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# Numerical investigation of CO<sub>2</sub> solubility trapping mechanisms for enhanced storage in saline aquifers

Zeeshan Tariq<sup>10</sup>\*, Jose Kevin Pauyac Estrada<sup>1,2</sup>, Bicheng Yan<sup>10</sup>\*, Jianchun Xu<sup>3</sup>, Youwei He<sup>4</sup>

<sup>1</sup>Energy Resources and Petroleum Engineering, King Abdullah University of Science and Technology, Thuwal 23955-6900, Saudi Arabia <sup>2</sup>Craft & Hawkins Department of Petroleum Engineering, Louisiana State University, Baton Rouge 70803, United States of America <sup>3</sup>Key Laboratory of Unconventional Oil and Gas Development, China University of Petroleum (East China)), Qingdao 266580, P. R.China <sup>4</sup>State Key Laboratory of Oil and Gas Reservoir Geology and Exploitation, Southwest Petroleum University, Chengdu 610000, P. R. China

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#### Abstract:

Geological Carbon Storage (GCS) faces significant challenges related to the potential leakage of CO<sub>2</sub> through cap rocks, posing risks of contamination to drinking resources and disruption to various ecosystems. Therefore, it is essential to develop and implement optimal injection strategies to minimize CO<sub>2</sub> escape from the formation. This study evaluates the effectiveness of three distinct  $CO_2$  injection strategies in complex saline aquifers: pure supercritical  $CO_2$  (SC-CO<sub>2</sub>), carbonated water (CW), and Water-Alternating-Gas (WAG). The results demonstrate that SC-CO<sub>2</sub> injection primarily relies on structural trapping, complemented by residual trapping and a minor contribution from solubility trapping. In contrast, CW injection significantly enhances solubility trapping to nearly complete levels, while structural and residual trapping are minimized. On the other hand, WAG injection strategies, characterized by varying cycle frequencies, exhibit a balanced trapping profile, with solubility trapping progressively increasing while maintaining structural and residual mechanisms to support overall storage. Previous studies have shown that SC-CO2 injection efficiently fills pore spaces and displaces resident brine within the storage formation. However, the buoyant nature of  $CO_2$  remains a challenge to secure long-term storage efficiency. CW injection emerges as a promising alternative by leveraging the solubility of CO<sub>2</sub> in resident brine. Dissolving CO<sub>2</sub> in water prior to injection mitigates gravity segregation between brine and  $CO_2$ , thereby improving volumetric sweeping efficiency within the formation. Additionally, WAG injection offers potential benefits by dynamically alternating  $SC-CO_2$  and water phases to enhance trapping and immobilization. Nevertheless, both CW and WAG injection strategies face challenges related to operational costs. CW injection requires a substantial volume of water to dissolve CO<sub>2</sub>, while WAG injection demands meticulous monitoring and precise control, resulting in increased energy consumption-particularly when highly compressed CO<sub>2</sub> is needed. These factors collectively contribute to the elevated cost of CW and WAG injection strategies, highlighting the need for further optimization to enhance their economic viability.

#### 1. Introduction

Fossil fuels including coal, oil, and natural gas have long been the backbone of the global economy, serving as the primary energy source for decades (Miguel et al., 2018). However, their extensive use has significantly increased emissions of  $CO_2$  and other greenhouse gases, accelerating climate change and environmental degradation (Holt and Lindeberg, 1992). To mitigate these emissions, Carbon Capture, Utilization, and Storage (CCUS) has emerged as a promising technology (Vilarrasa and Rutqvist, 2017). According to the International Energy Agency (IEA), CCUS could contribute to a 17% reduction in global  $CO_2$  emissions by 2050 (Raza et al., 2019). CCUS involves capturing  $CO_2$  from large-scale point sources (e.g., power plants), followed by uti-

Yandy<br/>Scientific<br/>Press\*Corresponding author.<br/>E-mail address: zeeshan.tariq@kaust.edu.sa (Z. Tariq); bicheng.yan@kaust.edu.sa (B. Yan);<br/>jpauya1@lsu.edu (J. K. P. Estrada); xujianchun@upc.edu.cn (J. Xu); youweihe\_cupb@163.com (Y. He).<br/>3007-5602 © The Author(s) 2024.<br/>Received August 9, 2024; revised September 13, 2024; accepted October 13, 2024; available online October 16, 2024.

lization, transportation, and injection into geological formations for long-term sequestration (GLOBAL, 2023). Potential storage sites include saline aquifers, depleted hydrocarbon reservoirs, and coal seams (Hassanzadeh et al., 2009; Motie and Assareh, 2020; Alkan et al., 2021). While geological  $CO_2$  sequestration (GCS) has been studied since the early 1990s, challenges such as storage risks, costs, and large-scale site availability remain significant barriers to implementation (Leonenko and Keith, 2008). Addressing even one-third of current global  $CO_2$  emissions through CCUS would require storing  $CO_2$  at an average rate of 15 km<sup>3</sup>/year at reservoir conditions-5,000 times the total volume currently injected in worldwide CCS projects (Leonenko and Keith, 2008). This highlights the immense scale required for CCUS to have a meaningful impact on climate mitigation.

Among the available geological formations, deep saline aquifers offer significant storage potential due to their vast capacity and multiple trapping mechanisms (Leonenko and Keith, 2008; Grobe et al., 2009; Ajayi et al., 2019). CO<sub>2</sub> can be retained through four primary mechanisms: structural trapping, where CO<sub>2</sub> accumulates beneath impermeable caprocks; solubility trapping, where CO<sub>2</sub> dissolves into resident brine; residual trapping, where CO<sub>2</sub> is immobilized within rock pores at irreducible gas saturation; and mineral trapping, where CO<sub>2</sub> reacts with host minerals to form stable carbonate precipitates (Hassanzadeh et al., 2009; Nghiem et al., 2009). Despite these mechanisms, buoyancy remains a key challenge, as supercritical CO<sub>2</sub> (SC-CO<sub>2</sub>) is 10-40% less dense than brine, leading to lateral migration and potential leakage through caprocks (Leonenko and Keith, 2008; Hassanzadeh et al., 2009).

