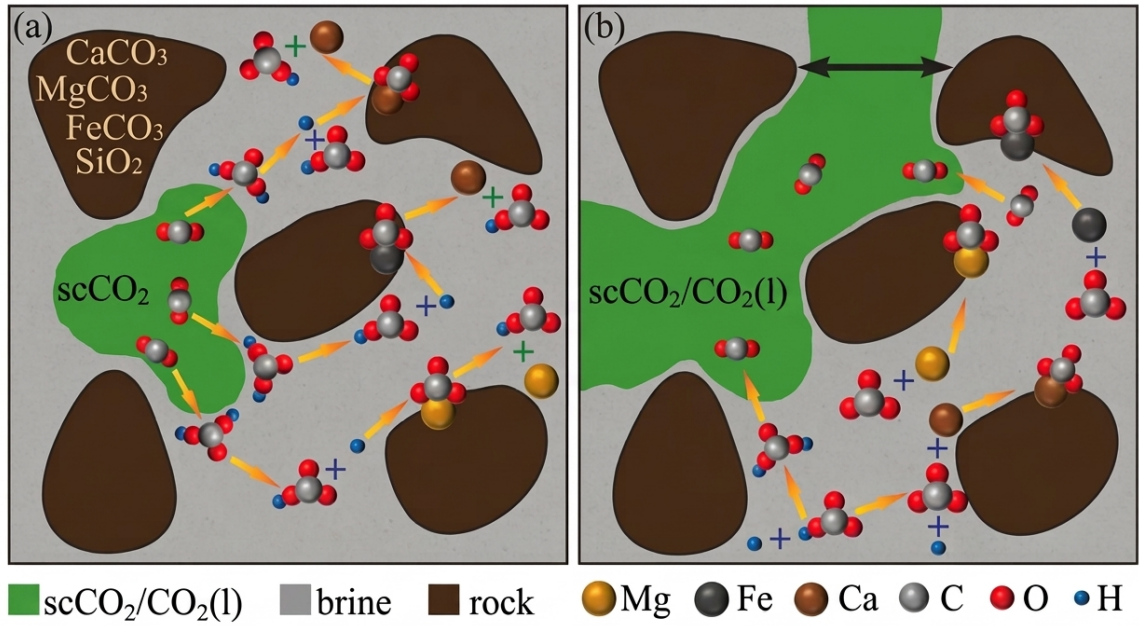


Figure 4. Pore-Scale Schematic of Mineral Trapping Mechanisms in Deep Saline Aquifers (Sun et al., 2023).

1.4 Conditions for CO₂ storage

Three main factors should be evaluated when selecting a saline aquifer for CO₂ storage. Capacity refers to the formation's ability to hold the required volume of injected CO₂. Containment describes the ability of the storage system to safely trap and retain the injected CO₂ over the long term. Injectivity reflects the formation's capability to receive CO₂ at an appropriate injection rate. Together, these factors determine whether a geological site is suitable for safe and effective carbon storage (Bachu, 2003; Koide et al., 1992; Raza et al., 2016).

1.4.1 Capacity

CO₂ storage capacity mainly depends on the available pore volume in the formation, so larger and thicker saline aquifers with higher porosity usually have greater potential for large-scale CO₂ storage (Celia et al., 2015). At a broader scale, however, the feasibility of CO₂ storage depends not only on geological conditions but also on economic factors. (Bradshaw et al., 2007) and (Bachu et al., 2007) proposed the techno-economic resource pyramid which useful for describing the geological and economic uncertainty associated with storage resources. A realistic estimate of storage capacity requires more than a simple evaluation of static pore volume. Gravity effects significantly affect the estimation of storage capacity. With low injection rates, CO₂ has more time to migrate and interact with brine. Water saturation also affects how much CO₂ can dissolve in brine. Additionally, geochemical reactions can change porosity, affecting the available pore space (Izgec et al., 2005; Obi & Blunt, 2006; Y. Wang et al., 2022).

Aquifer activity is another important factor because it controls the dynamic behavior of CO₂ in the subsurface. Reservoir properties associated with aquifer activity, such as permeability and porosity, hence influence both CO₂ migration and trapping (Bradshaw et al., 2007). Estimating CO₂ storage capacity in saline aquifers is complex challenge because the different trapping mechanisms operate over different time scales (Bachu, 2003, 2015). Structural and stratigraphic trapping can often be evaluated more directly, processes such as dissolution and mineral trapping develop gradually and are strongly time dependent. As a result, numerical modeling is often needed to obtain more reliable storage-capacity estimation for saline formations (Bachu et al., 2007).

Simulation studies indicate that mineral reactions affect pore properties differently depending on mineral composition. Quartz, illite, and kaolinite usually have only a minor influence, whereas calcite and dolomite may lead to more noticeable changes, although total pore-volume variations often remain limited even over long (Gibson-Poole et al., 2008; Khanal et al., 2024). Storage capacity is also shaped by connected pore volume, fluid properties, and CO₂ density under reservoir conditions (Gibson-Poole et al., 2008; Khanal et al., 2024). In addition, storage-capacity estimates should account both operational and geological factors, including injection rate, reservoir dip, heterogeneity, and structural closures along the migration pathway (Callas et al., 2023; De Silva & Ranjith, 2012; Gibson-Poole et al., 2008). Long-term evaluation should further account for the combined role of different trapping mechanisms, especially in saline aquifers where dissolution and mineral trapping become increasingly significant over time (Gibson-Poole et al., 2008; Kopp et al., 2009).

Besides estimating natural storage potential, studies have also explored ways to increase effective storage capacity. (Bachu, 2015) showed that pressure-management methods, especially brine extraction from distant wells, can significantly improve storage capacity. Injection at lower rates, through a larger number of wells, can improve storage performance.

1.4.2 Containment

Containment is a fundamental requirement for secure CO₂ storage (Celia et al., 2015; B. Chen et al., 2026). Storage security is heavily dependent on leakage pathways (B. Chen et al., 2026; Gholami et al., 2021). Safe operation also depends on proper drilling and completion of both injection and monitoring wells. Wells often receive special attention because they are the most direct and visible part of the storage system and are commonly associated with risks such as blowouts, groundwater contamination, and damage to the surface environment (Gholami et al., 2021). The IPCC also identified brine migration as a potential problem because of its possible impact on freshwater resources (IPCC, 2014). Studies have shown that upward brine migration

can affect groundwater systems, although the direct effect of dissolved CO₂ on groundwater chemistry is often limited, especially in high-quality drinking-water aquifers (Qafoku et al., 2017). Reservoir properties further influence containment performance. For instance, (Al-Khdheawi et al., 2018) showed that salinity strongly affects CO₂ plume migration and trapping behavior in a 3D heterogeneous reservoir. Their results demonstrate that lower salinity increases residual and solubility trapping and reduces CO₂ mobility and migration distance. Then low-salinity reservoirs may provide both higher storage capacity and improved containment security.

1.4.3 Injectivity

Injectivity is key requirement for CO₂ storage and describes the ability of a formation to accept CO₂ at the planned injection rate. Favorable injectivity generally depends on reservoir properties, especially permeability. However, it is not controlled by permeability alone, it is affected by porosity, formation thickness, reservoir size, relative permeability, pressure, temperature, brine salinity, and the properties of the injected CO₂ (Mathias et al., 2011). Temperature affects CO₂ density and viscosity and is therefore important for injectivity. As temperature increases, CO₂ viscosity decreases, which improves mobility and can enhance injectivity.

Near the wellbore, injectivity is influenced by fluid saturation, the pressure difference between the well and the reservoir, and fluid mobility, which depends on porosity and the relative permeability of CO₂ (Tawiah et al., 2020, 2021). Formation thickness and permeability also strongly affect pressure buildup during injection. Because injectivity is closely related to the permeability-thickness product, formations with higher kh values are generally more favorable for CO₂ storage (Hajiabadi et al., 2021). Aquifer geometry further influences plume spread within the reservoir. Irregular geometries may lead to nonuniform plume distribution, lower storage efficiency, and greater leakage risk. Therefore, acceptable injection rates depend on permeability, aquifer geometry, and the maximum allowable injection pressure (Celia et al., 2015; de Jonge-Anderson et al., 2024).

Several approaches have been proposed to improve injectivity in saline aquifers. These include using of horizontal wells, longer injection intervals, location of injection zones in deeper parts of the formation and hydraulic fracturing when it is economically feasible (K. Zhang et al., 2013). Previous studies have shown that hydraulic fracturing can substantially improve injectivity and increase storage capacity, particularly in narrow and low-permeability formations. Simulation results also indicate that fractured wells may provide significantly higher injectivity and storage capacity than unfractured vertical wells (Huerta et al., 2020).

Injectivity may also decline because of impurities in the injected gas and the salinity of the formation brine (Hajabadi et al., 2021). Salinity affects injectivity through its influence on CO₂ solubility, convective mixing, and gravity-driven flow behavior, and lower-salinity aquifers are generally considered more favorable for storage. Some studies have shown that impurities such as SO₂ can promote mineral reactions and salt precipitation, which may reduce permeability near the wellbore (Z. Wang et al., 2016). Likewise, salts such as MgCl₂ and CaCl₂ may cause more severe permeability damage than NaCl or KCl (Edem et al., 2020). In some cases, permeability declines markedly while porosity changes less significantly. Other studies have also reported that supercritical CO₂ can reduce permeability more than CO₂-saturated brine, especially under high-salinity conditions, because salt precipitation may block pore space and reduce the effective flow area. Overall, injectivity is a critical factor in evaluating saline aquifers for CO₂ storage because it determines whether CO₂ can be injected safely and efficiently. It reflects the combined effects of reservoir properties, fluid behavior, well design, and geochemical reactions. For this reason, injectivity must be carefully evaluated during site selection and storage development site (Yusof et al., 2021)

1.5 Parameters controlling CO₂ trapping mechanisms

CO₂ trapping in saline aquifers is governed by a combination of geological, petrophysical, and operational conditions, which are determining factors for CO₂ plume migration and retention. These factors not only control it individually, but also through complex interactions with one another. Examples of such parameters are porosity, permeability, wettability conditions, injection rate, injection duration, and others. Understanding the influence of the parameters is essential for estimating trapping mechanisms.

1.5.1 Porosity

Porosity is a key reservoir property in saline-aquifer CO₂ storage because it affects CO₂ migration, storage mechanisms, and overall storage capacity (Izadpanahi et al., 2024; X. Li & Yue, 2025). In general, higher effective porosity increases storage capacity and may improve structural, residual, and solubility trapping. However, porosity alone does not determine trapping efficiency, since pore connectivity, permeability, capillary behavior, and caprock quality also play important roles. Recent studies further shows that low-porosity formations usually demonstrate lower injectivity. However, they may improve long-term storage security by slowing plume movement and postponing breakthrough, which can reduce leakage risk (F. Chen et al., 2025).

1.5.2 Permeability

Permeability is a major control on CO₂ trapping in saline aquifers because it affects injectivity and the pressure response during injection. Higher permeability generally makes injection easier and enhances plume migration. In contrast, low-permeability aquifers usually have poorer injectivity and progressive pressure buildup near the well (Mijic et al., 2014). Permeability anisotropy is also important for plume geometry and trapping. (Han, Lee, et al., 2010a) showed that permeability heterogeneity affects CO₂ trapping mechanisms and buoyancy-driven flow. Permeability also influences solubility trapping because it controls convective mixing between CO₂ and brine. (Khatirzad & Jafarian, 2024) found that greater permeability leads to a faster onset of convection, higher fluid velocity, and greater mixing efficiency, which supports more effective dissolution of CO₂ into brine. Permeability affects structural, residual, and solubility trapping by controlling how easily CO₂ can be injected, how pressure changes and how the plume migrates, and how effectively CO₂ mixes with brine (Han, Lee, et al., 2010a). Permeability influences structural, residual, and solubility trapping by controlling how easily CO₂ can be injected, how pressure changes, and how the plume migrates and how effectively CO₂ mixes with brine.

1.5.3 Wettability

Wettability is a key pore-scale parameter because it controls spatial distribution of CO₂ and brine in pore space (Mirzaei-Paibaman & Okuno, 2024). In more water-wet rocks, CO₂ behaves more clearly as the non-wetting phase, which generally favors residual trapping after injection because brine can re-enter the pore system and disconnect the CO₂ into immobile ganglia (Khoramian et al., 2026a; H. Zhang et al., 2023). Water-wet conditions also tend to support stronger capillary sealing behavior, which is important for structural retention beneath the caprock. In contrast, when the system becomes less water-wet or more CO₂-wet, capillary immobilization may weaken and the sealing efficiency of the rock can decline, increasing the mobility of free-phase CO₂ (Iglauer et al., 2015). Wettability therefore has its strongest direct influence on residual trapping, but it also affects structural security and, through its influence on phase distribution and contact area, can indirectly modify dissolution and long-term geochemical evolution (Mirzaei-Paibaman & Okuno, 2024).

1.5.4 Capillary pressure and relative-permeability hysteresis

Capillary pressure and relative-permeability hysteresis are key controls on whether migrating CO₂ remains mobile or becomes immobilized during post-injection brine imbibition

(Krevor et al., 2015d). Capillary trapping occurs when CO₂ is left behind as disconnected ganglia surrounded by brine. This process is governed by pore-scale fluid and interfacial physics. Capillary pressure determines the entry threshold for non-wetting CO₂ into tighter rock. Therefore, it influences upward migration across low-permeability layers and the development of local capillary traps. In layered systems, capillary entry pressure can retain CO₂ beneath mudstone layers and control upward spill (Boulin et al., 2013). Relative-permeability hysteresis is especially important for residual trapping because it captures the difference between drainage during injection and imbibition after injection (Taku Ide et al., 2007). Numerical studies show that ignoring relative-permeability hysteresis leads to underestimation of snap-off trapping, while also biasing predictions of dissolution trapping. For this reason, capillary pressure and hysteresis are widely regarded as central controls on secure CO₂ immobilization in saline aquifers (Ershadnia et al., 2021; Juanes et al., 2006)

1.5.5 Pressure, temperature, and salinity

Pressure, temperature, and salinity primarily control of CO₂ phase behavior, density, interfacial properties, and brine solubility, so they are especially important for solubility trapping (Duan & Sun, 2003). Higher pressure generally increases CO₂ density and increases its solubility in brine, which tends to reduce plume volume for a given injected mass and strengthen dissolution trapping (B. Liu et al., 2021). Higher temperature usually has the opposite effect on solubility and can reduce the amount of CO₂ that dissolves into the aqueous phase (B. Liu et al., 2021; Y. Liu et al., 2011). Higher salinity also decreases CO₂ solubility, meaning that more saline brines are generally less favorable for dissolution and, by extension, for the mineral trapping that depends on dissolved CO₂ as an essential input (Kim et al., 2023b; Waldmann & Rütters, 2016). These thermodynamic variables also influence interfacial tension and contact angle behavior, so their effect extends beyond dissolution alone and can modify capillary and wettability-controlled trapping as well.

1.5.6 Caprock integrity

Caprock integrity is a key factor in both structural and stratigraphic trapping. It controls how long buoyant CO₂ remains trapped in the formation and gives slower trapping mechanisms time to act (Ajayi et al., 2019). Safe CO₂ storage depends on a caprock with low permeability, high capillary entry pressure, mechanical stability, and no transmissive faults or fractures. If the caprock acts as an effective seal, free-phase CO₂ can remain under it, while residual, dissolution,

and mineral trapping gradually improve storage security (Ajayi et al., 2019; Song et al., 2023). However, if the caprock is weakened by pressure buildup, fractures, geochemical reactions, or leakage through wellbores, mobile CO₂ may escape before these slower mechanisms become effective. Therefore, caprock integrity is essential not only for trapping, but also for long-term storage security.

1.5.7 Heterogeneity as a key control on CO₂ storage

From all the factors controlling CO₂ storage in saline aquifers, reservoir heterogeneity is a key control, which strongly influences plume migration, trapping efficiency, storage capacity, and containment security (Hovorka et al., 2004; Izadpanahi et al., 2024). In practice, geological formations are rarely homogeneous and commonly heterogeneous in different scales in the range between pore-scale and larger stratigraphic layering, faults and channel systems (C. W. Kuo & Benson, 2015; Ott et al., 2015).

