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Research Article

Influence of CO2 Injection Stream Impurities on CO2 Storage Efficiency in Deep Aquifers: A Gulf of Guinea Case Study

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ABSTRACT

This study investigates the impact of impurities in CO_2 injection streams on storage efficiency within deep saline aquifers. It focuses on the implications for CO_2 capture, transportation and geological storage operations. The paper has unfolded that CO_2 captured from industrial processes commonly contains contaminants such as non-condensable gases (N_2, O_2, Ar), acidic gases (SO_2, NO_x, H_2S), hydrocarbon gases (CH_4, CO) and residual water. Each of these aspects influence the storage in different manner. The presence of impurities especially modifies the thermodynamic behaviour of injected CO_2 streams, which in turn, affects phase behaviour, density, viscosity and solubility in formation waters. Simulations conducted using the Rio del Rey Basin case study have furhter illustrated that impurities significantly influence injectivity, plume migration, geochemical interactions and overall storage capacity. Scenarios containing lighter, low-solubility gases (e.g., CH_4, N_2, H_2) enhanced volumetric storage and injectivity by reducing density and viscosity, yet increased plume buoyancy and migration risks. Conversely, highly reactive impurities (e.g., H_2S, SO_2) showed reduced plume migration due to solubility-driven reactions but posed significant risks of geochemical alteration, mineral precipitation and reduced injectivity due to pore clogging. The findings highlight crucial trade-offs between purification costs and storage performance, suggesting that moderate impurity tolerance can economically benefit CO_2 storage projects if managed carefully. Ultimately, this study underscores the importance of precise impurity management and monitoring strategies to optimize storage efficiency, ensure geological integrity and comply with regulatory standards for safe, long-term CO_2 sequestration.

Keywords: CO_2 Injectivity; CO_2 Storage Efficiency; CCS; CCUS; Aquifer; Climate Change; numerical Simulation; CO_2 sequestration; CO_2 Injection Stream Impurities

Introduction

CO_2 that is captured from industrial processes, is seldom 100% pure; there can be a variety of contaminants present as per the source and method of capturing[1]. The impurity levels that are permissible, are typically set by transport and storage considerations well-adjusted alongside economic feasibility. In reality, streams of CO_2 are required to be predominantly CO_2 (often >90-95% by volume) to ensure efficient and safe storage. If there is an increase in the impurity content, the phase behaviour of CO_2 shifts, which can necessitate higher injection pressures to maintain a dense phase[2].

Classification of common impurities

Impurities in a CO_2 stream can be grouped by their nature and source:

Non-condensable gases (N_2, O_2, Ar): Nitrogen (N_2), argon (Ar) and oxygen (O_2) are the primary components of inert gas, that are largely introduced into the CO_2 stream from air utilized during combustion or industrial process streams. These gases, at the usual conditions of geological storage, remain in the form of gas and do not get liquefy because of their low critical temperatures and pressures[3]. As the consequence, their presence brings about dilution of the CO_2-rich phase, which significantly decreases the density and overall storage capacity of the injected fluid mixture. Given that nitrogen and argon are chemically inert, they exhibit negligible interaction with reservoir rocks or formation waters. However, in this respect, oxygen differs notably but it remain similarly in gasous state under storage conditions, which leads to actively promote microbial activity or participate in oxidative chemical reactions with reservoir minerals. As a result, there can be potential changes in dynamics of storage.

Acidic components (SO_2, NO_x, H_2S, CO_2's own byproducts): These are acid-forming gases that strongly interact with water. SO_2 and NO_x (NO and NO_2) originate from fuel sulfur and high-temperature combustion in air, respectively and can remain in the CO_2 stream if not completely scrubbed[4]. As noted by Chen[5], H_2S can accompany CO_2 from natural gas processing or pre-combustion capture of sulfurous fuels. In the presence of water, these form acids (sulfuric, nitric, sulfurous), which can corrode equipment and react with reservoir rocks. They are often limited to low concentrations due to corrosion and toxicity concerns (e.g. H_2S is poisonous).