To enhance  $CO_2$  storage efficiency and mitigate buoyancydriven migration, alternative injection strategies have been proposed, including carbonated water (CW) and Water-Alternating-Gas (WAG) injection (Jikich et al., 2003). CW injection, initially developed for Improved Oil Recovery (IOR), involves dissolving  $CO_2$  in water before injection. This approach enhances  $CO_2$  dissolution, reduces gravity segregation, and improves volumetric sweep efficiency (Jikich et al., 2003). Meanwhile, WAG injection, originally introduced as an Enhanced Oil Recovery (EOR) method, cycles between  $CO_2$  and water slugs to enhance residual trapping, promote dissolution, and control plume migration (Agarwal and Zhang, 2014). While WAG improves storage efficiency, its higher operational complexity and cost implications require further optimization.

Traditionally, pure CO<sub>2</sub> is injected in its supercritical phase due to its advantages in solubility and wellbore stability. SC-CO<sub>2</sub> dissolves more readily in brine than gaseous CO<sub>2</sub> and prevents hydrate formation, which can obstruct injection wells (Foroozesh and Jamiolahmady, 2018). However, the high buoyancy-driven mobility of SC-CO<sub>2</sub> can result in inefficient storage and increased leakage risk. CW and WAG injection strategies have been developed to counter these issues. CW injection improves solubility trapping, while WAG enhances residual and solubility trapping through cyclic water injection (Jikich et al., 2003). CW injection was initially introduced for improved oil recovery (IOR), where injecting CO<sub>2</sub>-saturated water facilitates CO<sub>2</sub> dissolution while reducing gravity segregation effects (Jikich et al., 2003). Similarly, WAG injection, originally developed for enhanced oil recovery (EOR), involves the alternating injection of water and  $CO_2$  to mobilize residual hydrocarbons. Beyond oil recovery, researchers have demonstrated that WAG injection can significantly enhance  $CO_2$  storage efficiency by reducing plume migration, improving residual trapping, and accelerating  $CO_2$  dissolution (Agarwal and Zhang, 2014). Although additional water injection increases operational costs, WAG remains a promising technique for optimizing long-term  $CO_2$  sequestration.

In geological sequestration, the mobility ratio between the non-wetting phase ( $CO_2$ ) and the wetting phase (brine) is a critical parameter for optimizing injection efficiency. The mobility ratio is defined as:

$$M = \frac{m_n}{m_w} = \frac{\mu_w k_{rw}}{\mu_n k_{rw}} \tag{1}$$

where  $\mu_w$  and  $\mu_n$  are the viscosities of the wetting phase and non-wetting phase, respectively;  $k_{rw}$  and  $k_{rn}$  are the relative permeabilities of the wetting phase and non-wetting phase, respectively. When M < 1, the displacement of the resident wetting phase (brine water) by the injected non-wetting phase is stable, otherwise, inefficient displacement occurs due to the formation of water/gas fingers.

Considering the intermittent  $CO_2$ -water injection as a pseudo-mixture entering the aquifer during WAG injection, the mobility ratio would be lower than that of pure  $CO_2$  injection. Moreover, the mobility ratio determines the velocity for buoyancy-driven  $CO_2$  migration (Agarwal and Zhang, 2014). The enhanced  $CO_2$  dissolution is also a favorable characteristic of the WAG technique. Numerous studies have been conducted to accelerate  $CO_2$  dissolution by injecting brine into the aquifer after  $CO_2$  injection (Bryant et al., 2008; Leonenko and Keith, 2008; Orr, 2010; Agarwal and Zhang, 2014), and promising results have been obtained from numerical simulations and feasibility analysis (Leonenko and Keith, 2008; Agarwal and Zhang, 2014).

Since  $CO_2$  is more soluble in water than other gases (Sohrabi et al., 2011), CW has also attracted significant attention in GCS. This strategy offers the dual benefit of utilizing the injected CO<sub>2</sub> for EOR and GCS purposes (Sohrabi et al., 2008; Burton and Bryant, 2009; Motie and Assareh, 2020), and reducing costs related to CO<sub>2</sub> capture and pressurization (Sohrabi et al., 2008; Burton and Bryant, 2009). Previous studies showed that CW injection has been an attractive strategy as a flooding agent for more than half a century, improving its efficiency in both lab and field scales (Foroozesh and Jamiolahmady, 2018; Esene et al., 2019; Sadati et al., 2020). Additionally, CW can eliminate many deficiencies of pure supercritical CO<sub>2</sub> injection, e.g., poor volumetric sweeping efficiency due to the high mobility of  $CO_2$  (Esene et al., 2019). When injecting water with dissolved CO<sub>2</sub> for EOR purposes, the dissolved CO<sub>2</sub> transfers from the injected water to the oil phase, leading to a more gradual front of  $CO_2$  than the water front. Due to density contrasts and lower CO<sub>2</sub> mobility in carbonated water, CW injection considerably enhances the sweeping efficiency and thus displaces more oil than water-flooding or pure CO<sub>2</sub> injection (Foroozesh and Jamiolahmady, 2018). What is more, CW presents a lower risk of gravity-driven leakage, as brine with dissolved CO<sub>2</sub> naturally sinks and remains at the bottom of the injection region due to gravity. Furthermore, CW is still feasible even with insufficient  $CO_2$  sources (Sohrabi et al., 2008; Burton and Bryant, 2009; Alizadeh et al., 2014; Bisweswar et al., 2020; Motie and Assareh, 2020). However, a critical drawback arises from  $CO_2$ 's limited solubility in water: although this property reduces the absolute  $CO_2$  volume required for injection (Foroozesh and Jamiolahmady, 2018), dissolving substantial amounts of  $CO_2$  necessitates large water volumes, significantly increasing operational costs (Bryant et al., 2008; Burton and Bryant, 2009). Despite this trade-off, CW remains a pragmatic compromise between efficiency, cost, and environmental safety.

To safely contain  $CO_2$  in aquifer, it is essential to understand the multiphase fluid flow processes occurring in storage reservoirs. In this study, the process of  $CO_2$  injection for geological sequestration is simulated using the physics-driven simulator CMG-GEM (Tariq et al., 2023), which models  $CO_2$ behavior from surface injection to long-term storage, allowing for detailed monitoring of plume migration over time.