Heterogeneity can occur in different forms such as faults, depositional variability, compartmentalization, channelized systems, and stratigraphic layering. In conventional petroleum reservoirs, it is often seen as unfavorable because it reduces sweep efficiency and leaves more hydrocarbons unrecovered. Natural heterogeneity in CO₂ storage may be beneficial, especially when low-permeability zones act as barriers that limit plume migration and reduce potential movement toward leakage (M. A. Flett et al., 2005; Saadatpoor et al., 2010b). In saline aquifers, heterogeneity also changes the balance between viscous and gravity forces by increasing effective permeability anisotropy (Shao et al., 2022). Its effect on plume evolution can be understood by considering how flow changes from the near-well region to the far field, as illustrated in **Figure 5**. Because heterogeneity is closely related to residual trapping and flow hysteresis and neglecting these coupled effects may result simulation errors (Y. Li et al., 2017b)

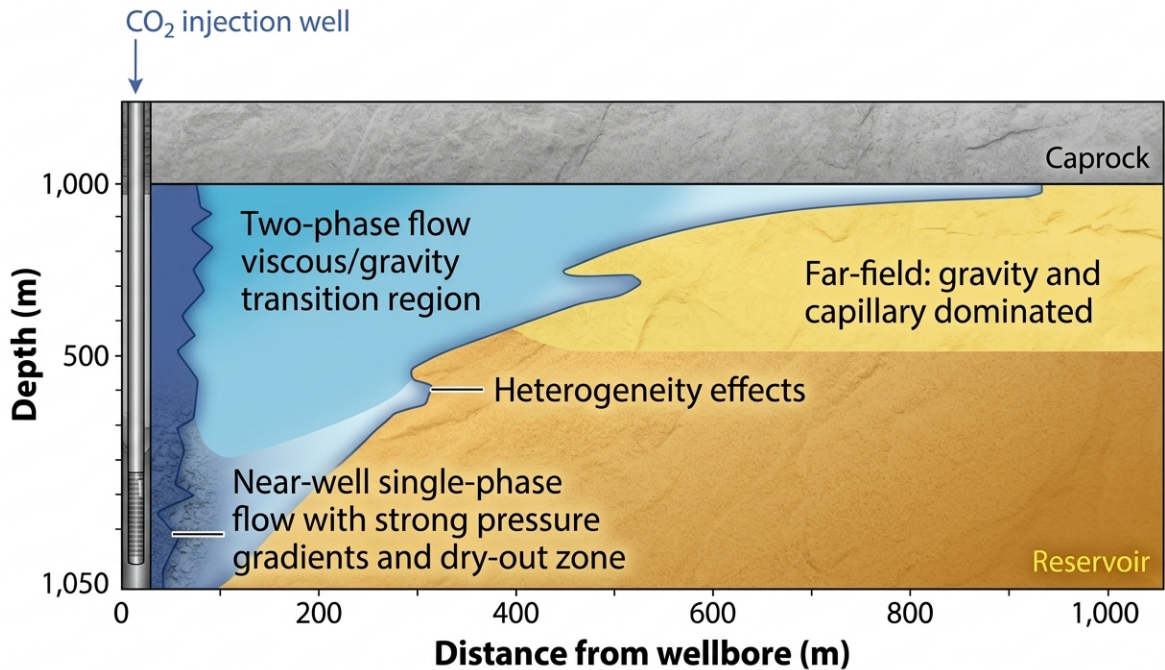


Figure 5 . Conceptual CO₂ plume evolution in a heterogeneous saline aquifer (Ringrose et al., 2021)

Permeability and porosity heterogeneity are major controls on CO₂ plume evolution. In layered reservoirs, vertical permeability is typically lower than horizontal permeability because of compaction and overburden stress. Under these conditions, low-permeability layers can act as baffles, restricting upward migration and reducing communication between layers, although fractures may locally provide vertical flow pathways. Ignoring fine-scale heterogeneity can lead overestimation of plume migration. Because homogeneous models do not capture local barriers, preferential flow paths, and capillary effects (B. Li & Benson, 2015; Onoja & Shariatipour, 2019).

The effect of heterogeneity also depends on its orientation. Layered heterogeneity generally improves storage security by restricting buoyancy-driven upward migration, reducing plume footprint, keeping more CO₂ deeper in the reservoir, and enhancing residual trapping and dissolution (Cavanagh & Nazarian, 2014; Strandli & Benson, 2013). Similar results were reported by (Singh & Bromhal, 2019), who found that thin baffles in heterogeneous formations reduce the areal plume extent. In contrast, horizontal heterogeneity promotes preferential flow through more permeable zones, producing fingering and a larger, more asymmetric plume (Frailey & Leetaru, 2009). In other words, some layers or zones are more permeable, more porous, or have different wettability or mineralogy than others; thus, they transmit and trap CO₂ differently. The importance of heterogeneity can be understood in two key ways: it determines where CO₂ will be stored and how it will be trapped over time.

Different parameters may exert either favorable or unfavorable effects on CO₂ trapping, as summarized in Table 1. The table further indicates that the influence of several parameters is not always consistently reported across studies, implying that certain variables may either enhance or reduce individual trapping mechanisms depending on reservoir conditions, fluid properties, and injection strategy.

In summary, although many factors effect on CO₂ storage in deep saline aquifers, reservoir heterogeneity is one of the most important because it controls plume migration, vertical communication, trapping efficiency and containment security. The preceding discussion shows that heterogeneity does not act in a simple or uniform way, its impact depends on the spatial distribution and orientation of reservoir properties, especially permeability. For this reason, understanding heterogeneity is essential for predicting storage performance and selecting suitable formations for long-term CO₂ sequestration. This importance motivates the next chapter, which reviews previous studies on heterogeneity and highlights the remaining gap concerning the effect of systematic vertical permeability trends on CO₂ trapping behavior.

Table 1. Integrated summary of the main controls, limiting factors, enhancement factors, risks, reversibility, and useful descriptors for CO₂ trapping mechanisms in saline aquifers.

Trapping class	Trapping mechanism	Key controls / parameters	What generally reduces it?	What generally enhances it?	Main risks / limitations	Reversibility	Useful quantitative descriptors	References
Physical	Structural / stratigraphic trapping	Caprock integrity, capillary entry pressure, seal continuity, trap geometry, porosity/permeability, injection pressure and rate, buoyancy–viscous balance	Weak or fractured caprock; transmissive faults/fractures/wells; excessive pressure buildup; poor seal continuity; low capillary entry pressure	Strong, continuous caprock; high capillary entry pressure; favorable structural closure; controlled injection pressure; pressure management; secondary seals	Leakage if caprock is weak or fractured; pressure buildup; old wells; fault reactivation; free-phase CO ₂ remains mobile	Highest reversibility because CO ₂ remains as a mobile separate phase if containment is lost	CO ₂ plume height; plume area; CO ₂ saturation; seal entry pressure; bottom-hole pressure; storage efficiency	(Ajayi et al., 2019; Celia et al., 2015; Izadpanahi et al., 2024)
Physical	Residual / capillary trapping	Wettability, capillary pressure, relative-permeability hysteresis, irreducible water saturation, residual CO ₂ saturation, pore size, porosity, permeability, heterogeneity	Intermediate- or CO ₂ -wet conditions; formation drying; large grain size; high irreducible water saturation; some impurities; weak capillary trapping	Water-wet conditions; higher porosity/permeability; suitable capillary behavior; small- to medium-scale heterogeneity; higher flow rate in some settings; horizontal or multiple wells	Sensitive to pore-scale properties and difficult to upscale; strongly dependent on wettability and hysteresis characterization	Largely irreversible at pore scale once CO ₂ is immobilized as disconnected ganglia	Residual CO ₂ saturation; irreducible water saturation; capillary pressure; relative-permeability hysteresis; contact angle; IFT	(Izadpanahi et al., 2024; Y. Li et al., 2017b)

Trapping class	Trapping mechanism	Key controls / parameters	What generally reduces it?	What generally enhances it?	Main risks / limitations	Reversibility	Useful quantitative descriptors	References
Chemical	Solubility trapping	Pressure, temperature, salinity, contact area/time, vertical permeability, density-driven convection, diffusion coefficient, heterogeneity	Higher temperature; higher salinity; weak mixing or limited contact area; low vertical permeability; some non-condensable impurities; weak convection	Higher pressure; lower temperature; lower salinity; greater contact area/time; stronger convection; higher vertical permeability; CO ₂ –brine co-contact strategies	Often slower than expected if convection is weak; strongly reservoir-specific; may be limited by low interface area and heterogeneity effects	Low to moderate reversibility; dissolved CO ₂ is less mobile than free-phase CO ₂ , but remains part of the aqueous system	CO ₂ solubility; diffusion coefficient; dissolved fraction; density increase of brine; Rayleigh number	(Bachu, 2015; Celia et al., 2015; Mim et al., 2023)
Chemical	Mineral trapping	Mineralogy, pH, groundwater chemistry, reactive cations (Ca ²⁺ , Mg ²⁺ , Fe ²⁺), pressure, temperature, reaction time, nucleation sites	Unreactive mineralogy; low pressure; low temperature; low pH; short residence time	Reactive mineral assemblage; suitable pH; nucleation sites; reactive Ca-, Mg-, or Fe-bearing ions/minerals; higher pressure; long residence time	Too slow to contribute much on short project timescales in many sandstone saline aquifers; may alter pore structure and injectivity	Lowest reversibility / most permanent because CO ₂ is fixed as solid carbonate minerals	Mineral reaction rate; carbonate precipitation extent; porosity/permeability change; dissolved-ion concentration	(Ajayi et al., 2019; Celia et al., 2015; Mim et al., 2023)

2 LITERATURE REVIEW

2.1 Review on Previous Studies

A wide range of studies has investigated the influence of reservoir heterogeneity on CO₂ trapping in saline aquifers. Collectively, these studies show that heterogeneity strongly affects plume evolution, storage capacity, and long-term containment by controlling the distribution of flow pathways, local capillary barriers, and vertical communication between layers. Depending on its type and spatial arrangement, heterogeneity can enhance trapping through plume spreading and increased dissolution.

Hovorka et al. (2004) carried out a site-scale case study for the Texas Gulf Coast to evaluate how geological heterogeneity affects CO₂ storage in brine formations. They used the TOUGH2 simulator to assess different geological conditions. This study compared homogeneous sandstone, a heterogeneous layered reservoir, and a compartmentalized setting; they also included dip and faults. Their results showed that heterogeneity with multiple low-permeability layers can improve CO₂ storage performance by distributing flow paths, increasing rock-CO₂ contact, and limiting the buoyancy effect. However, although such a setting can increase storage performance, the potential for leakage also increased.

Ghanbari et al. (2006) used reservoir simulation to examine how aquifer properties and geological heterogeneity affect long-term CO₂ storage in saline aquifers. Their model considered 30 years of CO₂ injection followed by 470 years of shut-in, allowing them to assess both short-term plume evolution and long-term trapping behaviour. They showed that solubility trapping was the dominant storage mechanism over hundreds of years, largely enhanced by convective mixing of CO₂-rich brine. Their sensitivity analysis further indicated that higher vertical-to-horizontal permeability ratio promoted dissolution trapping, whereas higher salinity reduced CO₂ solubility and weakened convective mixing. Among the heterogeneities examined, low-level random permeability variations had little overall effect, but shale layers strongly modified plume migration by inhibiting vertical movement and promoting lateral spreading beneath baffles. Faults mainly influenced plume distribution through the relative location of the injection well.

M. Flett et al. (2007) constructed full-scale 3D simulation models of heterogeneous saline formations to investigate how varying degrees of heterogeneity affect CO₂ containment and trapping over long timescales. Their study simulated 50 years of CO₂ injection followed by 950 years of post-injection migration and showed that increasing shale content progressively restricted vertical plume migration and promoted lateral spreading. They concluded that heterogeneity can

improve containment by reducing the amount of CO₂ accumulating beneath the top seal, although it also delays residual trapping because plume migration becomes more tortuous.

Lengler et al. (2010) applied stochastic Monte Carlo simulations to the Ketzin (a European onshore injection site of west Berlin, Germany) CO₂ storage site to investigate how small-scale spatial heterogeneity in permeability affects early plume migration and injectivity. Focusing on the first 21 days of injection, they showed that increasing heterogeneity reduced the sharpness of the CO₂ front, increased the reservoir volume affected, and led to a higher fraction of dissolved CO₂. They also found that greater anisotropy promoted fingering and earlier arrival probabilities, whereas injectivity generally decreased with increasing heterogeneity.

Han, Lee, et al. (2010b) systematically examined how permeability heterogeneity affects CO₂ trapping and plume migration using two-dimensional compositional simulations. A total of 27 scenarios were analyzed, including homogeneous systems, anisotropic cases, random log-normal permeability distributions, low-k lenses and correlated fields with different permeability variances and correlation lengths. The results indicated that higher mean permeability and lower variance increased residual trapping but also accelerated upward plume migration. Strong horizontal correlation lengths and low-permeability barriers promoted lateral spreading and greater immobilization. Solubility trapping was enhanced from better plume dispersion and structural trapping remained sensitive to permeability trends.

Rasheed et al. (2020) used numerical simulation with the CO2STORE module of Eclipse300 to evaluate how permeability heterogeneity affects CO₂ storage performance in saline aquifers. Heterogeneity was quantified using the Lorenz coefficient and classified into low, medium, and high levels, while CO₂ injection was simulated over 30 years. The results showed that increasing heterogeneity generally reduced storage capacity, decreased residual trapping, and shortened injection-rate stability, while dissolution trapping remained the dominant mechanism and free gas fractions stayed low. They concluded that aquifers with low to medium heterogeneity and good porosity (>20%) are more suitable for CO₂ storage.

Mahyapour et al. (2022) used randomly generated 2D and 3D permeability fields to investigate how permeability distribution variations affect dissolution trapping. Results showed that increasing the permeability standard deviation (i.e., making the permeability field more heterogeneous) leads to stronger and more unstable convective fingering, higher dissolution fluxes, and larger variability between realizations. The location and connectivity of high-permeability zones were found to control the development and merging of convective fingers, which influencing CO₂ dissolution patterns. Overall, fields with stronger permeability contrasts

enhanced mixing and increased dissolved CO₂ mass. This indicates that stronger permeability variations enhanced mixing and increased dissolution trapping in both 2D and 3D systems.

Q. Zhang et al. (2024) focused on solubility trapping and showed how permeability heterogeneity (vertical rhythms, abrupt k contrasts, and bedding layers) controls convective CO₂ dissolution. Structural and residual trapping were not modeled directly, and mineral trapping was referred to only indirectly as a potential long-term result of dissolution. Similarly, Fang et al. (2023) also focused on trapping solubility. The SGSIM and MRST simulations showed that heterogeneity variance is the main controlling factor under low-to-medium gravity index conditions. Under these conditions, stronger heterogeneity leads to higher dissolution efficiency. At a high gravity index, buoyancy forces dominated and the heterogeneity influence diminished.

Y. Wang et al. (2025) used high-resolution offshore saline aquifer simulations and found that strong horizontal layering enhanced lateral plume spreading and reduced leakage risk, whereas the vertical continuity of high-k channels accelerated upward migration and local capillary entrapment. It was found that the trapping behavior depended on injection rate. Residual trapping was dominant at low injection rates, whereas heterogeneity-induced structural and capillary trapping became more significant at higher rates, while solubility trapping remained limited.

Jing et al. (2025) examined layered aquifers in the Ordos Basin and showed that a reverse permeability rhythm enhanced structural trapping by concentrating CO₂ beneath the caprock while promoting higher dissolved fractions. In contrast, a positive rhythm improved injectivity but confined the plume deeper, limiting dissolution. Rezk & Ibrahim, (2025) went further with a 1000-year simulation, showing that heterogeneity initially favored structural trapping. However, over time, residual trapping declined while solubility trapping grew to dominate (~70% of the stored CO₂), highlighting dynamic shifts across mechanisms.

In related study, Z. Wang et al. (2024) analyzed the effect of permeability heterogeneity on CO₂ migration, injectivity, and trapping in deep saline aquifers. It used stochastic permeability fields with different correlation lengths and Dykstra-Parsons coefficients. Results showed that injectivity was highest at large horizontal and vertical correlation lengths, while storage efficiency was high at dimensionless correlation lengths of 0.1-0.2. In this range, frequent changes between high- and low-permeability zones increased residual trapping and slowed plume migration. This suggests that both correlation results and breakthrough time should be evaluated together when designing safer and more efficient CO₂ storage systems.