Hydrocarbon gases (CH_4, CO): Methane and occasionally carbon monoxide can appear especially in CO_2 streams from pre-combustion processes or natural gas processing. CH_4 is a component of natural gas that may slip through capture and CO can be present if combustion is incomplete or in synthesis gas streams. These components are combustible, but in the dilute concentrations within CO_2 streams they pose little flammability risk. Their main impact is on physical properties: CH_4, for instance, lowers the density of the CO_2 mix and raises its volatility, affecting storage volume and buoyancy. CO is typically very low if present at all, but is toxic and might be flagged in safety analyses.

Water (H_2O): Water vapor is often present in raw CO_2 from combustion (as a combustion product) and must be dried to low levels before transport and injection[6]. Any residual water in the CO_2 stream is considered an impurity as it can form carbonic acid with CO_2, leading to corrosion in pipelines and wells. In the reservoir, water will mostly stay in the aqueous phase, but the presence of water in the injected CO_2 can facilitate hydrate formation under certain conditions or enhance corrosion if liquid water condenses[7]. Generally, pipeline specs require very low H_2O (dew point control to avoid free water).

Other trace substances: Depending on the source, there may be trace amounts of substances like Argon (common with oxy-fuel capture since industrial O_2 is ~95–99% O_2 with Ar as the main impurity), Hydrogen (H_2) (from pre-combustion capture of syngas where H_2 can slip through), carbonyl sulfide (COS) (a sulfur species from fuel that can form during combustion/gasification), solvent degradation products (amines, ammonia from post-combustion capture solvents) or heavy metals/mercury (in flue gas, though mercury is usually captured by pollution controls; any that enters CO_2 stream must be extremely low due to toxicity)[8]. These are usually very minor concentrations but may require monitoring or cleanup to trace levels for safety.

Origins by capture technology

The impurity profile in a CO_2 stream is mainly determined by the capture process and fuel/source characteristics:

Post-combustion capture (e.g., amine scrubbing of flue gas): CO_2 separated from power plant flue gas or industrial exhaust will reflect the composition of flue gas[9]. Origin of impurities: Combustion in air introduces a large amount of N_2 (from air) and some residual O_2 into the flue gas, so if the capture process is not 100% selective, some N_2 and O_2 remain in the captured CO_2[10]. Fuel-derived impurities include SO_2 (if coal or high-sulfur fuel is used, any SO_2 not removed by pre-scrubbing can end up in the CO_2) and NO_x formed during combustion. Post-combustion amine systems also can carry over trace amine or degradation products (e.g. ammonia) into the CO_2 stream. Typical composition: Post-combustion CO_2 is often Ninety-plus percent CO_2 with a few percent air gases[11]. For example, coal plant CO_2 might come out ~95-99% CO_2, 1-3% O_2/N_2/Ar and ppm-level SO_2/NO_x if scrubbers are effective. Any water is usually condensed out after capture, but the CO_2 may hold some moisture if not thoroughly dried [12]. Because air-derived N_2/Ar are non-condensable, this scenario tends to yield CO_2 that is dilute and requires compression to higher pressures for supercritical injection[13].

Oxy-fuel combustion capture: Oxy-fuel involves burning the fuel in nearly pure oxygen, producing a flue gas of mostly CO_2 and H_2O. [14]After condensing water, the resulting CO_2 stream is high-purity but not 100%. Origin of impurities: Since air isn't used, N_2 is greatly reduced; however, the oxygen supply (from a cryogenic air separation unit) typically contains a small fraction of Argon and perhaps a residual ~1–3% N_2, which end up in the CO_2[2]. Also, any leak or ingress of air in the process can introduce N_2/O_2. Fuel-derived SO_2 and NO_x still occur (combustion in oxygen can actually create NO_x from nitrogen in the fuel if present and SO_2 from sulfur in fuel will be present unless scrubbed). Oxy-fuel systems often include a cleanup unit to remove SOx/NOx[15], but traces might remain. O_2 itself is often present in the CO_2 stream because it's challenging to consume all oxygen in combustion; a small excess O_2 ensures complete fuel burn, thus the CO_2 product may have some percentage of O_2 (a few percent typically). Typical composition: Oxy-fuel CO_2 can achieve ~95–98% purity; e.g., ~90+% CO_2, 2–5% O_2, a few percent Ar/N_2 combined and ppm levels of SO_2/NO_x (depending on cleanup). The high O_2 content is a distinguishing feature (compared to post-combustion), which raises considerations for storage (microbial growth, oxidative reactions)[16].