#### 2. Methodology

The primary goal of this research is to explore and analyze various  $CO_2$  injection strategies aimed at enhancing the sequestration of  $CO_2$  through increased solubility trapping within saline aquifers. The study delves into three distinct scenarios to assess their effectiveness in achieving this objective. The first scenario is the injection of supercritical  $CO_2$  (SC- $CO_2$ ); the second scenario is the injection of carbonated water (CW), which indicates brine with dissolved  $CO_2$ ; the third scenario is cyclic  $CO_2$ -brine injection, commonly known as WAG. Additionally, the research investigates five variations of cyclic injection in the WAG scenario, including scenarios WAG with 1, 2, 3, 5, and 6 cycles, respectively.

To prevent excessive pressure buildup in the reservoir during  $CO_2$  injection, a volume multiplier of  $10^6$  was applied at the lateral boundaries to simulate an infinite aquifer boundary condition. This adjustment mitigates pressure escalation and ensures stable injection conditions with low risk of cap-rock failure. The effect of this volume multiplier is particularly significant in CW injection due to its higher viscosity compared to SC-CO<sub>2</sub>, leading to a more pronounced pressure increase at the bottomhole.

#### 2.1 Model description

We take the GCS model from the 11<sup>th</sup> SPE Comparison Solution (11th SPE CSP) (SPE, 2023) in this work. Fig. 1 illustrates the sketch of the model. The reservoir is in the shape of anticline closure which elevates the central part of the domain by 150 m<sup>3</sup>. The formation size is  $8,400 \times 5,000 \times$ 1,200 m<sup>3</sup> along the x, y, and z-axis, respectively. The reservoir domain is discretized by a corner point grid system to honor the reservoir geometry, with in total  $86 \times 50 \times 60 = 25,800$ grid blocks along the x, y, and z-axis, respectively. The model presents two reservoir formations, each overlaid by a cap-rock with a very low permeability. The top of the lower and upper storage formations is at depths of 1,900 and 4,200 meters, respectively. The reservoir is initially fully saturated with water with a salinity equal to 57,000 ppm. The model is initially in hydrostatic equilibrium with an initial pressure at the top of the geometry equal to 196 bar. The reservoir has no-flow boundary conditions, and at the left and right boundary of the model, a pore volume multiplier is applied in order to avoid unphysical pressure increment, as specified in the 11<sup>th</sup> SPE CSP model description (SPE, 2023).



**Fig. 1**. Sketch of the Geometry for the CSP11C Case (SPE, 2023).

Two horizontal injection wells are considered. The horizontal part of the first injection well INJ0 follows the bending of the anticline, which is perforated between the points (5,100, 1,000, 700) meters and (5,100, 4,000, 700) meters. The horizontal part of the second well INJ1 is straight horizontal, which is perforated between the points (2,700, 1,000, 300) meters and (2,700, 4,000, 300) meters. Supercritical CO<sub>2</sub> is injected at the temperature of 40 °C and a maximum bottomhole pressure equal to 400 bar. As a result, if the injection pressure exceeds 400 bar, the well will be shut-in to stop the injection.

Three different  $CO_2$  injection strategies are assessed: SC-CO<sub>2</sub> injection, CW injection, and five WAG scenarios (1, 2, 3, 5, and 6 cycles). The simulation ensures comparability by maintaining an equal cumulative injection of  $CO_2$  and brine across all cases. Each WAG cycle consists of alternating  $CO_2$ and brine injection phases, with the duration of each phase adjusted to distribute the total 30-year injection period equally among the cycles. For instance, in the 1-cycle WAG scenario, each injection phase lasts 15 years; for 2 cycles, each phase is 7.5 years; for 3 cycles, 5 years; for 5 cycles, 3 years; and for 6 cycles, 2.5 years.

As seen in Fig. 2, there are two permeable porous storage formations in the model, which are separated by an impermeable layer, and the upper reservoir is overlaid by another impermeable layer. Thus, to store  $CO_2$  efficiently, two horizontal wells are perforated in each of the permeable formations: the well INJ0 is located in the lower storage formation, while the well INJ1 is perforated in the upper storage formation. Moreover, it is imperative to notice that the model presents four fault, as seen in Fig. 2(a). In order to make all injection scenarios comparable, the same (cumulative) amount of  $CO_2$ and brine is injected over the whole injection time. Table 1 shows the injection parameters for all cases.





WAG 1 WAG 2 WAG 3 WAG 5 WAG 6 Parameter SC-CO<sub>2</sub> CW cycle cycles cycles cycles cycles Max BHP [bar] 400 400 400 400 400 400 400 CO<sub>2</sub> mass rate 1.317 1.317 2.634 2.634 2.634 2.634 2.634 per well [Mton/y] Water mass rate 87.6 87.6 43.8 87.6 87.6 87.6 per well [Mton/y] Injected cumulative 39.501 39.501 39.501 39.501 39.501 39.501 39.501 CO<sub>2</sub> per well [Mton] Injected cumulative 1314 1314 1314 1314 1314 1314 water per well [Mton] Total amount of pore 5.082 E-3 3.150 E-4 5.398 E-3 5.398 E-3 5.398 E-3 5.398 E-3 5.398 E-3 volume injected PV PV PV PV PV PV PV (both wells)

Table 1. Model injection parameters.

#### 2.2 Relative permeability and capillary pressure

In this work, the relative permeability and capillary pressure functions for each facie in the model obeys the Brook-Corey correlation as specified in the spe11c description (SPE, 2023), and the formulation will not be repeated here. Fig. 3 shows the relative permeability and capillary pressure functions, respectively

#### 2.3 CO<sub>2</sub> solubility in aqueous phase

The equation of state (EOS) used in this work is the well known Peng-Robinson (PR) to calculate the  $CO_2$  thermodynamic properties.

Since the  $CO_2$  solubility in the aqueous phase is a quick process, a thermodynamic equilibrium between the gas and aqueous phases can be assumed, as shown in Eq. 2:

$$f_{ig} - f_{iw} = 0, \quad i = 1, 2, ..., n_g$$
 (2)

where  $f_{ig}$  and  $f_{iw}$  are the component *i* fugacities in the gas and aqueous phases.