Finally, L. Zhang et al. (2026) investigated the layered heterogeneity in saline aquifers composed of alternating sandstone (high permeability) and mudstone (low permeability) layers. The analysis showed that permeability contrast between layers strongly influences CO₂ plume

geometry. Instead of rising freely, the gas accumulates beneath mudstone layers, while low-permeability barriers redistribute CO₂ laterally across multiple sandstone intervals. This slows the vertical migration, increases the contact time between the brine and CO₂, and ultimately leads to higher dissolved CO₂ fractions. Their work shows that permeability heterogeneity increases pressure, reshapes the plume and controls dissolution, confirming that permeability rather than lithology alone, plays a major role in controlling CO₂ behavior in layered systems.

Table 2 summarizes the main findings of the literature reviewed in this study. Collectively, these studies indicate that heterogeneity is a major control on CO₂ storage in saline aquifers because it affects plume geometry, injectivity, and trapping efficiency. Nevertheless, the specific effect of systematic vertical permeability trends remains insufficiently studied. In particular, upward-increase and upward-decrease permeability trends have not been directly compared with respect to their influence on plume migration, trapping balance, and pressure response. Therefore, this thesis addresses this research gap.

Table 2. Summary of literature on the effects of heterogeneity on CO₂ storage in saline aquifers.

Study	Heterogeneity type	Method	Main finding on CO ₂ behavior	Main trapping implication
Hovorka et al. (2004)	Geological heterogeneity: homogeneous, layered, faults, compartments	TOUGH2 simulation	Stratigraphic heterogeneity dispersed flow, increased rock contact, and reduced upward migration; structural heterogeneity could raise leakage risk	Enhanced dissolution and storage effectiveness in layered systems
Ghanbari et al. (2006)	Random heterogeneity, shale layers, faults, kv/kh sensitivity	Reservoir simulation	Shale layers inhibited vertical migration and promoted lateral spreading; higher kv/kh promoted dissolution	Solubility trapping dominated long-term storage
M. Flett et al. (2007)	Varying shale content / layered heterogeneity	Full-scale 3D simulation	More shale reduced vertical migration and increased lateral migration	Improved containment, but delayed residual trapping
Lengler et al. (2010)	Small-scale stochastic permeability heterogeneity and anisotropy	Monte Carlo simulations	Increasing heterogeneity broadened plume footprint and increased dissolution; anisotropy promoted fingering	More dissolved CO ₂ , lower injectivity
Han, Lee, et al. (2010b)	Variance, correlation length, low-k lenses, anisotropy	2D compositional simulations	Higher mean k and lower variance enhanced residual trapping but accelerated upward migration; barriers increased lateral spreading	Residual and solubility trapping both affected by architecture

Study	Heterogeneity type	Method	Main finding on CO ₂ behavior	Main trapping implication
Rasheed et al. (2020)	Low, medium, high heterogeneity quantified by Lorenz coefficient	CO2STORE/ECLIPSE300	Greater heterogeneity lowered storage capacity and residual trapping; dissolution remained dominant	Low-medium heterogeneity with good porosity was more suitable
Mahyapour et al. (2022)	Random 2D/3D permeability distributions	Numerical simulations	Larger permeability variance strengthened convective fingering and mixing	Enhanced dissolution trapping
Fang et al. (2023)	Variance-controlled heterogeneity under different gravity index	SGSIM + MRST	Stronger heterogeneity improved dissolution efficiency at low-medium gravity index	Solubility trapping increased
Q. Zhang et al. (2024)	Vertical rhythms, abrupt contrasts, bedding	Numerical simulation	Heterogeneity controlled convective dissolution behavior	Solubility trapping emphasized
Z. Wang et al. (2024)	Correlation lengths + Dykstra-Parsons coefficient	Stochastic simulations	Injectivity highest at large correlation lengths; storage efficiency highest when high/low-k zones alternated frequently	Residual trapping enhanced under certain correlation structures
Y. Wang et al. (2025)	Horizontal layering vs vertical continuity of high-k channels	High-resolution offshore simulations	Horizontal layering promoted lateral spreading; vertically continuous high-k channels accelerated upward migration	Residual trapping dominated at low rates; structural/capillary trapping increased at high rates
Jing et al. (2025)	Positive vs reverse permeability rhythm in layered aquifers	Reservoir simulation	Reverse rhythm enhanced structural trapping and dissolved fractions; positive rhythm improved injectivity	Vertical rhythm strongly affected trapping style

Study	Heterogeneity type	Method	Main finding on CO ₂ behavior	Main trapping implication
Rezk & Ibrahim, (2025)	Heterogeneous layered system over long time		Heterogeneity initially favored structural trapping; over time solubility became dominant	Dynamic shift from residual/structural toward solubility trapping
L. Zhang et al. (2026)	Alternating sandstone-mudstone thin layers	3D TOUGH2/ECO2N	Low-k barriers slowed vertical migration and increased brine-CO ₂ contact time	Higher dissolved CO ₂ fractions, but higher pressure

2.2 Objectives of the Thesis

This thesis aims to investigate how vertical permeability heterogeneity influences CO₂ migration and trapping behavior in deep saline aquifers, with the help of numerical reservoir simulation. The study focuses on the role of systematic permeability trend. These trends can control the relative contributions of residual and solubility trapping during injection and long-term post-injection periods. Special attention is given to comparing upward-decrease and upward-increase permeability trends under different levels of heterogeneity.

The specific objectives of this thesis are:

1. To develop a numerical model of CO₂ injection in a deep saline aquifer using the CMG-GEM compositional simulator.
2. To construct a series of vertically heterogeneous reservoir models with systematic upward-decrease and upward-increase permeability trends with the same mean permeability.
3. To quantify the degree of heterogeneity in each model using the Dykstra-Parsons coefficient.
4. To investigate how vertical permeability trends affect CO₂ plume migration during the injection period and the post-injection monitoring period.
5. To evaluate the influence of heterogeneity level on the balance between residual trapping and solubility trapping.
6. To classify rock quality within the model using the Rock Quality Index and incorporate representative rock-type categories into the simulation framework.
7. To provide insights into how vertical permeability trend may influence the effectiveness of saline aquifers for long-term CO₂ storage.

2.3 Scope of Work

This study is limited to a simplified two-dimensional cross-sectional model of a deep saline aquifer developed in CMG-GEM. The model extends from 1200 to 1300 m depth and consists of 20 vertical layers with constant porosity, fixed salinity, temperature, and initial pressure conditions. A single vertical injection well is perforated across all layers, and supercritical CO₂ is injected for 5 years, followed by 195 years of post-injection monitoring to evaluate long-term storage behavior. The scope of the work includes the generation of multiple monotonic vertical permeability distributions representing different degrees of heterogeneity, all defined with the

same mean permeability and the same vertical anisotropy ratio. Both upward-decreasing and upward-increasing permeability trends are considered in order to isolate the effect of vertical ordering. The heterogeneity of each case is quantified using the Dykstra-Parsons coefficient. In addition, the study includes the calculation of the Rock Quality Index and the assignment of rock-quality categories to reflect variations in reservoir quality. The analysis focuses on how permeability heterogeneity influences CO₂ migration, plume distribution, and the relative importance of residual and solubility trapping. This work does not include geochemical reactions, geomechanical deformation, caprock failure analysis, fault leakage, or field-scale history matching. The reservoir geometry is intentionally simplified so that the effect of vertical permeability heterogeneity can be examined systematically and independently from other sources of complexity. As a result, the findings are intended to improve the understanding of trapping behavior under controlled heterogeneity conditions and to provide a basis for future, more realistic field-scale studies.

3 METHODOLOGY

To address the existing gap in understanding of how vertical permeability architecture influences the relative contributions of residual and solubility trapping, a static reservoir model of CO₂ injection into a deep saline aquifer was developed using the CMG-GEM compositional simulator. Vertical permeability heterogeneity was systematically incorporated while keeping the average permeability constant, allowing the effect of permeability distribution to be examined independently. The heterogeneity level in each case was quantified using the Dykstra-Parsons coefficient. Multiple scenarios were then generated and grouped into low-, medium-, and high-heterogeneity cases. This framework allowed direct comparison of plume evolution and trapping behavior across different heterogeneity levels and helped identify the conditions under which residual or solubility trapping becomes more dominant.

3.1 Static model characteristics

The geological model represents a simplified two-dimensional (2D) cross-section of a deep saline aquifer extending from 1200 to 1300 m depth. Which lies within the typical 800-3000 m range for CO₂ storage, where CO₂ remains in a dense supercritical state and storage efficiency is higher (Birkholzer et al., 2009).

The formation was divided into 20 layers, each with a uniform thickness of 5 m, which makes up a total vertical extent of 100 m. The grid resolution consists of 125 cells in the i-direction, 1 cell in the j-direction, and 20 cells in the k-direction. This approach allows a detailed representation of vertical heterogeneity and to maintain lateral homogeneity. The reservoir conditions were set as follows: temperature = 50 °C, pressure = 1710 psi, salinity = 50,000 ppm NaCl, and pH = 7.0. The porosity was held constant at 0.18 across the model domain. Permeability heterogeneity discussed in the next section was varied systematically to investigate its influence on CO₂ migration and trapping. A single vertical injection well was perforated in the last bottom layer to inject supercritical CO₂ from left to right. The bottom-hole pressure constraint was fixed at 6500 psi, which corresponds to a safe operation below the fracture limit. The CO₂ injection rate was set to 10,000 m³ day⁻¹ for a period of 5 years, followed by 195 years of post-injection monitoring. No volume modifier was applied to this base configuration. The model configuration and boundary conditions were selected to represent typical saline aquifers suitable for CO₂ storage. Porosity is 0.1-0.3, horizontal permeabilities on the order of 10-1000 mD, and formation thicknesses of 20-100 m (Chadwick, 2008; Metz, 2005). Following best-practice CO₂ storage modeling, sufficiently large model extents were used to minimize boundary effects so that flow

and trapping behavior are primarily governed by reservoir heterogeneity and wettability rather than artificial boundary constraints (Metz, 2005).

3.2 Model heterogeneity

The permeability was defined as lateral anisotropic, with $k_x = k_y$ and a vertical reduction of $k_z = 0.1 k_x$. Eleven monotonic permeability distribution scenarios were generated to examine the role of vertical heterogeneity at a constant bulk capacity, each maintaining a modelwide mean permeability of 110 mD. The reservoir model consists of 20 layers, with Layer 20 (the injection layer) fixed at 250 mD in all cases to represent the high-permeability injection interval.

Permeability was assigned to the remaining 19 layers following the ranges listed in Table 3. For the by upward-decreasing (UD) cases, permeability is higher at the base and lower toward the top, whereas for the upward-increasing (UI) cases, the arrangement is reversed, with lower permeability at the base and higher permeability toward the top. **Figure 6** shows the corresponding permeability histograms for the base case and Cases 1-10, illustrating the progressive widening of permeability distribution as heterogeneity increases. The degree of vertical heterogeneity was quantified using the Dykstra-Parsons coefficient, defined using Equation (8). **Figure 7** illustrates an example of a vertically heterogeneous upward-decreasing permeability configuration across 20 vertical layers. The shown realization corresponds to $V_{DP} = 0.1124$, with permeability values ranging from approximately 250 mD at the bottom to 87 mD at the top. Similar layered permeability distributions were constructed for all investigated V_{DP} values to represent different degrees of vertical heterogeneity in Equation.

$$V_{DP} = \frac{k_{50} - k_{84.1}}{k_{50}} \quad (8)$$

where: k_{50} and $k_{84.1}$ denote the 50th and 84.1st percentile permeabilities, respectively.

The coefficient ranges from 0, representing a perfectly homogeneous reservoir, to 0.9262, which corresponds to a highly heterogeneous system. It therefore provides a quantitative measure of stratification contrast within the permeability field. Based on this definition, the model set was designed to cover the full heterogeneity range, from nearly uniform to strongly stratified formations, while keeping the mean permeability constant at 110 mD. The base case represents a moderate heterogeneity level with $V_{DP} = 0.5083$, whereas Cases 1-10 progressively increase from 0.1124 to 0.9262, as summarized in Table 3.

Table 3. Permeability distributions and Dykstra-Parsons' heterogeneity coefficients for the 20-layer aquifer model were calculated.

ID	UD/UI $k_{\min}-k_{\max}$ (mD)*	V_{DP}
Base	20 - 200/ 200 - 20	0.5083
1	87 - 137/137 - 87	0.1124
2	68 - 168/ 168 - 68	0.2109
3	51 - 208/ 208 - 51	0.3080
4	36 - 261/ 261 - 36	0.4036
5	24 - 330/ 330 - 24	0.4974
6	14 - 423/ 423 - 14	0.5892
7	7 - 548/ 548 - 7	0.6786
8	2 - 320/ 320 - 2	0.7652
9	0.7 - 962/ 962 - 0.7	0.8483
10	0.06 - 1313/ 1313 - 0.06	0.9262

*Note: All cases share a mean permeability of 110 mD and a vertical anisotropy of $k_z = 0.1 k_x$. UD, upward-decrease trend; UI, upward-increase trend.

For sensitivity to vertical ordering, each of the above cases was also replicated as an upward-increasing (UI) profile, where permeability is low at the base and high at the top, while the original configurations represent upward-decreasing (UD) profiles (high at the base and low at the top). Each UI counterpart retains the same $(k_{\min}, k_{\max}, \bar{k})$ as its UD counterpart, which ensures identical statistical properties but inverse stratification.

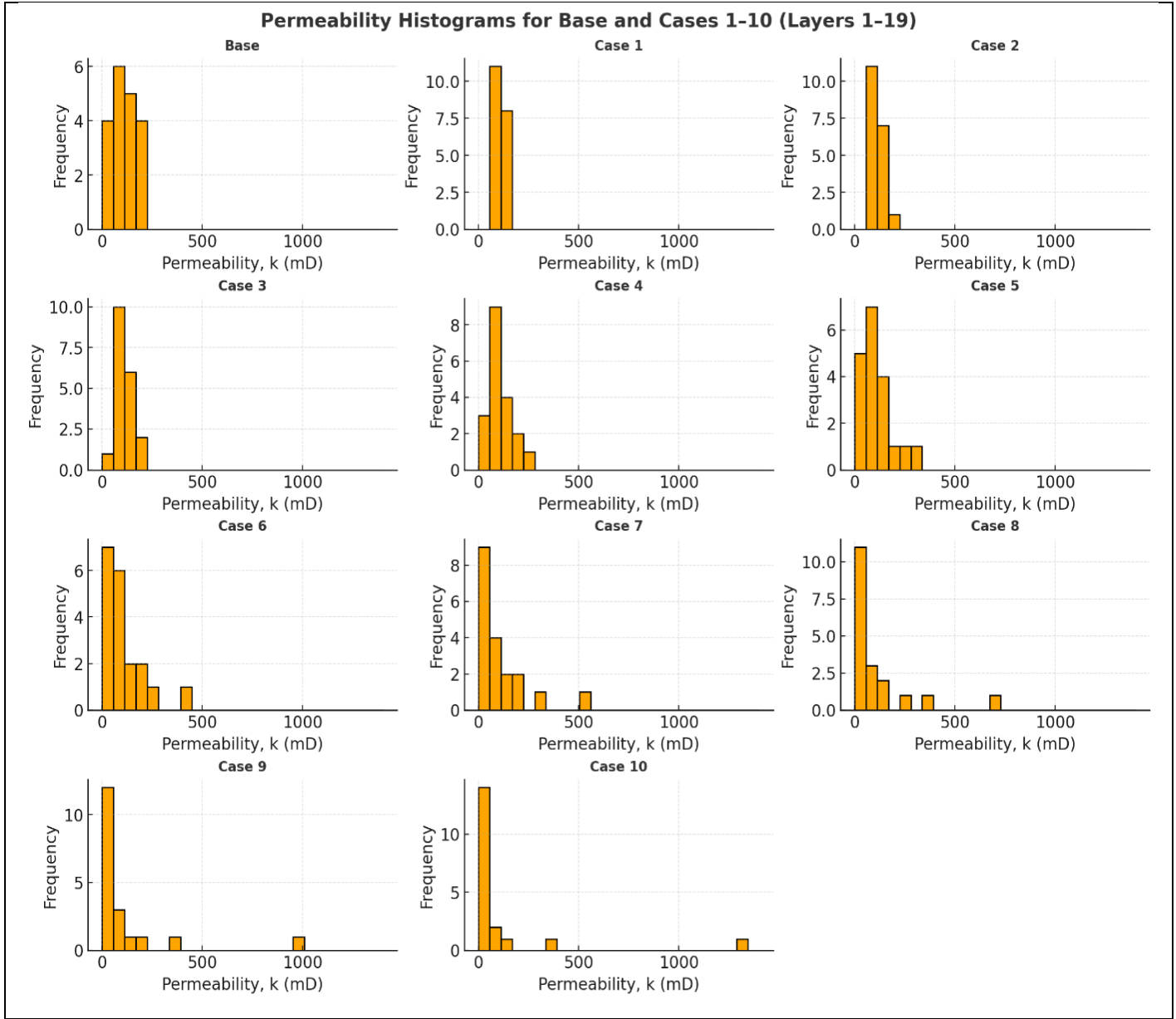


Figure 6. Permeability histograms for the base case and Cases 1-10 (Layers 1-19). The spread of permeability widens systematically in different cases, which reflects the controlled increase in heterogeneity ($V_{DP} = 0.1124 - 0.9262$).