Pre-combustion capture (Gasification/Shift and Separation): In pre-combustion (applicable to IGCC power plants or hydrogen production), carbon in fuel is converted to CO_2 (via gasification and water-gas shift reactions) before combustion and CO_2 is removed from a high-pressure syngas mixture[17]. Origin of impurities: The syngas contains H_2, CO, CO_2, H_2S (if sulfur in fuel), CH_4 (if gasification is incomplete or for certain reforming processes) and other minor gases. Capture processes like Selexol™ or Rectisol™ can co-remove CO_2 and H_2S together or separately. If designed to only remove CO_2, some H_2S might slip with the CO_2; conversely, if designed for sulfur removal, the CO_2 stream might carry very little H_2S. Hydrogen can also slip through unless a polishing step is used (usually we try to keep H_2 out of the CO_2, but small fractions may remain). Also, any inert gases from the oxidant (oxygen or air used in gasifier) could be present (e.g., Argon if oxygen-blown). Typical composition: Pre-combustion captured CO_2 is often high-purity (because separation is done by physical solvents or membranes at high pressure)[18]. We might see >98% CO_2 in many cases. But possible impurities include H_2 (up to a few % if not fully captured for use), CH_4 or CO (small percentages if the shift/gasifier didn't convert everything), H_2S (which could range from ppm to a couple percent depending on process setup) and N_2/Ar from any air input. An example case: a coal gasification might yield CO_2 with ~2% H_2 and some hundred ppm H_2S if a single-column Selexol is used. These components all have different impacts (H_2 is super-light, affecting compression; H_2S is reactive and toxic; CH_4 adds gas phase volume)[19].

Natural gas processing and other industrial sources: In natural gas sweetening (removing CO_2/H_2S from raw gas) and some industrial processes (e.g., ethanol fermentation, ammonia production), CO_2 streams can have unique impurity profiles[20]. Natural gas processing: Often yields "acid gas" mixtures of CO_2 with significant H_2S (since both are removed together from sour gas). In petroleum provinces (like parts of the Gulf of Guinea), CO_2 streams might contain 5-30% H_2S in some cases if used for co-sequestration (a practice common in Canada's acid gas disposal wells). Such streams may also contain light hydrocarbons (C_1-C_3) that slip through the amine unit and minor nitrogen[21]. Industrial sources: e.g., fermentation CO_2 is relatively pure CO_2 with some moisture and trace organics; steel or cement plant CO_2 (if captured) would be similar to post-combustion flue gas CO_2 with N_2/O_2 and some CO (from incomplete combustion in kilns or blast furnaces). Each source will thus contribute its signature impurities, which must be identified and managed[22].

Thermodynamic behaviors of impurities under storage conditions

In this section, we have reviewed how these impurities behave physically in the environment of deep aquifer storage (high pressure, characteristically 100-200+ bar; temperatures often 80–120 °C in deep reservoirs):

Phase behavior and critical point: Pure CO_2 has a well-known critical point (~31 °C, 7.38 MPa). Introducing other gases shifts the phase diagram[23]. For example, N_2 or CH_4, being less condensable, tend to widen the two-phase region and raise the minimum pressure needed to keep the mixture in a single dense phase. As impurity levels increase, the critical pressure of the mixture rises and the mixture's critical temperature may shift. In practice, this means a CO_2 stream with a lot of non-condensables might require higher injection pressure to stay supercritical/dense in the reservoir. Conversely, very condensable impurities (e.g. SO_2, which has a higher critical temperature than CO_2) can actually make the mixture more easily liquefiable[24] - potentially increasing the density of the fluid phase at reservoir conditions.