 $f_{ig}$  is calculated from the PR EOS while  $f_{iw}$  uses Henry's law that relates the fugacity of a component to its concentration as shown in Eq. 3:

$$f_i = x_{iw} * H_i \tag{3}$$

where  $x_{iw}$  is the mole fraction of component *i* in the liquid

phase,  $H_i$  is Henry's constant, which is a function of pressure, temperature, and aqueous phase salinity.

Thus, since  $CO_2$  solubility in the aqueous phase plays a significant role, it is crucial to know the amount of  $CO_2$ dissolved ( $CO_2$  concentration) in the aqueous phase under certain pressure and temperature conditions. The United States Geological Survey has developed a software called PHREEQC to calculate the  $CO_2$  solubility in the aqueous phase, as seen in Fig. 4.



**Fig. 4.**  $CO_2$  solubility at high pressures with no salinity (Parkhurst and Appelo, 2013).

Fig. 4 shows the comparison between experimental data (points) and the simulator PHREEQC (solid lines). The data



Fig. 3. Brooks-Corey relative permeability (a) and capillary pressure (b) for each facie.

points were taken from experimental data provided by Duan et al. (2006), and Spycher et al. (2003). As mentioned previously, one of the cases studied in this work is the co-injection of  $CO_2$  and brine (CW), thus, it is crucial to know the  $CO_2$  concentration (molality) in brine so that 100% of the injected  $CO_2$  will be dissolved in the aqueous phase (injected brine). Fig. 5 shows the  $CO_2$  molality dissolved in water with different salinity (0 and 2 molal) at different pressures and temperatures calculated using PHREEQC.



Fig. 5. CO<sub>2</sub> solubility comparison with no salinity and salinity.

As seen from Fig. 5, it can be seen that the  $CO_2$  solubility increases when increasing the pressure but decreases as temperature and salinity of the water increases. This behavior was previously reported by (Sadati et al., 2020; Addassi et al., 2021).

#### 3. Governing Equations

Several studies showed that when supercritical  $CO_2$  is injected into a deep saline aquifer, a two-phase fluid flow is created (brine-CO<sub>2</sub>) (Celia et al., 2015; Zamani et al., 2024). The CO<sub>2</sub> is slightly miscible with the brine with up to a few percent by mass dissolving into the brine, and an even smaller H<sub>2</sub>O fraction (less than 1 %) can evaporate into the CO<sub>2</sub> phase (Celia et al., 2015).

When  $CO_2$  dissolves into the resident brine, the pH of the aqueous phase decreases, driving a sequence of geochemical reactions in the saline aquifer and aquitard rocks and in well cements. Similarly, H<sub>2</sub>O partitions into the CO<sub>2</sub>-rich phase

creates "wet"  $CO_2$ , which can be much more corrosive to metal piping compared to "dry"  $CO_2$  (Celia et al., 2015).

#### 3.1 Mass balances and constitute equations

 $CO_2$ -brine system involves basic balance equations, written either for the bulk phases or for the major components of the phases. The mass balance equation for each component in the system is described by Eq. 4 (Celia et al., 2015):

$$\sum_{\alpha} \left[ \frac{\partial (\rho_{\alpha} \phi s_{\alpha} m_{\alpha}^{i})}{\partial t} + \nabla (\rho_{\alpha} u_{\alpha} m_{\alpha}^{i} + j_{\alpha}^{i}) \right] = \sum_{\alpha} \psi_{\alpha}^{i} \qquad (4)$$

where  $\rho_{\alpha}$  is the density of the phase  $\alpha$ ,  $\phi$  is the porosity,  $s_{\alpha}$  is the saturation of the fluid phase  $\alpha$ ,  $m_{\alpha}^{i}$  is the mass fraction of component *i* in the phase  $\alpha$ ,  $u_{\alpha}$  is the volumetric flux vector (Darcy flux) for phase  $\alpha$ ,  $j_{\alpha}^{i}$  is the non-advective flux vector (diffusion and mechanical dispersion) for component *i* in phase  $\alpha$ ,  $\psi_{\alpha}^{i}$  is the external sources or sinks of mass for component *i* in phase  $\alpha$ . In the equation, components represent CO<sub>2</sub>, H<sub>2</sub>O, NaCl, and others if any  $i = CO_2, H_2O, NaCl, ...$  and phases called brine and CO<sub>2</sub>.

The mass balance equation needs to be augmented by constitutive equations and equations of state, including the multiphase extension of Darcy's equation (Celia et al., 2015):

$$u_{\alpha} = -\lambda_{\alpha} k (\nabla p_{\alpha} - \rho_{\alpha} g) \tag{5}$$

where  $k_{r,\alpha}$  is the relative permeability, taken as a scalar and a function of the phase saturation  $s_{\alpha}$ , k is the intrinsic permeability tensor,  $\mu_{\alpha}$  is the phase viscosity,  $\lambda_{\alpha}$  is the phase mobility,  $p_{\alpha}$  is the phase pressure, g is the gravitation acceleration vector directed downward with the positive vertical direction pointed upward.

Additional equations include:

$$\sum_{\alpha} m_{\alpha}^{i} = 1 \tag{6}$$

$$\sum_{\alpha} s_{\alpha}^{i} = 1 \tag{7}$$

#### 3.2 Equations for horizontal wells

Horizontal wells can greatly improve both injectivity and storage capacity, as well as lead to a higher CO<sub>2</sub> dissolution rate compared to the vertical injection well when waterchasing injection is applied.

In CMG, for a horizontal well, the wellbore (flowing bottomhole) and the pressure at the grid block containing the well are related by the Eq. (8) (Peaceman, 1993):

$$p_{wf} = p_o - \frac{q\mu}{2\pi (k_x k_z)^{1/2} \Delta y} \ln \frac{r_o}{r_w}$$
(8)

For an an anisotropic medium:

$$r_o = \frac{0.14(k_z/k_x)^{1/2}\Delta x^2 + (k_x/k_z)^{1/2}\Delta z^2}{0.5[(k_zk_x)^{1/4} + (k_x/k_z)^{1/4}]}$$
(9)

#### 4. Results and discussions

#### 4.1 Efffect of carbonated brine injection

Fig. 6 illustrates the global CO<sub>2</sub> mole fraction within the horizontal (XY) and vertical (YZ) planes across the storage porous formations, considering both pure SC–CO<sub>2</sub> and CW injection scenarios for both horizontal wells. For both cases, the injection rate of CO<sub>2</sub> and brine for both wells is equal to  $1.93 \times 10^7$  mol/d (about 1.32 MMton/y) and  $1.2 \times 10^8$  kg/d (about 43.8 MMton/y), respectively.