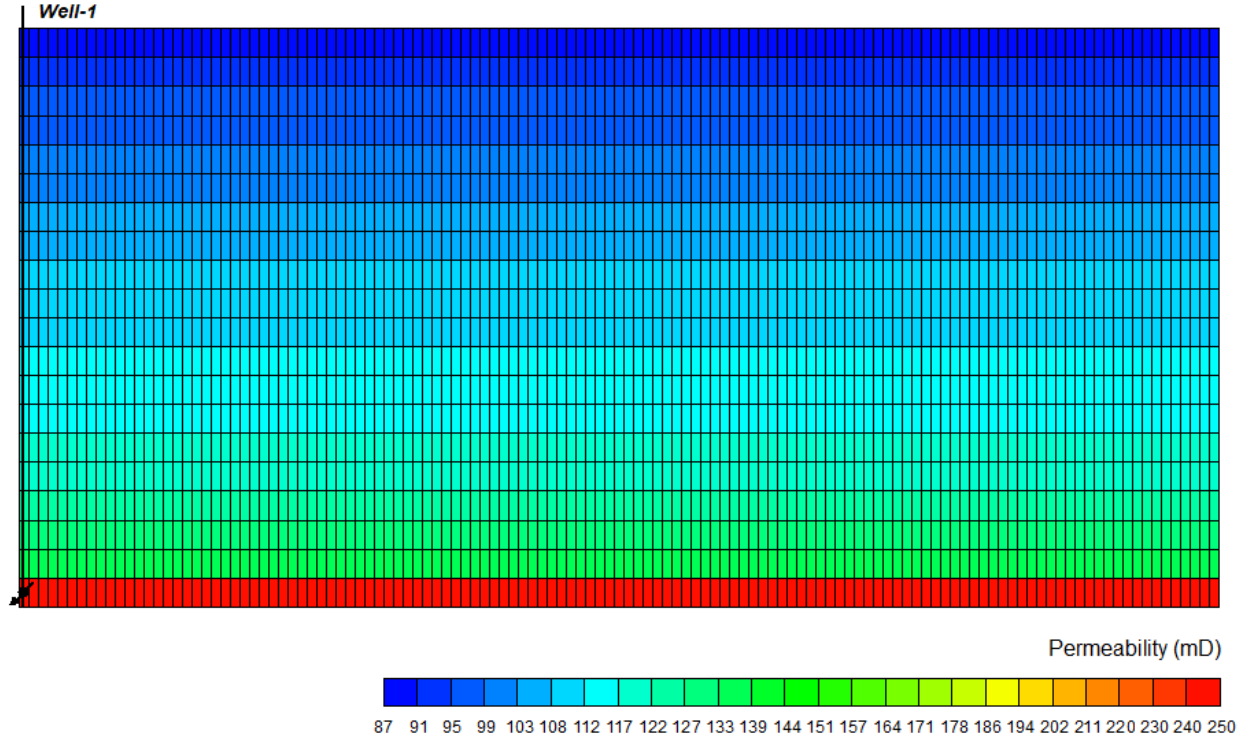


Figure 7. IK view - upward-decrease vertical permeability distribution ($V_{DP} = 0.1124$)

3.3 Rock Quality Classification Based on RQI

To better reflect realistic reservoir conditions, the model incorporated several rock types with distinct petrophysical and flow characteristics. The Rock Quality Index (RQI), which combines permeability and porosity into a single indicator of reservoir flow quality, was calculated for each grid cell using Equation (9). This RQI-based classification was used not only to differentiate permeability variations, but also to assign multiphase flow and capillary behavior in a manner consistent with pore-scale rock quality.

$$RQI = 0.0314 \sqrt{\frac{k}{\phi}}, 0.49 < RQI < 2.05 \quad (9)$$

where: k is the absolute permeability (mD) and ϕ is the porosity (fraction).

The calculated RQI values were then mapped to four separate rock-quality categories applied in property tables and flow functions:

Category 1: ($0.49 < RQI < 0.65$)

Category 2: ($0.65 < RQI < 1.11$)

Category 3: ($1.11 < RQI < 1.50$)

Category 4: ($1.50 < RQI < 2.05$)

This classification preserves the same overall mean permeability and vertical anisotropy across all cases, which allows us to systematically compare (i) the degree of heterogeneity (narrow versus

wide k ranges) and (ii) the vertical arrangement of permeability (UD versus UI) influence CO₂ plume migration, capillary and dissolution trappings under comparable average rock quality conditions. The **Figure 8** presents the corresponding distribution for one representative upward-decrease case selected as an example from the ten investigated cases.

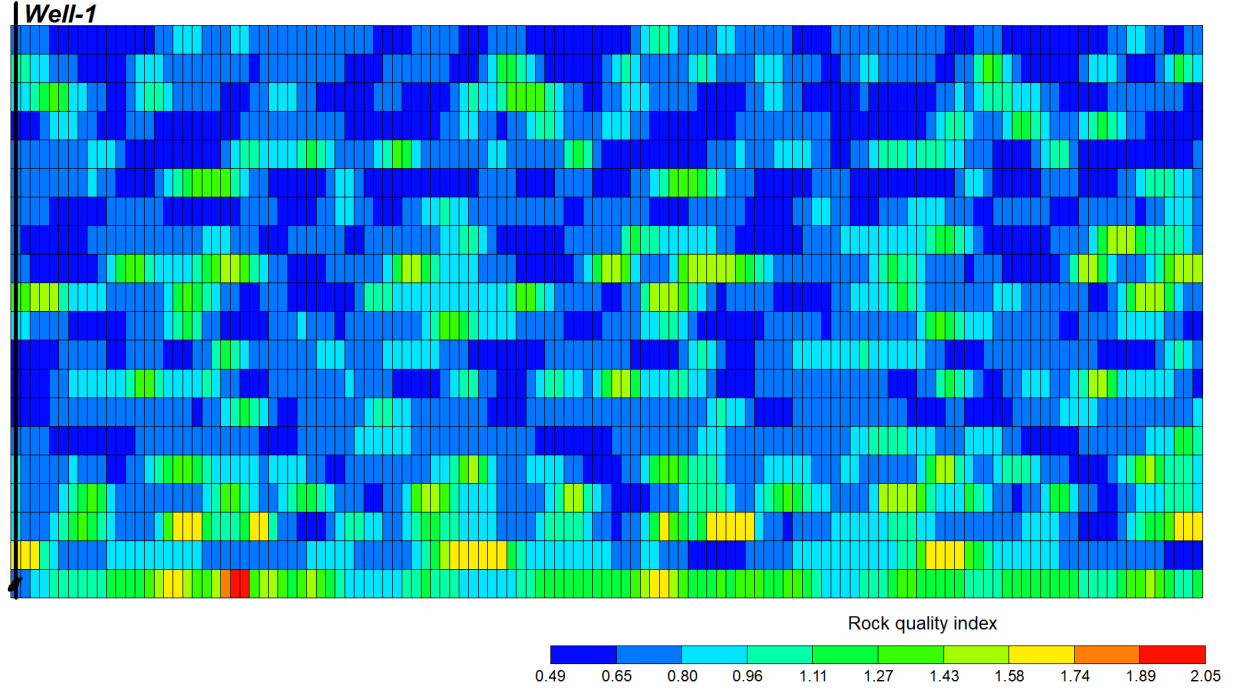


Figure 8. The spatial distribution of reservoir rock types based on the rock quality index was calculated.

3.4 Wettability Definition

A uniformly water-wet system was assumed throughout the reservoir, in which brine acts as the wetting phase and CO₂ as the non-wetting phase. Wettability effects were represented using relative permeability and capillary pressure functions derived from the Brooks-Corey formulation, which was selected because it provides a simple and widely used framework for describing two-phase flow and capillary behavior in porous media. The governing equations are given in Equations (10-14).

$$k_{rg} = (1 - S_w^*)^{0.5} \left[1 - (S_w^*)^{\frac{1+\lambda}{\lambda}} \right]^2 \quad (10)$$

$$k_{rw} = (S_w^*)^{\frac{4+5\lambda}{2\lambda}} \quad (11)$$

$$S_w^* = \frac{(S_w - S_{wr})}{(1 - S_{wr} - S_{gr})} \quad (12)$$

$$S_w^* = \frac{(S_w - S_{wr})}{(1 - S_{wr} - S_{gc})} \quad (13)$$

$$P_c = P_e (S_w^* \frac{1}{\lambda} - 1) \quad (14)$$

Here, S_w is the water saturation, S_{wr} the residual water saturation, S_{gr} the residual gas saturation (hysteresis factor between drainage and imbibition), S_{gc} the critical gas saturation, λ the pore-size distribution index, and P_e the entry pressure. The values of S_{wr} and S_{gc} were set to 0.25 and 0.05, respectively, following (Khoramian et al., 2026b), while $\lambda=0.7$ was adopted based on (Al-Khdheawi et al., 2017a). The hysteresis factor (S_{gr}) was represented by a land trapping coefficient of 0.40 for the water-wet condition, which is consistent with that reported by (C. Khan et al., 2015). These parameters were selected to maintain consistent wettability and capillary behavior across all simulations, allowing the impact of layered permeability heterogeneity on CO₂ migration and trapping to be examined independently. **Figure 9** represents the relative permeability curves used in this study.

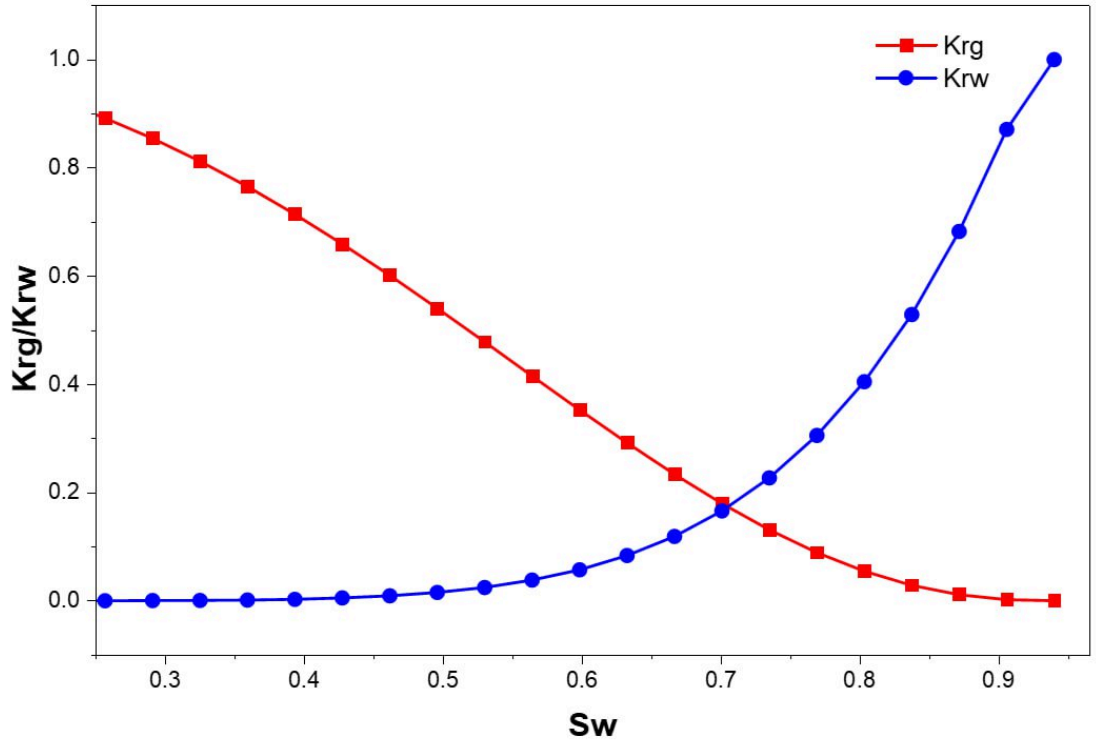


Figure 9. Relative permeability curves used in this study.

Capillary pressure functions were also modeled using the Brooks-Corey formulation, with four rock types defined according to their pore-size distribution index (λ) scaled relative to the base value of 0.7. These multipliers capture the variation in pore throat size across different rock quality categories derived from the RQI classification (Section 3.2):

Rock type 1: $\lambda = 1 \times 0.7 = 0.7$

Rock type 2: $\lambda = 2 \times 0.7 = 1.4$

Rock type 3: $\lambda = 5 \times 0.7 = 3.5$

Rock type 4: $\lambda = 10 \times 0.7 = 7.0$

This approach ensures that the capillary pressure functions are consistent with the assigned rock quality categories. **Figure 10** shows the capillary pressure curves used to characterize the wettability conditions in this study.

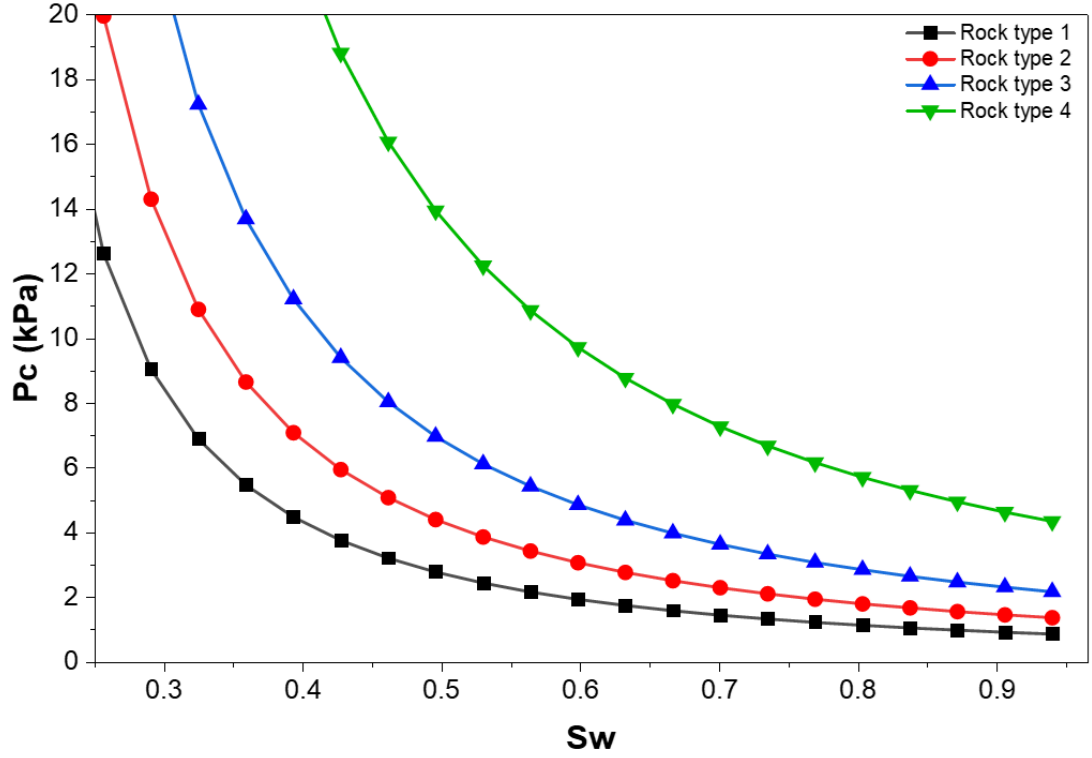


Figure 10. Capillary pressure curves are used to represent different wettability conditions used in the simulation.