Density and viscosity: Impurities alter the density of the CO_2-rich phase. Non-condensable gases like N_2, O_2, CH_4 lower the average molecular weight of the mixture[25], so the dense-phase CO_2 in the reservoir becomes less dense than pure CO_2 would be at the same P/T. For instance, a few percent of N_2 can measurably reduce fluid density, which directly reduces the amount of CO_2 (by mass) that can be stored in a given pore volume. On the other hand, highly condensable or heavier impurities (SO_2 has MW ~64, higher than CO_2's 44) can increase the mixture density at given conditions, slightly enhancing the mass of fluid per volume[26]. Viscosity tends to decrease with lighter components - CO_2 is already a low-viscosity fluid and adding CH_4 or N_2 can lower viscosity further, potentially improving mobility. However, viscosity changes are relatively small compared to density changes[27]. At high pressures, the viscosity reduction from impurities might help injection (reducing pressure drop), whereas density reduction can negatively impact how much CO_2 can be pushed into the formation. The net effect on injectivity is a balance (discussed in 5.2.1).

Solubility in brine: Different impurities partition differently between the supercritical CO_2 phase and the brine phase. SO_2 and NO_2, for example, are highly soluble in water (and will dissolve into formation brine until equilibrium, creating acidic solutions)[28]. H_2S is also quite water-soluble (it will significantly partition into water, forming bisulfide ions), whereas CH_4 and N_2 are only sparingly soluble (most of those will remain in the CO_2 phase as free gas). O_2 has moderate solubility in water but can be consumed by reactions (with any organics or minerals)[29]. Water itself, if any is in the CO_2, will condense into the aquifer's water phase because the reservoir is water-saturated; however, a small water content in CO_2 can also lead to minor formation of hydrates (ice-like solids of CO_2/CH_4) if temperatures are low near the wellbore – though at deep reservoir temperatures, hydrate formation is not a concern except possibly in wells or pipelines[30].

Reservoir condition implications: Under deep aquifer conditions (e.g., 100 bar, 80 °C), pure CO_2 is a dense supercritical fluid[31]. With impurities, two scenarios can occur: (1) If reservoir pressure is high enough, the CO_2 mixture will stay in a single supercritical phase albeit with altered properties; (2) If reservoir pressure/temperature is near the two-phase boundary of the mixture, impurities could cause the CO_2 to split into a gaseous CO_2-rich phase and possibly a liquid phase (if heavy components condense)[32]. Generally, operators aim to inject above the mixture's supercritical pressure to avoid two-phase flow in the reservoir because a gas-liquid CO_2 mixture could have complex flow behavior[31]. Thus, understanding the mixture's phase envelope is key – often simulation tools or equations of state are used to predict if a given impurity mix will remain supercritical in situ. In summary, impurities modify PVT (pressure-volume-temperature) relations: non-condensables make the CO_2 more gas-like (compressible, lower density), while condensable impurities can make it more liquid-like (higher density). Both types will be considered in how they affect injection and storage efficiency next[33].

Effects of Impurities on Key CO_2 Storage Parameters

Injectivity and flow behavior

Phase behavior and injectivity: The presence of impurities can require maintaining higher well pressures to inject CO_2 in a dense phase[34]. If impurities shift the phase envelope such that CO_2 would be gas-phase at reservoir conditions, injection could lead to a two-phase region near the well (e.g., a gas pocket forming if pressure drops during injection). Gas-phase CO_2 has much lower density, which provides less drive for displacement and can dramatically lower injectivity (more gas volume must flow for the same mass of CO_2)[35]. Therefore, operators might need to pump to higher pressures at the wellhead to keep the CO_2 stream supercritical in the formation. This higher injection pressure can strain facilities and approach fracture pressures if not carefully managed. In short, impure CO_2 demands closer control of injection pressure to maintain favorable phase conditions for flow[36].