**Fig. 6.** Global  $CO_2$  mole fraction for the SC- $CO_2$  and CW injection cases for both INJ0 and INJ1 horizontal wells after 30 years in XY, YZ, and XZ planes.

Additionally, since a small section of the well INJ1 is perforated in a low-permeability zone ( $K_i = 0.1 \text{ mD}$ ) as seen from Fig. 2(a), a slight leakage can be seen in Fig. 6 (YZ plane) when injecting CW. However, this slight leakage does not happen when injecting SC-CO<sub>2</sub> since it tends to flow upwards due to gravity effects. From Fig. 2(a), a sealing fault can be seen in the upper storage formation where the well INJ1 is located. When injecting CW into the formation, the CO<sub>2</sub> plume reaches the sealing, not allowing the CO<sub>2</sub> to flow through it. However, the CO<sub>2</sub> can flow through neighboring lower cells, and thus, CO<sub>2</sub> plume can be seen on the left side of the sealing (XY and YZ planes). Furthermore, it is imperative to mention that CO<sub>2</sub> follows the permeability distribution along the storage formations easier when injection injecting pure SC-CO<sub>2</sub> than CW. Although supercritical CO<sub>2</sub> indeed combines characteristics of both liquids and gases, the CO<sub>2</sub> tends to exhibit a lower viscosity when it is injected pure rather than injecting it dissolved in the aqueous phase (carbonated water). This lower viscosity allows SC-CO<sub>2</sub> to flow through porous formations more readily, navigating the permeability distribution with reduced resistance. Thus, it can be seen in Fig. 6 from the XZ plane that the CO<sub>2</sub> plume follows the permeability field shown in Fig. 2(a) when injecting it pure through the horizontal well INJO.

Since CW is basically water containing dissolved CO<sub>2</sub>, it increases the amount of CO2 that can be dissolved in the formation resident brine. Thus, as seen in Fig. 6, when injecting CW into a saline aquifer, the CO<sub>2</sub> spreads through a higher area than in the case of pure SC-CO<sub>2</sub>. This can be seen in Fig. 7. Structural trapping arises from the behavior of free (buoyant) CO<sub>2</sub> nature during its injection into geological formations, being trapped within the geological structure of the reservoir. In other words, structural trapping relies on the  $CO_2$  molecules becoming physically trapped in the pore space and, thus, forming structures that prevent their movement. In the context of the CW injection, where the  $CO_2$  is already dissolved in brine prior to injection, the CO<sub>2</sub> buoyant nature is eliminated. However, as the CW solution flows from the surface to the subsurface formation, temperature changes attributed to the geothermal gradient-may induce the release of CO<sub>2</sub> from the CW solution. For this reason, structural trapping contribution is significantly lower for the CW injection case, as seen in Fig. 7. Additionally, when  $CO_2$  is injected in its supercritical state, the resident fluid in the storage formation is displaced as the CO<sub>2</sub> flows through the porous media, and small portions are left behind as residual droplets in the porous rock. Moreover, when injecting SC-CO<sub>2</sub>, it tends to remain in this state, being more effectively trapped by capillary forces in the pore space. In contrast, the injected CW is more mobile and, thus, may not be effectively trapped in the pore space over the long term. Fig. 7 shows that the  $CO_2$  residual trapping contribution is significantly less for the CW case than for the SC-CO<sub>2</sub> case.



**Fig. 7**.  $CO_2$  trapping mechanisms relative contribution for both SC- $CO_2$  and CW injection cases.

Table 2 shows the quantity of CO<sub>2</sub> trapped by solubility, structural, and residual mechanisms for the SC-CO<sub>2</sub>, and CW injection cases.

Table 2. Amount of  $CO_2$  trapped by different mechanismsfor the SC-CO2 and CW cases after 30 years of continuousinjection.

Trapping mechanism	SC-CO <sub>2</sub>	CW
Structural (Supercritical CO <sub>2</sub> )	7.710E11 mol	1.601E7 mol
Residual (Trapped CO <sub>2</sub> )	2.275E11 mol	1.601E7 mol
Solubility (Dissolved CO <sub>2</sub> )	1.277E11 mol	8.978E11 mol

## **4.2** Effect of Water-Alternating-Gas (WAG) injection

In this work, the WAG method was also studied for GCS in saline aquifer for two horizontal wells. Five cases were simulated: i) WAG injection with one cycle, ii) WAG injection with two cycles, iii) WAG injection with three cycles, iv) WAG injection with five cycles, and v) WAG injection with six cycles. One complete cycle is when SC-CO<sub>2</sub> injection is followed by brine injection. For simplicity, we set that each cycle is identical with equal time of injection phase. Fig. 8 represents a schematic representation of the considered WAG injection.

In this section, we focus on only the first scenario case (WAG injection with one cycle) to compare it to the baseline case of SC-CO<sub>2</sub> injection. And, in the next section, the impact of the number of cycles on the global  $CO_2$  mole fraction will be studied.



Fig. 8. WAG injection schematic representation.

In order to make WAG case comparable to the previous ones (SC-CO<sub>2</sub> and CW), the same amount of CO<sub>2</sub> and water (cumulative) should be injected over the whole injected period (30 years). Thus, the rate of the injected CO<sub>2</sub> and brine for both cyclic cases is equal to  $1.64 \times 10^8$  mol/d (about 2.64 MMton/y) and  $2.4 \times 10^8$  kg/d (about 87.6 MMton/y), respectively through each well.

Fig. 9 presents the global  $CO_2$  mole fraction within the horizontal (XY) and vertical (YZ and XZ) planes across the storage zone, comparing scenarios of the SC-CO<sub>2</sub>, and WAG with one cycle. Fig. 9 shows that the WAG injection enhances the sweeping efficiency of  $CO_2$  along the storage zone, reaching a higher distance in comparison with the pure SC-CO<sub>2</sub> case, but a lower distance than when injecting CW. When injecting brine cyclically after  $CO_2$  (two phases and not one as in the CW injection case), it can be clearly observed that the buoyancy effect of the  $CO_2$  plume is minimized. In the case of WAG injection with one cycle, SC-CO<sub>2</sub> is injected for the first 15 years, and then, brine is injected for the following 15 years.