3.5 Interpretation and role of the trapping indices

To quantify the main CO₂ trapping mechanisms, simulation outputs were post-processed at each reporting time to calculate trapping indices for residual trapping and dissolution. For each case, the mass of CO₂ associated with each mechanism was extracted from the simulator at the field scale over the entire model domain and normalized by the cumulative injected CO₂ mass. This normalization yields dimensionless indices that allow direct comparison between scenarios regardless of differences in the absolute amount of stored CO₂. The trapping indices are defined in in Equations (15) and (16).

$$RTI = \frac{\text{Total mass of CO}_2 \text{ trapped as residual (tons)}}{\text{Total mass of injected CO}_2 \text{ (tons)}} \quad (15)$$

$$STI = \frac{\text{Total mass of CO}_2 \text{ dissolved in saline aquifer (tons)}}{\text{Total mass of injected CO}_2 \text{ (tons)}} \quad (16)$$

Here, the residual trapping index (RTI) represents the fraction of injected CO₂ immobilized in the pore space by capillary forces as residually trapped gas, whereas the solubility trapping

index (STI) represents the fraction of injected CO₂ dissolved in the formation brine. These indices are time-dependent and were evaluated consistently across all scenarios at identical reporting times during and after injection to enable direct comparison of the relative contribution and evolution of each trapping mechanism.

The proposed model is particularly useful because it isolates the effect of vertical permeability architecture on CO₂ plume migration and trapping while maintains the same mean permeability, porosity, and vertical anisotropy in all scenarios. The model includes controlled heterogeneity design, RQI-based rock typing, fixed wettability assumptions and time-dependent trapping indices. These features together make it possible to compare residual and solubility trapping in a physically meaningful way. Although the model is simplified by its two-dimensional geometry and uniform water-wet conditions, these assumptions help to isolate the effect of layered reservoir structure. The analysis quantifies key performance indicators that includes CO₂ plume geometry (extent, continuity, and vertical migration), the residual trapping index (RTI), the solubility trapping index (STI), and bottom-hole pressure (BHP) as an indicator of injectivity. These parameters are evaluated consistently across all scenarios to determine how vertical permeability trend affects trapping mechanisms, plume shape, and pressure response. Which provides a direct connection to the results and discussion presented in the next chapter.

4 RESULTS AND DISCUSSION

This section examines the impact of heterogeneity and vertical permeability distribution on the dynamic behavior of CO₂ storage in deep saline aquifers. The focus is on plume geometry evolution and the distribution of CO₂ between residual and dissolution trapping mechanisms. Bottom-hole pressure trends are also analyzed to evaluate injectivity and overall storage performance. The section compares upward-decrease and upward-increase permeability trends to identify the main factors that control plume shape, trapping efficiency, and pressure response. These factors support better reservoir selection and help estimate the relative contribution of each trapping mechanism.

4.1 Evolution of CO₂ plume geometry

CO₂ plume geometry is an important component of CCS performance and storage security. It influences migration pathways, access to trapping structures and monitoring strategy. In this study, heterogeneity levels were classified into low, medium, and high categories based on the Dykstra-Parsons coefficient (V_{DP}). Low heterogeneity refers to V_{DP} values of 0-0.31, medium heterogeneity to 0.31-0.59, and high heterogeneity to 0.59-1.

Figure 11 presents the effect of vertical permeability trends on total CO₂ saturation and capillary-trapped CO₂ under weak, moderate, and strong heterogeneity conditions. It illustrates systematic changes in plume continuity, vertical migration, and trapping behavior. Total gas saturation helps capture the overall plume migration, which shows the extent and continuity of the CO₂ as it moves through the reservoir. In contrast, capillary-trapped gas represents the portions of CO₂ that are immobilized due to capillary forces, which offers insight into residual trapping. These parameters together allow for a comprehensive analysis of both plume movement and the effectiveness of CO₂ trapping mechanisms.

At low heterogeneity ($V_{DP} = 0.1124, 0.2109, \text{ and } 0.308$), permeability differences between layers are small, so vertical connectivity remains good in both upward-increase and upward-decrease permeability trends. Under these conditions, buoyancy dominates CO₂ migration, and the plume rises to form a largely continuous accumulation near the top of the reservoir. In the upward-decrease case, CO₂ spreads somewhat more within the more permeable lower layers before rising, whereas the upward-increase case promotes a more direct upward migration and earlier concentration in the upper reservoir.

As V_{DP} increases within this low range, plume geometry only slightly changes. The upward-decrease cases show minor plume variations, local flow diversion, and a few additional disconnected capillary-trapped pockets. In upward-increase cases retain a smoother, more vertically focused plume with fewer isolated trapped-gas zones. Even so, vertical flow pathways remain open in all three cases, so snap-off and bypassing are limited. Structural trapping therefore remains the dominant storage mechanism, while residual trapping is limited to a few localized zones. Overall, under low heterogeneity conditions, CO₂ storage is controlled mainly by buoyancy and the influence of reservoir architecture remains secondary.

At medium heterogeneity ($V_{DP} = 0.4036, 0.4974, \text{ and } 0.5892$), permeability contrasts become strong enough to noticeably affect vertical connectivity, which leads to a clearer divergence in plume behavior between the two vertical permeability trends. Gravity still affects CO₂ upward in all cases, the permeability architecture increasingly controls how continuous this upward migration remains.

In the upward-increase trend, the higher permeability toward the top maintains better vertical flow pathways, which allows the plume to flow upward more efficiently and maintain a laterally continuous upper gas accumulation. This results in thicker and more coherent high-saturation zone near the top of the reservoir and limits the extent of disconnected capillary-trapped gas. In contrast, in the upward-decrease trend, the reduction in permeability toward the upper layers increasingly restricts upward migration and promotes lateral spread of CO₂ within the lower and intermediate layers. As a result, the plume becomes less vertically efficient, and a larger number of disconnected capillary-trapped pockets develop under and along the margins of the main accumulation.

As V_{DP} increases from 0.4036 to 0.5892, the difference between the two trends becomes clearer. The upward-decrease cases develop a more irregular plume and more widely distributed residual trapping, while the upward-increase cases remain more connected. However, localized trapped-gas pockets begin to appear. Under medium heterogeneity the system is no longer controlled mainly by buoyancy. Instead, vertical permeability becomes more important in deciding whether CO₂ keeps moving upward and stays structurally trapped or becomes residually trapped.

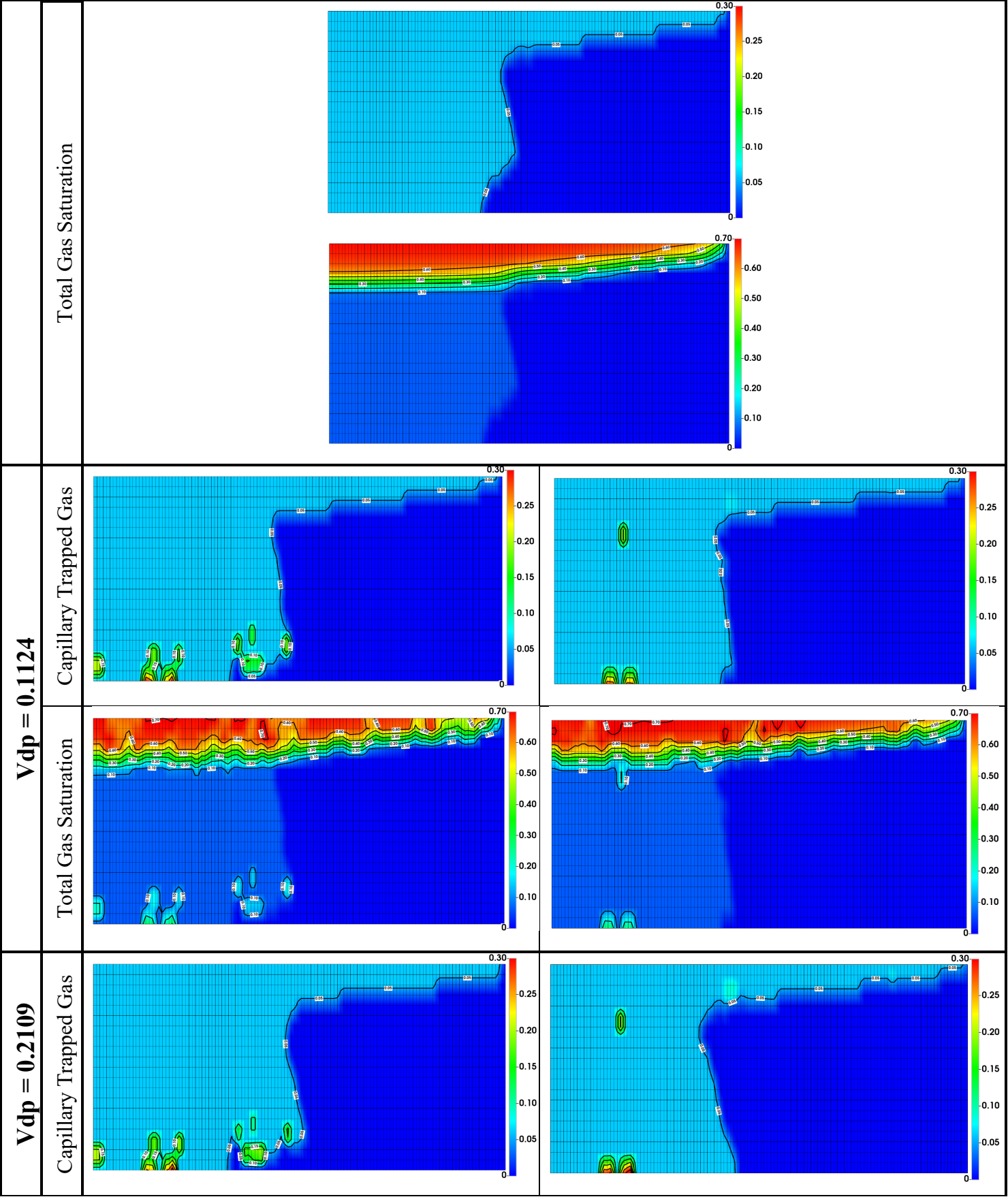
Under high heterogeneity ($V_{DP} = 0.6786, 0.7652, 0.8483, \text{ and } 0.9262$), strong permeability contrasts control plume evolution, and the vertical permeability trend becomes the main factor that controls the CO₂ migration and trapping. In the upward-decrease case, the sharp reduction in permeability toward the upper reservoir acts as a barrier to vertical flow and slows the upward rise of CO₂. The plume migrates upward in a stepwise manner and repeatedly loses connectivity at low-permeability layers. This leads to strong plume breakup, frequent snap-off, and more CO₂

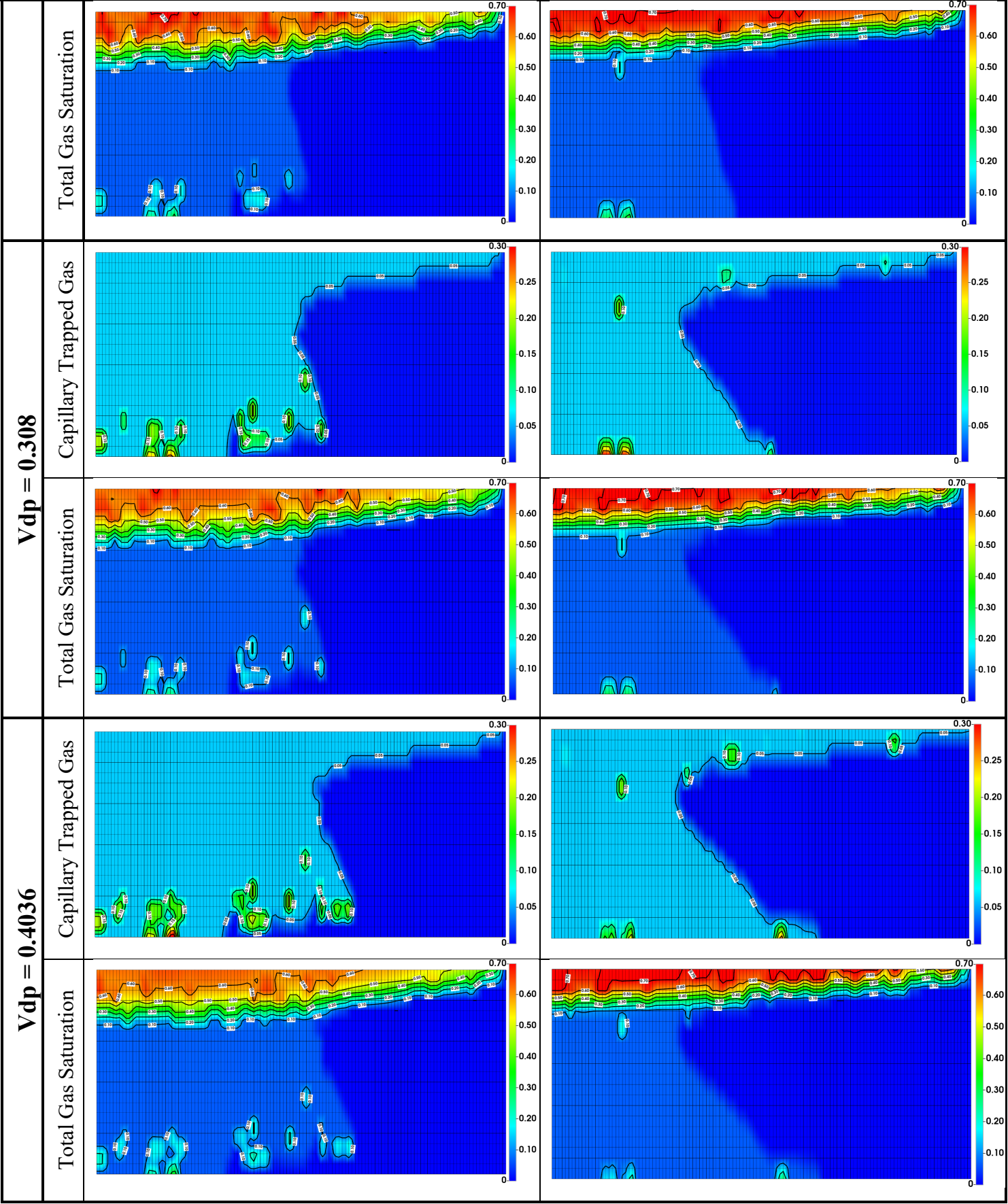
becoming residually trapped. The buoyant accumulation in the upper reservoir stays small and discontinuous, and lateral spreading is limited by poor vertical communication. By contrast, the upward-increase case still preserves preferential vertical pathways even at high heterogeneity, so CO₂ remains more connected as it moves upward. Although the flow becomes more tortuous and locally diverted, which makes the buoyant accumulation thinner and more irregular. However, the plume is still much more continuous than in the upward-decrease case. As a result, structural trapping linked with buoyant accumulation remains dominant, while residual trapping is less significant because snap-off and disconnection occur less often.