Density and viscosity impacts: Impurities alter the fluid properties that govern injectivity (the ease of injecting fluid into the formation)[35]. A less dense CO_2 mixture means for a given injection pressure, fewer moles of CO_2 enter per unit volume - effectively, injectivity (in terms of mass flow) is reduced when density is lower. Also, a lower density CO_2 exerts less pressure head in the wellbore (less hydrostatic help), so more surface pumping pressure might be needed. However, on the flip side, reduced viscosity due to light impurities can improve injectivity by lowering frictional pressure losses in the reservoir. According to study, the net injectivity of an impure CO_2 can be lower than pure CO_2 at the same conditions, until a certain pressure threshold is reached where the viscosity reduction compensates for density loss[37]. For example, Lee, et al.[38] reported that above some pressure, an impure stream's injectivity might "catch up" to that of pure CO_2 because the viscosity becomes so much lower[34]. Overall, at typical aquifer conditions, non-condensables tend to initially reduce injectivity compared to pure CO_2, whereas a heavy impurity like SO_2 (in small amounts) could slightly increase fluid density and thus potentially improve injectivity (all else equal).

Mobility and displacement efficiency: The mobility ratio between the CO_2 phase and the resident brine is a key factor in how the CO_2 moves through the aquifer[36]. CO_2 is a non-wetting phase and usually less viscous than brine, so it tends to finger through water. If impurities like N_2 or CH_4 make the CO_2 even less viscous or more gas-like, this mobility contrast increases. A higher mobility ratio can lead to unstable displacement – the CO_2 fingers more and may bypass some parts of the formation, reducing sweep efficiency. Also, increased gas-phase content means higher compressibility; the CO_2 plume might expand rapidly but carry less mass, potentially causing earlier breakthrough to observation wells or boundaries[34]. Buoyancy is another factor: a less dense CO_2 plume (due to light impurities) will rise more quickly within the reservoir, which can focus flow toward the top of the formation and reduce the vertical sweep of CO_2 across the reservoir thickness. This can leave more residual brine un-contacted at lower portions and thus reduce overall storage efficiency in terms of volume utilized[35]. In contrast, a denser CO_2 (with heavy components) is slightly less buoyant and may stay more stratified where placed. For injectivity, high buoyancy might mean the CO_2 quickly accumulates under the caprock above the well, potentially raising local pressure (impacting injectivity over time). Hence, impurities that decrease density/viscosity tend to increase CO_2 mobility – which can be a double-edged sword: easier to inject initially (less viscous), but possibly less efficient sweep and earlier gravity override[38].

Near-wellbore effects and well integrity: Impurities can also affect the injection well vicinity. If SO_2 or NO_x are present, the injected CO_2 (initially dry) will start dissolving into formation water and generating acid[36]. Near the well, where CO_2 first contacts brine, this could enhance rock dissolution (potentially enlarging pore space and increasing injectivity locally). However, it could also lead to precipitation (e.g., sulfate minerals) if the chemistry allows, which would decrease injectivity by clogging pore throats[34]. Notably, co-injection of H_2S and SO_2 has a known risk of producing elemental sulfur via redox reactions (the "Claus reaction" in the reservoir), which can deposit as a solid in the near-well region. Elemental sulfur precipitation could significantly impair injectivity by plugging pores around the well. Operators need to be aware of this when considering co-sequestration of H_2S and SO_2 - it may warrant keeping those below certain ratios or implementing measures to avoid sulfur drop-out[35]. Another well-related issue is corrosion: during active injection, the well is usually dry (the CO_2 dries out the near-well environment), so corrosion is limited. But once injection stops and moisture re-enters, any acidic impurities (SO_x, NO_x, etc.) can corrode well casing and cement[34]. This long-term integrity aspect doesn't directly change injectivity during injection, but it affects the well's ability to be used for future injection or its sealing after closure. Material selection (corrosion-resistant alloys, proper cement) mitigates this, but those are part of practical considerations[35].