During the pure  $SC-CO_2$  injection phase, the  $CO_2$  tends to accumulate in the upper part of the perforated section of the well INJ0, but then, when the brine injection phase starts, the water minimizes the segregation effect of the previously injected SC-CO<sub>2</sub>, and displaces the CO<sub>2</sub> from the nearwellbore zone to the upper part of the formation. Moreover, as explained before, the water improves the CO<sub>2</sub> dissolution and sweeping efficiency, making the CO<sub>2</sub> plume reach a further horizontal distance as seen from YZ and XZ planes.



**Fig. 9.** Global  $CO_2$  mole fraction for the SC- $CO_2$  and WAG with one-cycle cases for both INJ0 and INJ1 horizontal wells after 30 years in XY, YZ, and XZ planes.

Moreover, similar to the SC-CO<sub>2</sub> case, the CO<sub>2</sub> plume in the WAG with one cycle case also follows the highpermeability channels. As seen in Fig. 2(a), the lower and upper storage zones are connected through a tiny channel in the left part of the reservoir domain. Since the brine injection leads to an improved CO<sub>2</sub> sweeping efficiency, the CO<sub>2</sub> plume reaches a longer horizontal distance, flowing from the lower to the upper formations. Depending on the injection rate, a higher or lower amount of CO<sub>2</sub> will flow from the lower to the upper formation.

Fig. 10 shows the relative contribution of the different  $CO_2$ trapping mechanisms (structural, residual, and solubility) over time for the supercritical CO<sub>2</sub>, CW, and WAG with single cycle cases. From Fig. 10, it can be seen that the CW injection case brings highest solubility trapping but lowest structural trapping since the CO<sub>2</sub> prior to injection is comprehensively dissolved in the aqueous phase eliminating the buoyancy effects, improving the storage efficiency. As mentioned previously, in order to make all cases comparable, the same amount of CO<sub>2</sub> (cumulative) should be injected over the whole simulation time (30 years), thus, the injection rate for the WAG injection case with one cycle is twice the rate for the pure SC-CO<sub>2</sub> case. For this reason, even though pure SC-CO<sub>2</sub> is injected during the first 15 years, a higher amount of  $CO_2$  is trapped in the formation (higher solubility trapping). Then, as the subsequent 15-year phase of pure brine injection starts, it improves the CO<sub>2</sub> dissolution into the in-situ formation brine, significantly increasing the solubility trapping. As for the other two cases, during the first 15 years of continuous injection, the structural



Fig. 10. Relative contributions of different  $CO_2$  trapping mechanisms for the SC-CO<sub>2</sub>, CW, and WAG with a single cycle cases.

trapping is higher for the cyclic case than for the pure SC- $CO_2$ , even though pure SC- $CO_2$  is injected for both cases in this period. This is because the injection rate for the cyclic case is twice the rate for the pure SC- $CO_2$ , leading to a higher amount of buoyant SC- $CO_2$  in the formation. On the other hand, as brine injection starts for the cyclic case for the subsequent 15 years, the  $CO_2$  in the reservoir is displaced, and its buoyancy nature is minimized by the injected brine, decreasing the amount of free  $CO_2$  in the storage formation, being slightly lower than for the pure SC- $CO_2$  case, as seen from Fig. 10.

Fig. 10 shows the CO<sub>2</sub> residual trapping mechanism for all cases studied in this section, being the lowest for the CW case. For the first 15 years, the residual trapping is higher for the cyclic case than for the SC-CO<sub>2</sub> case, since more CO<sub>2</sub> is injected. Then, as the brine injection phase occurs for the subsequent 15 years, the residual trapping decreases. This is because the brine improves the CO<sub>2</sub> dissolution into the formation brine, altering the phase behavior of CO<sub>2</sub> and potentially reducing its ability to be trapped in the pore spaces.

Table 3 shows the quantity of  $CO_2$  trapped by solubility, structural, and residual mechanisms for the SC-CO<sub>2</sub>, CW, and WAG with single cycle injection scenarios.

#### **4.3 Effect of WAG injection with multiple cycles**

Previously, we explored the effect of WAG injection with a single cycle on various  $CO_2$  trapping mechanisms, with a specific emphasis on solubility trapping. In this section, we extend our investigation to encompass different injection strategies with multiple cycles. Specifically, four additional cases are studied, characterized by 2, 3, 5, and 6 cycles. The objective is to assess the impact of the number of injection cycles on the efficacy of trapping mechanisms.

Fig. 11 presents the global  $CO_2$  mole fraction within the horizontal (XY) and vertical (YZ and XZ) planes across the storage porous zones, considering the WAG with 1, 2, 3, 5, and 6 cycles cases for both horizontal wells. From the plane XY in Fig. 11, when injecting the fluid through both wells, it can be seen that the  $CO_2$  global mole fraction increases in the near-wellbore area. This phenomenon can be attributed to the increased number of cycles, leading to a reduction in the duration of each cycle. This shortened cycle time allows for more frequent injections of pure supercritical  $CO_2$  and brine, contributing to the observed rise in the  $CO_2$  concentration near the wellbore area. Consequently, with an increased frequency of pure  $CO_2$  injections, there is a corresponding accumulation of  $CO_2$  in the near-wellbore regions. Furthermore, a higher number of brine injections results in the  $CO_2$  plume traveling a greater distance from the well, attributed to an improved  $CO_2$ sweeping efficiency, as illustrated in the preceding section. Thus, the more times pure  $CO_2$  is injected, the more it accumulates in the near-wellbore region. Additionally, the more times brine is injected, the  $CO_2$  plume travels a further distance from the well due to an enhanced  $CO_2$  sweeping efficiency, as demonstrated in the previous section.



**Fig. 11.** Global  $CO_2$  mole fraction for the WAG case with 1, 2, 3, 5, and 6 cycles for both INJ0 and INJ1 horizontal wells after 30 years in XY, YZ, and XZ planes.