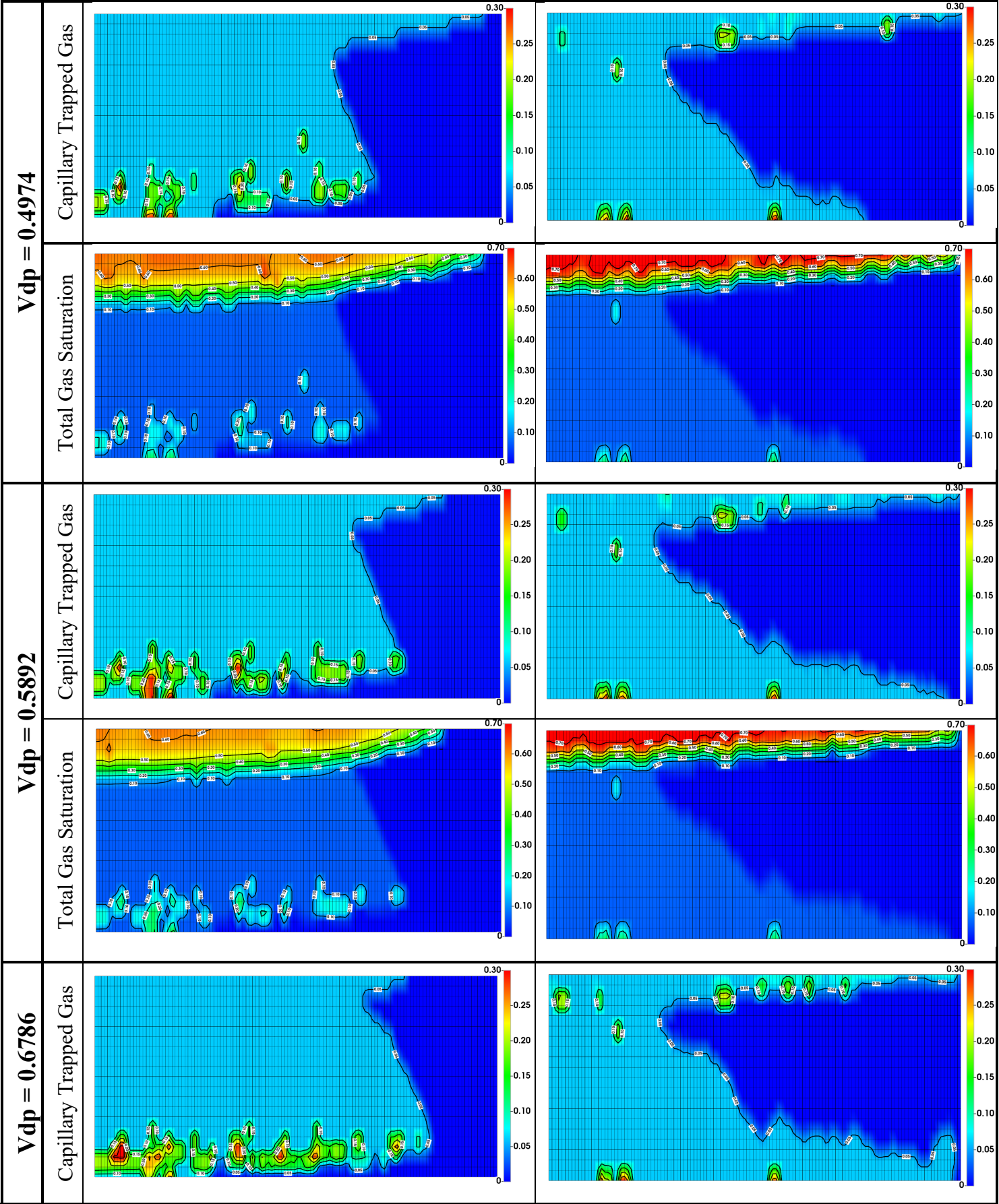
At $V_{DP} = 0.8483$ and especially 0.9262, the plume boundary becomes more irregular, local segmented zones develop and isolated trapped-gas pockets appear even in the upward-increase case. Under high heterogeneity, the upward-increase trend still favors better plume continuity and stronger buoyant accumulation than the upward-decrease. However, the upward-decrease trend shows greater plume breakup and greater residual trapping. High heterogeneity levels show that plume behavior in both cases is controlled more by reservoir connectivity rather than by buoyancy alone.

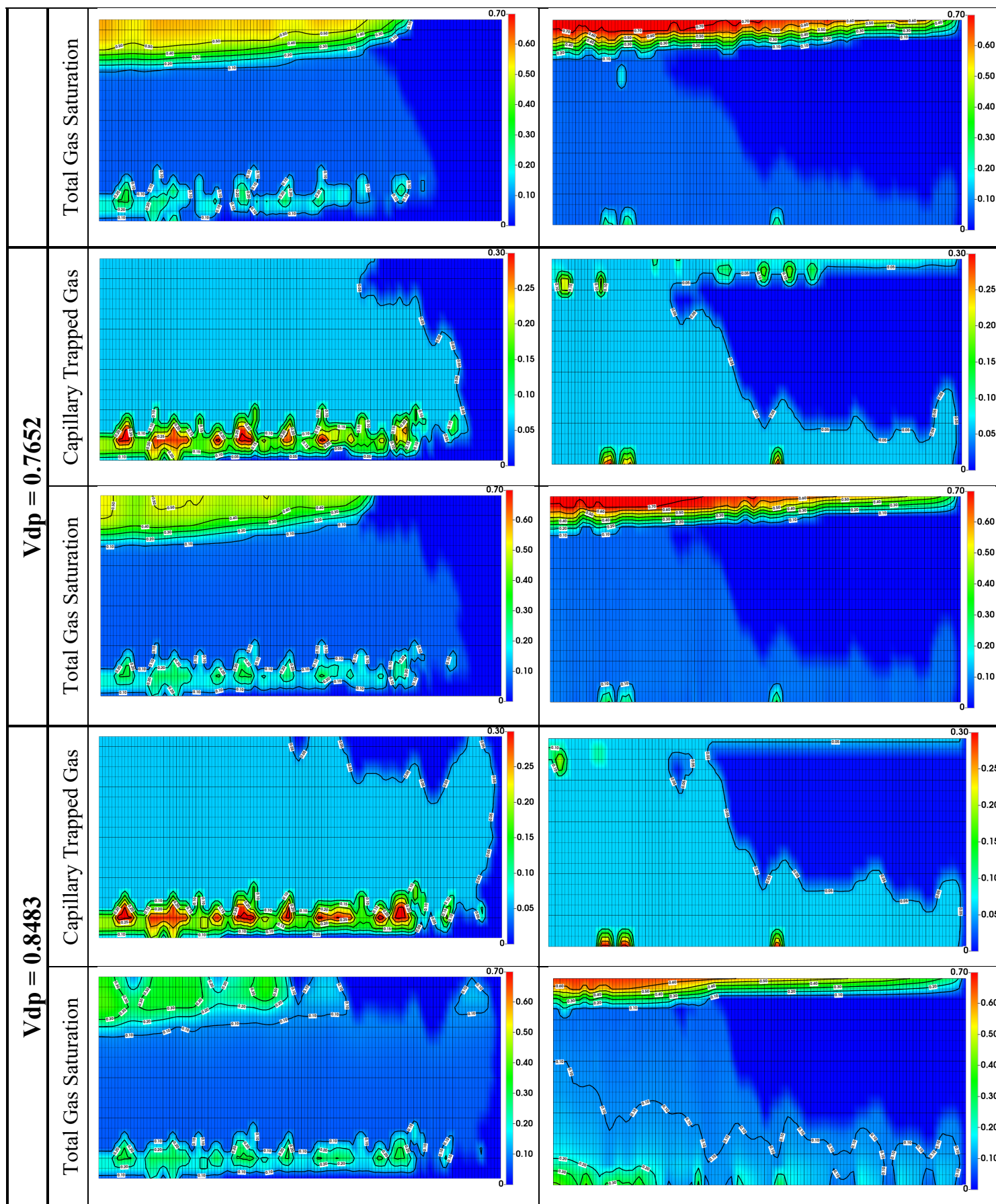
At high heterogeneity level CO₂ movement is controlled less by buoyancy and more by layer connectivity. When permeability decreases upward, the upper layers act as barriers, causing the plume to break into disconnected parts and increasing residual trapping. In the upward-increase case upward flow of CO₂ plume occurs easily, and the plume remains more connected, so less becomes residually trapped.

		Upward-decrease	Upward-increase
Vdp = 0	Capillary Trapped Gas		









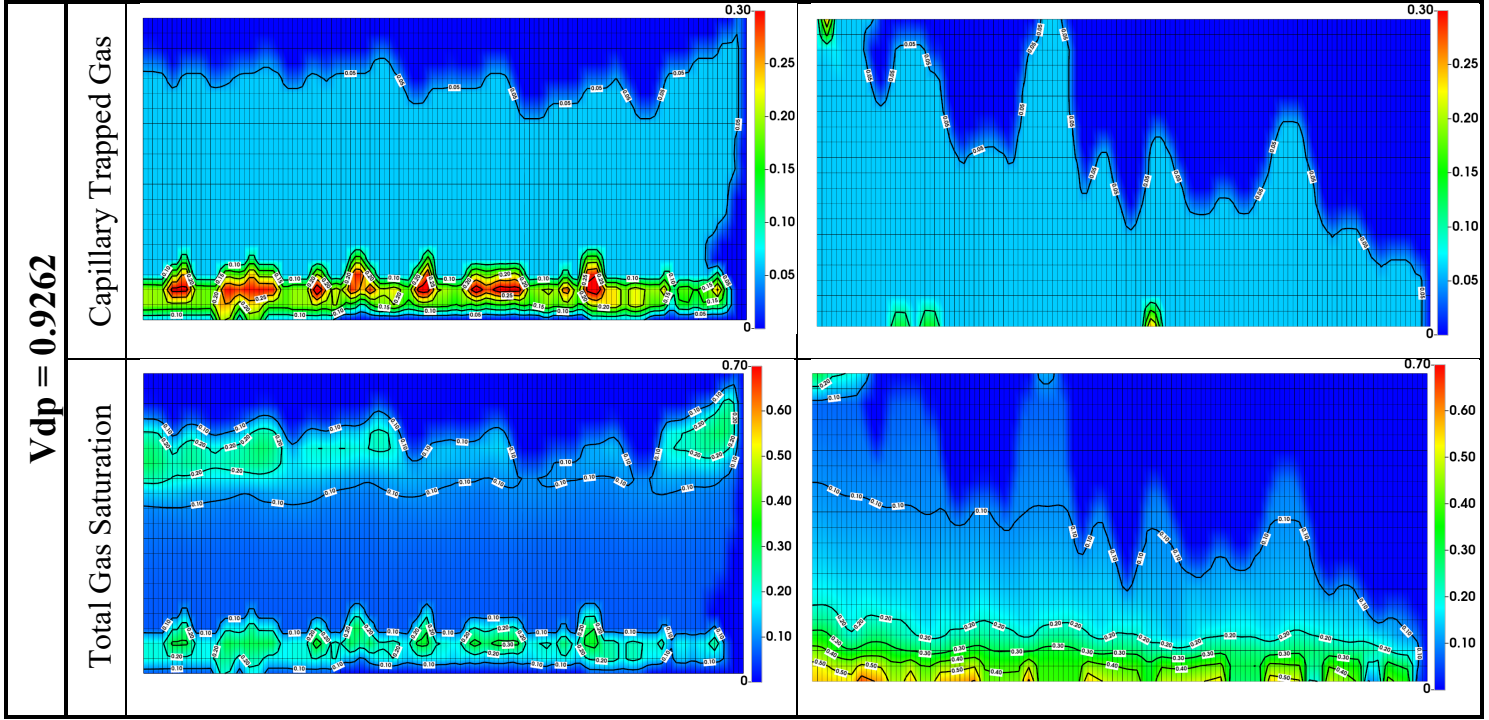


Figure 11. Effect of permeability trend on total gas saturation and capillary-trapped gas for low, medium, and high heterogeneity values

4.2 Effect of heterogeneity on CO₂ dissolution and residual trapping

The analysis shows how reservoir heterogeneity, measured by the Dykstra-Parsons coefficient, affects CO₂ dissolution and residual trapping distribution under two permeability trends. For each trend, the dependence on V_{DP} is evaluated at 10, 30, 50, 100, 150, and 200 years. This allows time-resolved comparison of which trapping mechanism increases most strongly and how heterogeneity shifts the balance between them. Field studies indicate that sandstone and carbonate reservoirs exhibit different ranges of heterogeneity, as reflected by their Dykstra-Parsons coefficients. Following the heterogeneity rankings of (Nabawy et al., 2023) and (Tiab & Donaldson, 2012) as reported, $V_{DP} \sim 0.25-0.50$ is considered moderately heterogeneous and $V_{DP} \sim 0.50-0.75$ highly heterogeneous. Reported sandstone reservoirs commonly fall within the 0.3-0.5 range, representing moderate heterogeneity, whereas carbonate reservoirs, particularly fractured systems, often exhibit V_{DP} values greater than 0.5.

4.2.1 Dissolution trapping

Figure 12 shows CO₂ dissolution during early, intermediate, and late time periods for both permeability trends. During the early period (10-50 years), dissolution evolved through distinct

regimes. At 10 years, dissolution is mainly controlled by near-injection behavior. In the upward-decrease architecture, lower-permeability upper layers limit early vertical migration. It promotes lateral spread in brine-rich lower layers and increase of the CO₂-brine contact, which leads to higher dissolution. For upward-increase trend CO₂ moves upward more easily and reduces contact near the injector and leads to lower dissolution. By 30 years, buoyancy effects strengthen and the trends begin to separate. The upward-decrease case generally shows higher dissolution because partial vertical restriction maintains stratified mixing. Upward-increase case reaches higher layers and more brine, but preferential pathways may reduce local mixing. Over the 50 years, CO₂ has spread across a larger vertical interval, and dissolution is increasingly governed by both vertical connectivity and residence time. As a result, the early advantage of the upward-decrease case becomes less pronounced.

At 100 years, CO₂ dissolution is in a transition stage, so both connectivity and retention are important. In the upward-increase case, better vertical connectivity helps CO₂ reach more brine at moderate heterogeneity, which leads to increased dissolution trapping. CO₂ movement in high heterogeneity levels goes preferential pathways too quickly with less time spending in mixing zones and reducing dissolution gains. Upward movement remains more restricted in the upward-decrease case and CO₂ remains in brine-rich layers for longer, and dissolution increases as heterogeneity increases. At 150-200 years, long-term residence time dominates dissolution. The upward decrease increasingly supports sustained contact and continued dissolution growth with heterogeneity. But the upward increase can show flattening or decline at very high heterogeneity as preferential pathways shorten the mixing-zone contact.

4.2.2 Residual trapping

CO₂ residual trapping during the early, middle, and late periods under different heterogeneity levels is shown in **Figure 13**. Residual trapping is governed by how often and effectively the CO₂ phase is broken, disconnected, and immobilized during migration by capillary forces. Unlike dissolution, it does not primarily depend on the contact area with brine but on flow interruption, snap-off, and repeated redistribution within heterogeneous pore structures.

In the upward-decrease permeability trend, lower-permeability layers progressively restrict upward migration toward the top. As CO₂ rises from the injection interval, it cannot move continuously upward. Instead, it repeatedly accumulates and spreads laterally. Each spreading event increases the likelihood of capillary snap-off, which leaves behind disconnected CO₂ clusters that become trapped in the residual state. As heterogeneity increases, permeability contrasts increases layer by layer and plume becomes less continuous. Residual trapping increases almost

monotonically with V_{DP} and time. In contrast, the upward-increase architecture promotes smoother and more continuous upward migration due to higher permeability toward the top. This reduces the number of flow interruptions and snap-off events. At moderate heterogeneity, some increase in residual trapping still occurs due to local fingering. However, at higher heterogeneity, preferential vertical pathways begin to develop. This allows CO_2 bypass intermediate layers rather than being repeatedly redistributed within them. As a result, the opportunity for additional capillary trapping diminishes, causing residual trapping to level off or even decline at high V_{DP} and late times.

At early times, the differences are modest because residual trapping is still developing near the injection zone. Intermediate times, the contrast becomes more clearer as repeated redistribution in the upward-decrease case accumulates trapped CO_2 . At late times (150-200 years), residual trapping is dominated by long-term flow segmentation. With increasing heterogeneity, the upward-decrease trend continues to enhance CO_2 immobilization. By contrast, the upward-increase trend approaches a saturation point, where further heterogeneity produces little additional trapping.