Reservoir stability and geochemical reactivity

Rock–fluid chemical interactions: Introducing CO_2 with impurities into a reservoir triggers a series of geochemical reactions, some of which are significantly different from pure CO_2 injection. Pure CO_2 dissolves in water to form carbonic acid (weak acid), gradually reacting with minerals. If SO_2 is co-present, it forms sulfurous acid, which can further oxidize to sulfuric acid – a much stronger acid. NO_x can form nitrous/nitric acids. These strong acids lower the pH of formation water more dramatically than carbonic acid alone, leading to accelerated mineral dissolution[36].

Mineral dissolution: Carbonate minerals (like calcite, dolomite common in many aquifers) will dissolve rapidly if pH drops, potentially enlarging pore spaces. Silicate minerals (clays, feldspars) also start dissolving more when pH is very low[34]. This can enhance porosity and permeability in some zones (favorable for injectivity), but it also means higher concentrations of cations (Ca^{2+}, Fe^{2+}, etc.) are released into the brine. As the acidic plume moves and gets buffered by rock, the pH will start rising again and secondary minerals can precipitate: e.g., calcium released from calcite may combine with sulfate from dissolved SO_2 to precipitate gypsum ($CaSO_4 \cdot 2H_2O$) or anhydrite ($CaSO_4$). Iron released from minerals could react with H_2S to form pyrite (FeS_2) or with CO_2 to form siderite ($FeCO_3$). These precipitates can clog pore spaces[35]. The IEAGHG analysis indicated SO_2-related sulfate precipitation might reduce porosity/injectivity less severely than initially feared, but it is still a concern to monitor. Especially, the combination of H_2S and SO_2 was highlighted: they can react to form elemental sulfur, a solid that can seriously block pore space near the mixing fronts[34].

Caprock and seal integrity: The geochemical effects extend to the caprock (sealing formation). Caprocks are often composed of shales or mudstones with clays and minor carbonates[36]. Acidic fluids (low pH from impurities) can attack caprock minerals: for instance, dissolve carbonate nodules or cements within the caprock, potentially creating micro-permeable pathways. Clays might be less soluble but could undergo ion exchange or structure changes if the water chemistry shifts drastically (e.g., sodium clay converting to calcium clay if Ca^{2+} increases, potentially affecting clay swelling). There is also the risk of weakening caprock: if acid dissolves some material, it could increase caprock permeability or reduce mechanical strength[34]. On the other hand, some precipitation reactions might seal fractures in the caprock: e.g., if iron or calcium precipitate as new minerals in cracks, that could reduce permeability. It's a complex balance and reactive transport models are used to predict net effects. The safe assumption is that impurities increase the potential for caprock alteration. Therefore, one must ensure the caprock has sufficient thickness and mineral buffering or design the injection to minimize acidic plume reaching the caprock in high concentration[35].

Wettability and fluid properties changes: Impurities can indirectly alter the wettability and interfacial tension in the CO_2-brine-rock system. For example, if SO_2 leads to extensive mineral dissolution, the rock surface mineralogy might change (exposing more quartz or clay as carbonates dissolve), which could shift the wettability toward more water-wet or CO_2-wet depending on the scenario. Precipitation of certain minerals could coat pore surfaces (e.g., gypsum lining the pores), possibly making them more water-wet (gypsum is moderately water-wet). A more water-wet rock improves residual trapping of CO_2 but could reduce relative permeability to CO_2[36]. Conversely, some studies suggest that high H_2S/CO_2 mixtures can reduce interfacial tension between CO_2 and brine[39,40], which might allow CO_2 to penetrate smaller pores (potentially increasing microscopic sweep). Also, any introduction of microbes (see below) or organic reactions could produce biosurfactants or other agents altering IFT/wettability. While these effects are secondary compared to the physical impacts, they can influence how much CO_2 is trapped residually versus migrates.