Moreover, from the plane XZ, for the WAG case with a single cycle, it can be seen that the  $CO_2$  flows from the lower to the upper formation through the interconnected permeable region when injected through the well INJ0, as seen in Fig. 6 and Fig. 11. However, this behavior is minimized when increasing the number of cycles. When injecting brine more frequently, the buoyancy effects of the  $CO_2$  are diminished. Consequently,  $CO_2$  tends to settle at the bottom due to gravity segregation with brine, leading to a reduction in the amount

**Table 3.** Amount of  $CO_2$  trapped by different mechanisms for the SC-CO2, CW, and WAG with 1 cycle injection cases after30 years of continuous injection.

Trapping mechanism	SC-CC	$D_2$ (	CW	WAG-1 cycle	
Structural (Supercritical CO2	2) 7.71E1	1 mol	1.60E7 mol	5.54E11 mol	
Residual (Trapped CO <sub>2</sub> )	2.27E1	1 mol	1.60E7 mol	2.71E11 mol	
Solubility (Dissolved CO <sub>2</sub> )	1.27E1	1 mol 8	8.97E11 mol	3.43E11 mol	
SC CO <sub>2</sub>		CW	WAG	1 cycle	
\$ <sup>100</sup>	100		100		
5 80	80		90		
rtio	80		801		
	60		60		
put					
Ŭ 40	40		40		
	20		20		
U Structural Residual	20 Structural Residual		20 Structural Residual		
	0 Solubility	1 2017 2024	O Solubility	2017 2024	
2004 2011 2017 2024 Year	2004 201	1 2017 2024 Year	2004 2011 Y	2017 2024 'ear	
WAG 2 cycles WAG	G 3 cycles	W	AG 5 cycles	WAG 6 cycles	
100		100		100	
80		80 -		80	
60		60		60	
40 40		40		40	
20.		20		20	
20 Structural Residual		Structural Residual		Residual	
	1 2017 2024	0 Solubility	011 2017 2024	0 Solubility	
2004 2011 2017 2024 2004 201 Vear	Year	2004 20	Year	2004 2011 2017 2024 Year	

**Fig. 12**. CO<sub>2</sub> trapping mechanisms relative contribution for the SC-CO<sub>2</sub>, CW, and WAG with 1, 2, 3, 5, and 6 cycles injection cases.

of buoyant SC-CO<sub>2</sub> in the upper part of the lower storage formation. This behavior is further evident in the YZ plane when injecting fluids through the horizontal well INJ1, where the global CO<sub>2</sub> mole fraction exhibits a decrease in the upper sections of both the upper and lower formations.

Relative Contribution (%)

Fig. 12 shows relative contribution of the different  $CO_2$  trapping mechanisms (structural, residual, and solubility) over time. It can be seen that the contribution of the solubility trapping is the highest for the CW injection case since the injected aqueous phase eliminates the buoyancy effects, improving the storage efficiency. For the cyclic cases, since the  $CO_2$  mass rate is two times higher than for the SC- $CO_2$ , a higher amount of  $CO_2$  is trapped in the formation brine (higher solubility trapping).

Moreover, to gain a clearer understanding of the cyclic cases, we will segment the 30 years of continuous injection into twelve distinct frames, each lasting 2.5 years. During the initial 2.5-year period, where all cyclic cases involve  $CO_2$  injection exclusively, the solubility trapping mechanism remains consistent. However, as the subsequent 2.5-year phase begins, the case with six cycles introduces the injection of brine. This results in a notably higher quantity (sharper increment of  $CO_2$  being dissolved into the formation brine compared to the other cyclic cases, where pure SC-CO<sub>2</sub> injection persists, except for the case with 5 cycles. In this instance, the brine injection initiates after 3 years, leading to a slightly higher solubility trapping than the case with 6 cycles. This pattern continues throughout the timeline, signifying that the injection of  $CO_2$ 

contributes to an increment of the amount of dissolved  $CO_2$  within the formation brine. Simultaneously, the introduction of brine injection leads to a sharper increment of the solubility trapping. At the end of 30 years of continuous injection, the trend becomes evident-the amount of dissolved  $CO_2$  increases when the number of cycles increases.

In the context of structural trapping, a similar trend is observable. Fig. 12 shows that the contribution of the structural trapping is the lowest for the CW case. For the cyclic cases, specifically during the first 2.5 years of pure SC-CO<sub>2</sub> injection, the amount of free CO<sub>2</sub> trapped in the reservoir structure remains constant. However, when the brine injection phase starts, structural trapping decreases as the aqueous phase displaces the buoyant SC-CO<sub>2</sub> in the reservoir, enhancing CO<sub>2</sub> dissolution. Furthermore, another notable observation is that during the first (initial) pure SC-CO<sub>2</sub> injection phase, the structural trapping is considerably higher for all cyclic cases compared to the pure SC-CO<sub>2</sub> case. This is due to the significantly higher CO<sub>2</sub> injection rate for the cyclic cases compared to the pure SC-CO<sub>2</sub> case.

However, at the end of the whole injection period (after 30 years), Fig. 12 shows that the structural trapping contribution is the highest for the pure  $SC-CO_2$  case since no brine is injected at all. For the cyclic cases, as explained before, when the brine injection phase starts, it increases solubility trapping but decreases the amount of buoyant  $SC-CO_2$  in the reservoir, and thus, the structural trapping reduces. Additionally, it can be seen that the structural trapping decreases when the number of

**Table 4.** Amount of CO2 trapped by different mechanisms for the SC-CO2, CW, and WAG with 1, 2, 3, 5, and 6 cyclesinjection cases after 30 years of continuous injection. (Unit: mol)

Trapping mechanism	SC-CO <sub>2</sub>	CW	WAG-1 cycle	WAG-2 cycles	WAG-3 cycles	WAG-5 cycles	WAG-6 cycles
Structural							
(Supercriti- cal CO <sub>2</sub> )	7.7107E11	1.6019E7	5.5418E11	4.9500E11	4.6277E11	3.9617E11	3.3753E11
Residual							
((Trapped CO <sub>2</sub> )	2.2755E11	1.6015E7	2.7161E11	2.2826E11	2.1052E11	1.8787E11	1.6845E11
Solubility							
((Dissolved CO <sub>2</sub> )	1.2778E11	8.9787E11	3.4324E11	3.9372E11	4.3775E11	5.0514E11	5.3273E11

cycles increases. This phenomenon is attributed to the higher frequency of brine injection following the phase of pure SC- $CO_2$  injection.