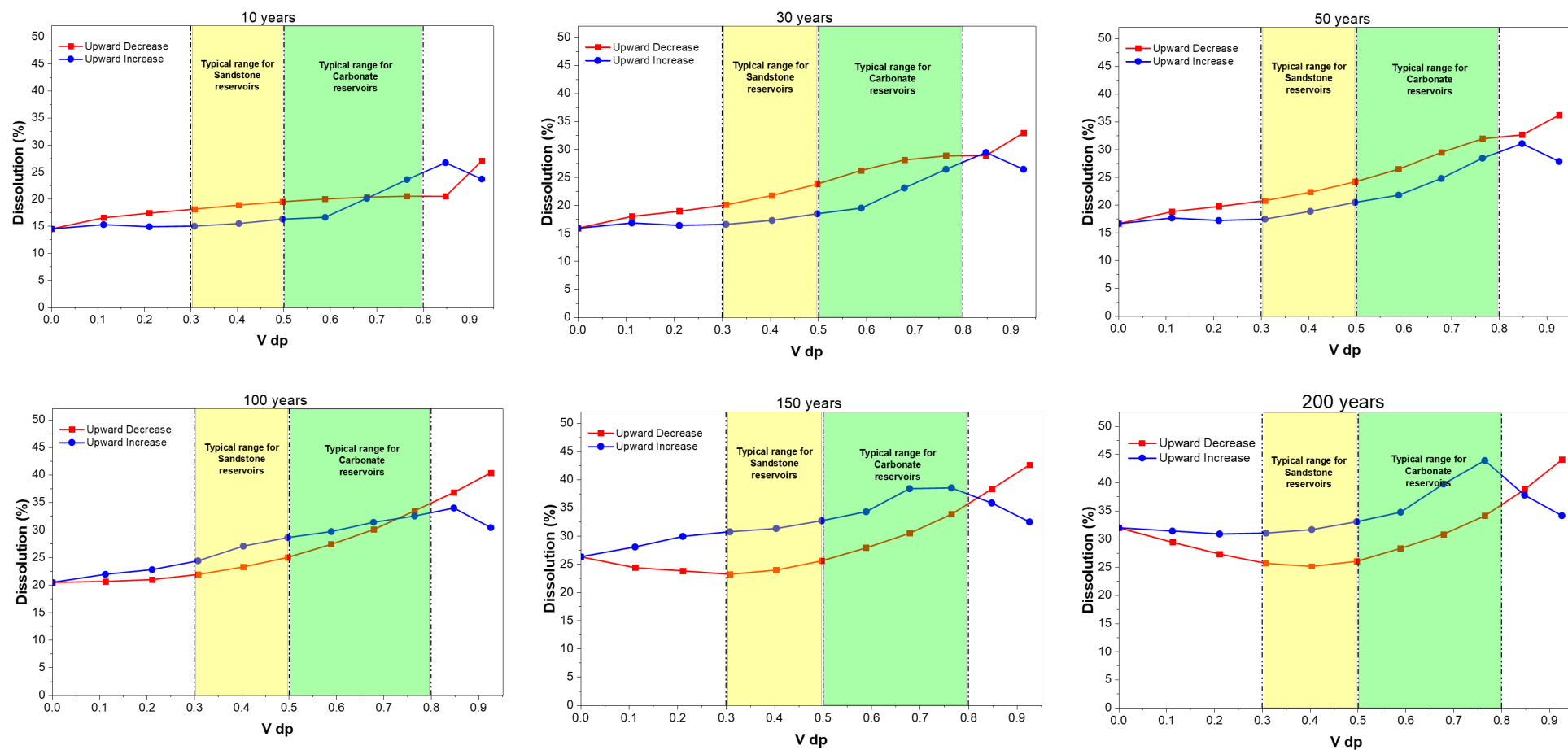


Figure 12. Effect of heterogeneity (V_{DP}) on dissolution over time for upward decrease vs upward increase.

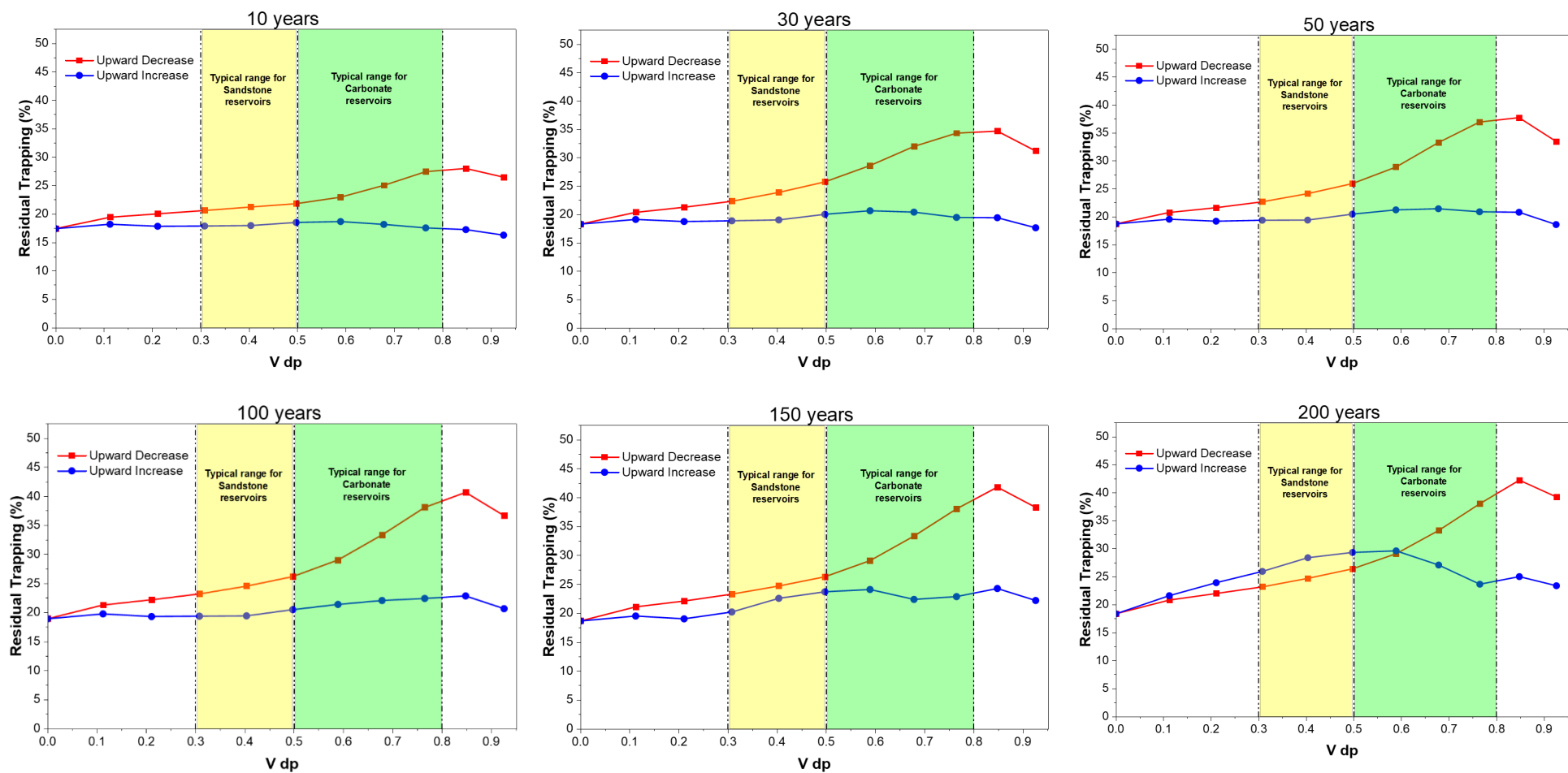


Figure 13. Effect of heterogeneity (V_{DP}) on residual trapping over time for upward decrease vs upward increase.

Figure 14 illustrates the temporal evolution of CO₂ dissolution and residual trapping for the upward-decrease and upward-increase permeability trends. For three representative heterogeneity levels: low heterogeneity ($V_{DP}=0.1124$), moderate heterogeneity ($V_{DP} = 0.4974$) and high heterogeneity ($V_{DP} = 0.8483$).

At low heterogeneity, both permeability trends exhibit relatively smooth CO₂ migration and modest increases in dissolution over time. As shown in **Figure 14 (a)**, decreasing permeability toward the top does not form effective vertical barriers. Thus, dissolution rises rapidly at early times and then gradually approaches a quasi-steady regime by approximately 100 years. In **Figure 14 (b)**, upward migration is efficient from early times, but the limited structural contrast restricts residence-time enhancement, producing a similarly gradual and stabilized dissolution trend. Residual trapping at this heterogeneity level remains low and increases, as shown in **Figure 14 (d)**, but only slightly with time for the upward increase case, reflecting limited disruption of flow and snap-off.

At moderate heterogeneity, permeability contrasts become stronger to influence flow behavior. In the upward-decrease trend in **Figure 14 (a)** and **14 (c)**, the partial restriction of upward migration keeps CO₂ longer within layered zones rich in brine, and dissolution and residual trapping to continue increasing over time. Upward-increase trend is illustrated in **Figure 14(b)**. Enhanced dissolution trapping between 30 and 100 years can be observed, most likely due to better vertical connectivity, which allows CO₂ plume to reach the higher layers. **Figure 14 (d)** shows a delayed increase in residual trapping after 120 years, consistent with late invasion of additional layers and renewed snap-off. **Figure 14 (c)** shows early formation and stabilization, this means early capillary trapping saturation in the upward-decrease case.

At high heterogeneity, the permeability structure has the strongest effect. In the upward-decrease case **Figure 14 (a)**, strong permeability contrasts create effective vertical baffles that retain CO₂ in the stratified regions. This leads to the highest dissolution and residual trapping across all times **Figure 14 (c)**, with a sharp early increase followed by continued growth toward a high limited value. In the upward-increase case **Figure 14 (b)**, strong vertical connectivity drives rapid early dissolution, but preferential pathways later reduce CO₂-brine contact, slowing dissolution growth and limiting residual trapping relative to upward-decrease. Residual trapping in **Figure 14 (d)** is higher at $V_{DP}=0.8483$, because stronger permeability

contrasts promote snap-off and disconnection, whereas $V_{DP} = 0.4974$ maintains more continuous flow paths and therefore results in lower capillary trapping of CO_2 .

Overall, the curves demonstrate that with increasing VDP, both dissolution and residual trapping increase, but the controlling mechanism depends on the permeability trend. The upward-decrease trend favors long-term storage and prolonged trapping, whereas the upward-increase trend promotes faster redistribution and an earlier plateau in trapping efficiency, particularly at high heterogeneity.

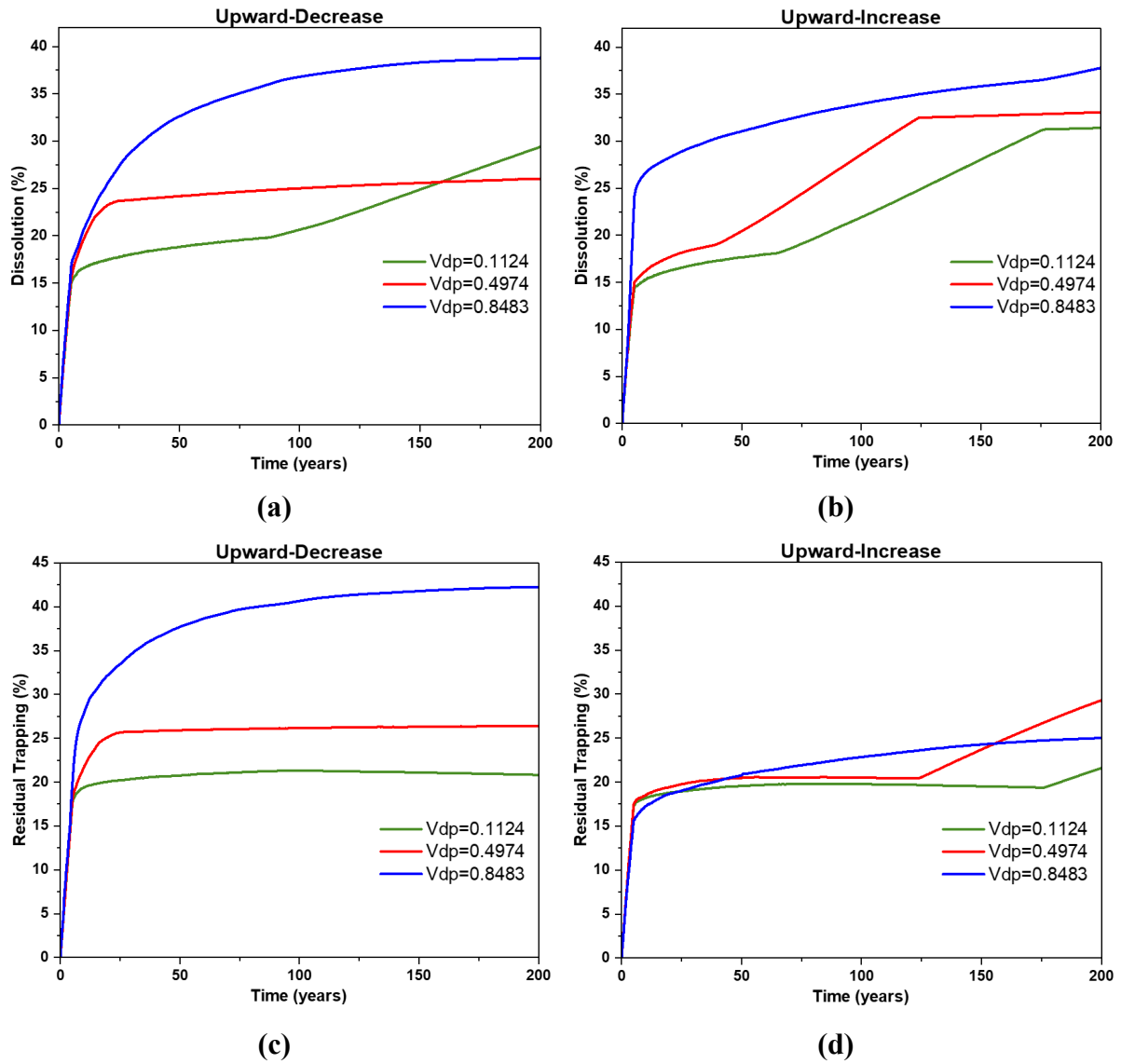


Figure 14. Time evolution of dissolution and residual trapping for different levels of heterogeneity.

Figure 15 represent net impact of heterogeneity Δ dissolution and Δ residual trapping relative to the homogeneous case at 50 and 200 years. At 50 years, heterogeneity is consistently beneficial for the upward-decrease architecture. Both trends increase with V_{DP} , whereas

the upward-increase case shows smaller, mainly positive gains that become clearer at moderate-high V_{DP} . By 200 years, the separation strengthens: upward-decrease remains strongly positive and grows with V_{DP} , whereas upward-increase can be negative at low V_{DP} due to preferential flow, but turns positive again at high V_{DP} especially for residual trapping, because stronger contrasts promote phase disconnection and immobilization.