Furthermore, Fig. 12 shows the contribution of the residual trapping mechanism of  $CO_2$ , being the lowest for the CW case. The residual trapping is significantly higher for the cyclic cases compared to the pure SC-CO<sub>2</sub> case during the first CO<sub>2</sub> injection phase. This is because the injection rate for the cyclic case is twice the rate for the pure SC-CO<sub>2</sub> case.

Subsequently, similar to the observed trend for the  $CO_2$  structural trapping mechanism, the quantity of  $CO_2$  trapped in the porous space decreases during the brine injection phase. This can be attributed to the increased sweeping efficiency of  $CO_2$  by the brine, and enhanced  $CO_2$  dissolution within the formation brine. Fig. 12 underscores the impact of the number of cycles on the residual trapping. As the number of cycles increases, the amount of  $CO_2$  trapped in the porous space decreases due to the higher frequency of displacement and dissolution of  $CO_2$ .

Table 4 shows the quantity of CO<sub>2</sub> trapped by solubility, structural, and residual mechanisms for all cases.

Fig. 13 supplements the insights from Fig. 12, providing a more nuanced understanding of each CO<sub>2</sub> trapping mechanism's contribution after 30 years of continuous injection. It can be clearly seen that the contribution of the solubility trapping is significantly higher for the CW case than for the SC-CO<sub>2</sub> case. And, when introducing the WAG injection, the solubility trapping increases as the number of cycles increments. In contrast, the pure SC-CO<sub>2</sub> case exhibits the highest degree of structural trapping, while the WAG case with a single cycle excels in residual trapping. Moreover, the amount of  $CO_2$  trapped by both structural and residual mechanisms reduces as the number of cycles increases. For the case of the CW injection scenario, both structural and residual trapping mechanisms contribute little to the overall amount of trapped CO<sub>2</sub>, playing a minor role, as seen in Fig. 13. Importantly, it is emphasized that the solubility trapping stands out as the primary contributor to GCS when injecting carbonated water into the storage formation. And, its contribution increases when incrementing the number of

cycles for the WAG injection.



Fig. 13. Contribution of different CO<sub>2</sub> trapping mechanisms.

#### 4.4 Impact on the bottomhole pressure

The injection of  $CO_2$  into a saline aquifer significantly increases pressure in the vicinity of the wellbore. Depending on the injection rate, this pressure increment can be substantial and potentially damage the formation. To mitigate the risk of uncontrolled pressure buildup, a volume increment of  $10^6$  was applied at the lateral boundaries of the reservoir, effectively simulating an infinite aquifer, as seen in Fig. 14.



Fig. 14. Volume multiplier.

With the incremental volume at the lateral boundaries by  $10^6$ , the pressure experiences a slight increase during the injection of pure Supercritical CO<sub>2</sub> (SC-CO<sub>2</sub>), remaining



Fig. 15. Bottomhole pressure for the SC-CO<sub>2</sub>, CW, and WAG with single and multiple cycles injection cases.

relatively constant. In contrast, when employing Carbonated Water (CW) injection, the higher viscosity of CW, compared to pure SC-CO<sub>2</sub>, induces a pronounced pressure surge at the bottomhole, as evident in Fig. 15.

Furthermore, in the cyclic injection scenarios, the pressure remains relatively steady during the injection of pure SC-CO<sub>2</sub>, as previously mentioned. However, the subsequent injection of brine, characterized by its incompressibility, triggers a sharp rise in pressure. Additionally, it is noteworthy that due to the deeper location of well INJ0 compared to INJ1, the pressure at the bottom is higher. This pressure variation is illustrated in Fig. 15.

#### 5. Conclusions and recommendations

In this work, different  $CO_2$  trapping mechanisms were studied with a focus on solubility trapping. To achieve this goal, three injection strategies were analyzed: pure supercritical  $CO_2$  (SC-CO<sub>2</sub>), carbonated water (CW), and wateralternating-gas (WAG) with 1, 2, 3, 5, and 6 cycles, in which the same amount of  $CO_2$  and brine in term of mass were injected over the whole injection period (30 years) through two horizontal wells. This comprehensive study reveals the effectiveness of these injection strategies and highlights the role of solubility trapping as a prominent and sustainable mechanism for long-term  $CO_2$  geological storage since it is the most effective way to safely store  $CO_2$  underground because it prevents the  $CO_2$  from escaping from the storage formation. Based on the insights gathered from the results, the following conclusions can be inferred:

- The CW injection strategy is the most favorable among the options, as it enhances sweeping efficiency and CO<sub>2</sub> dissolution, reducing gravity segregation and minimizing residual and structural trapping. This results in safer and more secure geological CO<sub>2</sub> sequestration.
- The WAG injection strategy shows that increasing cycling frequency enhances solubility trapping compared to pure

 $SC-CO_2$  injection. However, as the cycle count rises, the duration of each cycle decreases, eventually resembling continuous CW injection. WAG also reduces  $CO_2$  leakage by breaking the gas into smaller, immobilized blobs and minimizing gravity effects, leading to a more uniform reservoir sweep. Despite its technical advantages, selecting the best injection strategy requires economic analysis, as both CW and WAG involve high water demand, making them costly options.

- 3) A detailed analysis of the effect of increasing WAG cycles (1-6) on CO<sub>2</sub> trapping mechanisms shows that structural trapping is progressively reduced as more cycles are introduced, while solubility trapping increases. Residual trapping remains significant but is influenced by the rate at which CO<sub>2</sub> is displaced by brine. This suggests that while WAG enhances solubility trapping, an optimal number of cycles must be determined to balance efficiency and operational complexity.
- 4) While WAG and CW injection strategies offer improved CO<sub>2</sub> sequestration efficiency, their feasibility depends on economic and operational factors. The high water demand for both methods presents a significant challenge, increasing costs and logistical complexity. Further economic feasibility studies are required to assess the trade-offs between improved sequestration efficiency and operational costs.

#### **Conflict of interest**

The authors declare no competing interest.

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