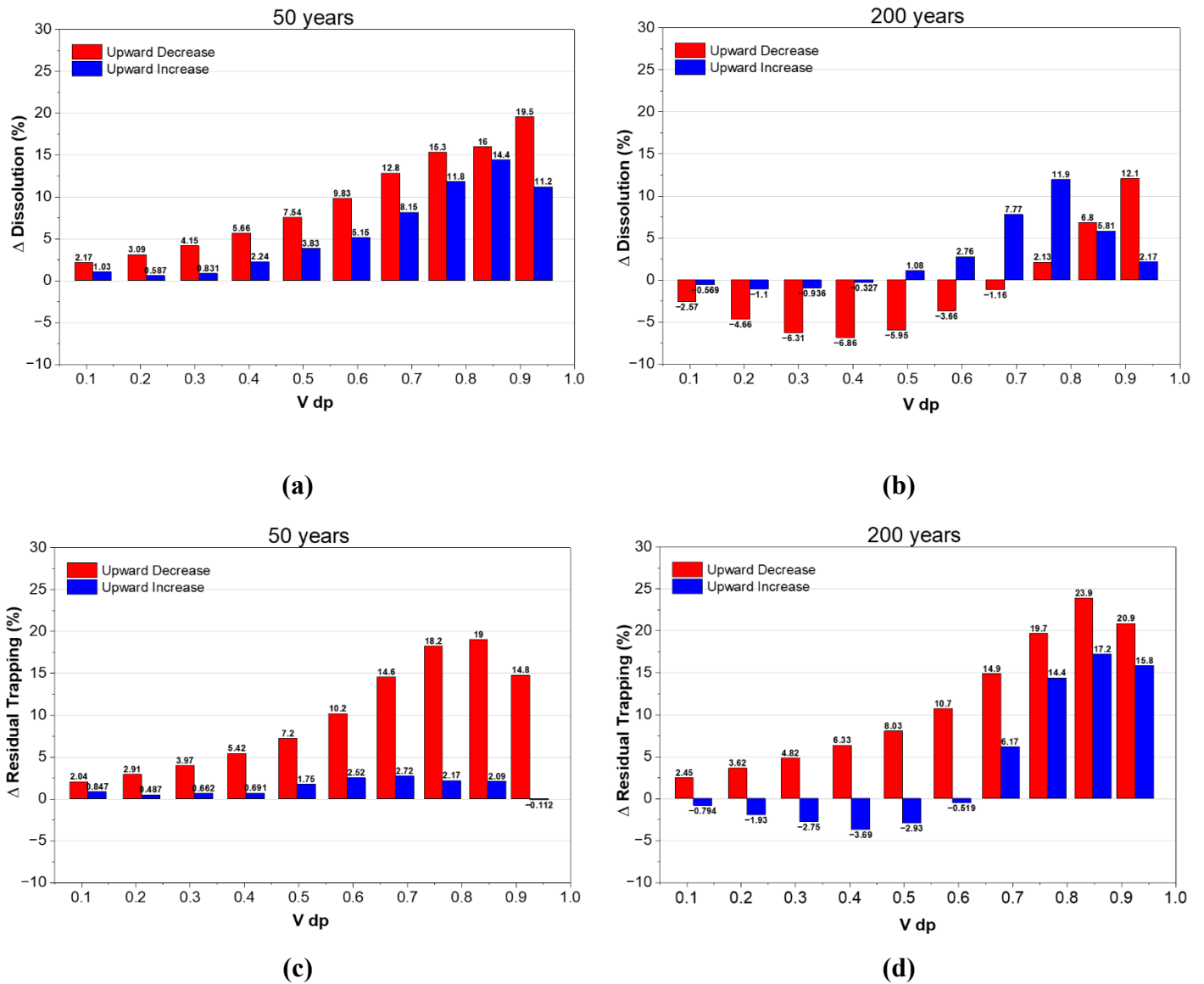


Figure 15. The net effect of heterogeneity on CO₂ dissolution and residual trapping relative to the homogeneous case for upward-decrease and upward-increase permeability trends.

4.3 Injectivity behavior under different vertical permeability trends

Figure 16 shows the time evolution of bottom-hole pressure (BHP) for different Dykstra-Parson's heterogeneity levels V_{DP} during 5 years of CO₂ injection followed by shut-in

for two vertical permeability architectures: (a) upward-increase and (b) upward-decrease. **Figure 16** illustrates how BHP responds to heterogeneity and vertical permeability structure over time, rather than the absolute “effect” of BHP.

In **Figure 16 (a)** the upward-increase configuration, BHP rises rapidly during injection and separates strongly with increasing V_{DP} . Higher heterogeneity leads to higher BHP because the low-permeability base near the well acts as a vertical choke, limiting early upward pressure diffusion. CO₂ therefore accumulates in the near-well region, gas saturation increases, water relative permeability decreases, and a higher pressure is required to maintain the imposed injection rate. After shut-in, BHP decreases slowly and stays relatively high. This is more noticeable at high V_{DP} , where flow near the well remains limited even as the CO₂ plume gradually connects vertically. This behavior indicates reduced injectivity and strong sensitivity of BHP to heterogeneity when the tightest layers are located near the well.

In **Figure 16(b)**, the upward-decrease configuration shows lower BHP and much weaker sensitivity to V_{DP} during injection. Here, the high-permeability base under the well allows efficient vertical pressure diffusion; thus, pressure does not build strongly in the near-well region even as heterogeneity increases. As a result, the BHP curves are tightly clustered, and the injectivity remains relatively high across all V_{DP} values. After shut-in BHP declines faster than in the upward-increase case and this behavior is consistent with easier pressure redistribution away from the wellbore. The sharp pressure peak near 0.01 years (approximately 3.7 days) is interpreted as an early transient effect that occurs immediately after the start of injection. At this stage, CO₂ first enters the near-well region, which causes rapid gas-phase appearance. This leads to abrupt changes in relative permeability and temporary local pressure buildup. Because the spike appears only at the start and disappears quickly, it likely reflects an initial simulation adjustment rather than long-term reservoir behavior. After that, the BHP trends stabilize and better show the effect of heterogeneity and vertical permeability on injectivity.

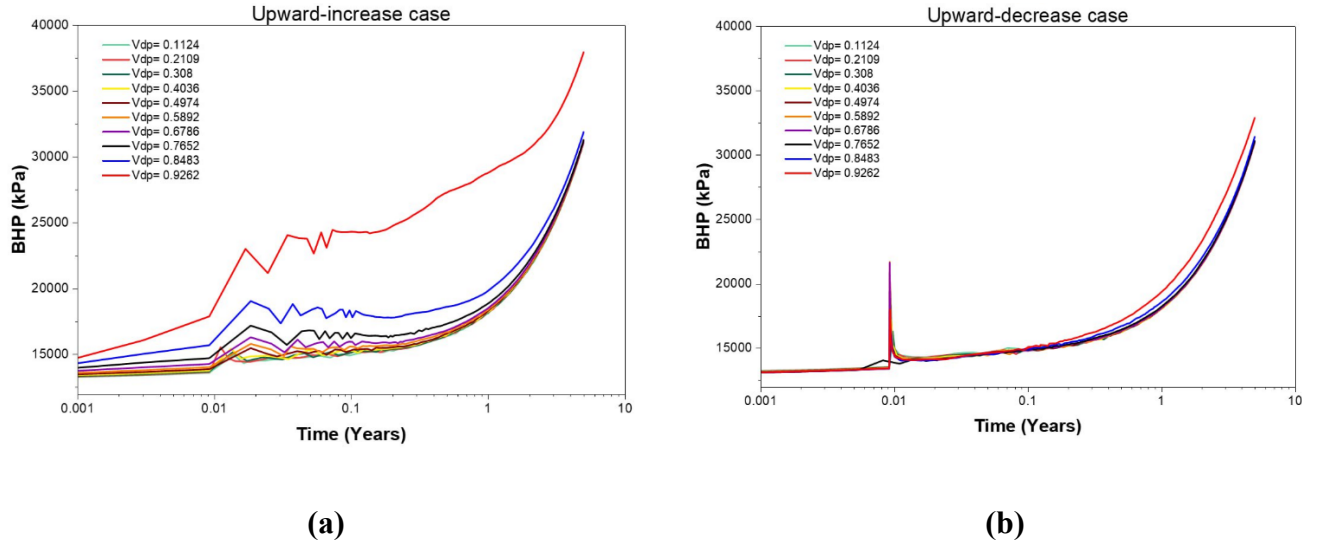


Figure 16. Bottom-hole pressure (BHP) evolution for different Dykstra–Parsons (VDP) heterogeneity levels under two vertical permeability trends: **(a)** upward-increase and **(b)** upward-decrease permeability cases.

The late-time BHP upturn observed near the end of injection in both configurations reflects the following: increasing gas saturation and reduced two-phase mobility around the well as the gas zone grows; this effect is much stronger in the upward-increase case, where the near-well flow restriction is already significant. Any sharp spikes at very early times are transient numerical effects phase appearance or timestep control and do not affect the sustained pressure trends. The BHP evolution mainly depends on where the tightest permeability occurs relative to the well. A tight base (upward increase) produces higher, V_{DP} sensitive BHP and slower post-shut-in pressure decline, whereas a permeable base (upward decrease) yields lower, V_{DP} insensitive BHP and faster falloff after injection.

4.4 Practical implications and guidance for reservoir selection

The results provide clear guidance for reservoir selection and operational strategy, as it connects heterogeneity level, vertical permeability trend, trapping mechanisms, and injectivity.

Sandstone reservoirs

Sandstone reservoirs are typically characterized by moderate heterogeneity ($V_{DP} \approx 0.3$ -0.5). They are particularly suitable for CO_2 storage when the main aim is to enhance early-stage CO_2 dissolution. The moderate heterogeneity of such reservoirs provides a balanced distribution of permeability across the reservoir, which leads to efficient CO_2 plume migration and good injectivity. An upward-increase permeability trend in these reservoirs creates

favorable conditions for rapid upward plume migration, due to increased vertical connectivity. This increased connectivity allows CO₂ to spread more efficiently through the reservoir, which provides early brine- CO₂ contact and improves dissolution trapping in the first 10-50 years after injection. The upward-increase trend also contributes to relatively low bottom-hole pressure, which results in favorable injectivity and reduces the risk of pressure buildup and subsequent well damage. Furthermore, the enhanced vertical permeability in such reservoirs promotes rapid CO₂ plume migration, which reduces the risk of stagnation and capillary trapping.

In contrast, an upward-decrease permeability trend in sandstone reservoirs restricts the vertical migration of CO₂. This restriction increases the residual trapping of CO₂, but at the cost of higher bottom-hole pressure when tighter layers are located near the well. These tight layers can create pressure buildup near the wellbore, which leads to poor injectivity and a limited volume of CO₂ that can be injected. This trend also leads to more lateral spreading of the CO₂ plume and the formation of capillary-trapped gas pockets in the lower layers, which can result in a more heterogeneous plume distribution.

For sandstone reservoirs aiming to optimize early CO₂ dissolution, the upward-increase permeability trend is more favorable. The rapid upward migration improved vertical flow pathways, and subsequent CO₂-brine contact enhance early-stage dissolution, making it an ideal scenario for maximizing CO₂ storage during the initial 10-50 years of injection. For long-term storage, the upward-decrease permeability trend may also be useful, but it is better for situations where residual trapping is the primary storage mechanism. Nonetheless, these trends require careful management of injection pressures to avoid reduced injectivity and mitigate the risks of high bottom-hole pressure.

Thus, sandstone reservoirs with an upward-increase trend are more favorable for early dissolution-dominated storage strategies. This is due to their ability to improve CO₂ migration and early dissolution, whereas upward-decrease trends are more advantageous for long-term storage, where the focus is more on residual trapping and maximizing CO₂ containment in isolated zones.

Carbonate reservoirs

Carbonate reservoirs, typically with high heterogeneity ($V_{DP} \gtrsim 0.5$), demonstrate unique challenges and advantages for CO₂ storage. The upward-decrease permeability trend is particularly beneficial in carbonate reservoirs for long-term CO₂ immobilization, typically over 100 to 200 years. The strong permeability contrasts, coupled with a reduction in permeability

toward the top of the reservoir, help to increase CO₂ residence time by restricting the upward flow of CO₂. This results in more CO₂ being trapped through residual trapping mechanisms, as the upward-decrease trend promotes CO₂ snap-off and trapping in low-permeability layers.

The increased vertical heterogeneity, with less permeability in the upper layers, limits the upward migration of CO₂ and promotes the formation of more disconnected gas pockets. This mechanism contributes to a greater portion of CO₂ being residually trapped within the lower and intermediate layers. Although the upward-decrease trend leads to higher bottom-hole pressure and reduced injectivity, especially if tight layers are near the well, the long-term containment provided by this trend outweighs the short-term challenges. The trapped CO₂ is more securely immobilized in the reservoir, with reduced risk of migration, providing enhanced storage security over a longer timescale.

On the other hand, an upward-increase permeability trend in carbonate reservoirs can still allow for some vertical flow but generally leads to a more continuous migration path for CO₂. In highly heterogeneous carbonates, this trend can maintain plume connectivity, which helps the direct migration of CO₂. However, this trend may reduce long-term trapping efficiency as it allows CO₂ to move preferentially through high-permeability pathways, which can lead to less residual trapping in the lower sections of the reservoir. Even though the plume remains more connected with lower bottom-hole pressure, the efficiency of long-term CO₂ immobilization is reduced.

For carbonate reservoirs, the upward-decrease permeability trend is typically the most favorable conditions for long-term CO₂ storage. The reduced vertical permeability helps to create multiple capillary barriers and isolated zones. However, for more efficient injectivity during the early stages of CO₂ injection, the upward-increase trend may still be useful, as it provides better vertical flow pathways and greater plume mobility.

Therefore, carbonate reservoirs with upward-decrease permeability trends are ideal for long-term storage applications, particularly in cases where residual trapping and CO₂ immobilization are prioritized over short-term injectivity. The upward-increase trend, while favorable for initial migration and plume connectivity, should be employed with caution, as it may reduce the efficiency of long-term trapping and storage security.

5 CONCLUSIONS AND RECOMMENDATIONS

This study used numerical reservoir model to investigate the effect of vertical permeability trends on CO₂ trappings, plume evolution and injectivity. Upward-decrease and upward-increase permeability trends with different heterogeneity were systematically evaluated. The results confirmed that vertical permeability trend has a major control over plume geometry, trapping mechanisms, and pressure response.

The first main conclusion is that permeability architecture becomes more important as heterogeneity increases. When heterogeneity is low, gravity is still the main factor, and CO₂ accumulates near the top. In this case, structural trapping is dominant, while residual trapping is small and limited to local areas. At medium heterogeneity, vertical connectivity starts to clearly affect plume shape and trapping mechanisms. Under high heterogeneity, the vertical permeability trend becomes the main factor affecting plume behavior. The upward-decrease trend breaks vertical continuity, while the upward-increase architecture keeps a better-connected upward flow path and allows a larger buoyant gas accumulation.

The second major conclusion is that upward-decrease and upward-increase trends improve different trapping mechanisms. The upward-decrease trend creates partial vertical barriers in the upper reservoir. These barriers slow upward migration, which leads to increased lateral spreading and plume compartmentalization. As a result, residual trapping occurs faster, and dissolution is enhanced at later times because CO₂ remains in contact with brine-rich zones for a longer period. In contrast, the upward-increase trend provides better vertical connectivity, which allows CO₂ to flow directly upward and accumulate as a continuous gas cap. This creates more favorable conditions for structural trapping, but it reduces long term trapping, compared with the upward-decrease case. This effect becomes even more pronounced at higher heterogeneity levels.

The third conclusion is related to the temporal evolution of dissolution and residual trapping. Dissolution and residual trapping do not respond to heterogeneity in the same way or on the same timescale. In the upward-decrease architecture, both trapping indices generally increase with heterogeneity and time, particularly during the long-term post-injection period, because restricted upward movement increases residence time and repeated snap-off. In the upward-increase architecture, early vertical access can support dissolution under moderate

heterogeneity, but at very high heterogeneity preferential flow paths reduce sustained mixing-zone contact and limit late-time gains. Residual trapping follows a similar contrast: it continues to grow in the upward-decrease cases due to repeated flow interruption, whereas in the upward-increase cases it tends to level off once preferential pathways become established.

The fourth conclusion is that injectivity is also strongly controlled by vertical permeability arrangement. Bottom-hole pressure trends show that when lower-permeability layers are positioned near the base of the system, the near-well region behaves as a vertical choke, causing stronger pressure buildup and greater sensitivity to heterogeneity. When the more permeable layers are located near the base, pressure diffusion is more efficient, bottom-hole pressure remains lower, and post-shut-in pressure decline is faster. Therefore, permeability architecture affects not only how CO₂ is trapped, but also how efficiently it can be injected. Overall, this thesis fills an important gap by demonstrating that two reservoirs with identical average permeability can exhibit substantially different CO₂ storage behavior depending only on how permeability is vertically arranged.

Based on these findings, several recommendations can be made. For reservoir screening and site selection, vertical permeability ordering should be evaluated together with heterogeneity level, rather than relying only on average permeability or porosity. Reservoirs with upward-decrease architecture are more favorable when the main objective is long-term immobilization of CO₂ through residual and dissolution trapping, especially in highly heterogeneous formations. Reservoirs with upward-increase architecture may be attractive where stronger plume connectivity or structural accumulation is acceptable, but pressure buildup and reduced long-term immobilization must be carefully assessed.

Future work should focus on more realistic representations of reservoir models. Such models should account for geochemical reactions, geomechanical effects. Additionally, it should include caprock integrity evaluation, and pressure management strategies.

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