Microbial activity (O_2 Effects): The presence of oxygen in an otherwise anaerobic deep aquifer is a wild card. O_2 can enable the growth of aerobic bacteria if nutrients are available[34]. In oil reservoirs, O_2 is known to cause souring – stimulating sulfur bacteria that oxidize hydrocarbons or reduce sulfate to H_2S, etc., but in a saline aquifer with little organic matter, microbial activity might be limited. However, even slight microbial growth could have effects: biofilm formation that clogs pore spaces (reducing permeability around injection zones), consumption of O_2 and any biodegradable impurities (possibly mitigating O_2 but producing biomass and CO_2). If there are any residual hydrocarbons or organic materials in the formation (not uncommon in saline formations that are near hydrocarbon-bearing zones), O_2 could cause degradation of those, producing CO_2 or organic acids[35]. In summary, O_2 is generally an unwanted impurity because it introduces unpredictability - hence it's often limited to very low levels (ppm) in CO_2 streams to avoid these issues.

Implications for mineral trapping

- In the long term, impurities can change the ultimate trapping mechanisms of CO_2. Pure CO_2 storage relies on residual trapping, solubility trapping (CO_2 dissolving into brine) and mineral trapping (CO_2 reacting to form carbonates)[36]. With impurities:
    - H_2S can actually enhance mineral trapping by forming sulfide minerals (pyrite) if iron is present, effectively sequestering sulfur but not contributing to CO_2 mineralization (though co-precipitation might trap some CO_2 indirectly).
    - SO_2 doesn't directly form a CO_2 mineral, but by reacting with Ca/Mg it might precipitate as $CaSO_4$, which consumes Ca that otherwise could form $CaCO_3$. That could delay or reduce carbonate mineral trapping but instead trap sulfur. Over very long times, once SO_2 is spent and if pH rebounds, carbonate trapping might resume.
    - NO_x likely ends up as nitrate or nitrite in the water; these could be taken up by clays or react with organic matter, but generally NO_x will not enhance CO_2 trapping. It's more of a contaminant in the water phase.
    - CH_4/N_2 do not partake in trapping reactions and tend to remain in gas phase or dissolve a bit. CH_4 might even exsolve later and be mobile. Thus, their presence means a fraction of the gas is not participating in dissolution or mineral trapping at all (essentially, they reduce the fraction of gas that can be trapped as CO_2 because they occupy space and remain mobile).
    - Water impurity doesn't change trapping fundamentally (since the formation is water-saturated anyway), but if free water in CO_2 caused any early carbonate precipitation (unlikely at injection time), that might slightly alter local trapping.

In sum, reactive impurities (SO_2, H_2S) might introduce alternate trapping pathways (sulfur minerals) but also can compete with or delay classical CO_2 trapping, while inert impurities (N_2, CH_4) just reduce the proportion of CO_2 available for dissolution/mineral trapping (dilution effect).

Pressure buildup and containment

Pressure buildup dynamics: When injecting any fluid into a confined aquifer, reservoir pressure rises. With impure CO_2, to inject the same mass of CO_2, a larger volume of fluid is injected (because impurities take up volume but don't contribute to stored CO_2 moles). Non-condensable impurities particularly cause a larger pressure footprint. Essentially, for a given mass of CO_2 injected, the presence of (for instance) 10% N_2 means you're injecting 10% more moles of gas to get the same CO_2 mass, which will occupy more pore volume and raise pressure more. Studies have quantified[34] that storage capacity (in terms of mass of CO_2 sequestered per pore volume) drops with impure streams - e.g., 10% N_2 can lead to >30% reduction in effective CO_2 storage efficiency in the formation. This means pressure builds up faster for the same amount of CO_2 injected, reaching operational pressure limits sooner. Field operators might need to stop injection earlier or use more injection wells to spread out the CO_2, to stay below fracture pressure or regulatory limits. On the other hand, if an impurity like SO_2 increases density, the pressure buildup for a given mass might be slightly less (since that mass occupies a bit less volume than pure CO_2 would, due to higher density). But in most practical cases, the impurities of concern are lighter gases, so the net effect is higher pressure rise and lower storage capacity per well/reservoir. Wang et al. (IEAGHG) found that non-condensables reduce CO_2 structural trapping capacity more than their molar fraction would suggest (a disproportionate decrease) - in part due to this pressure/volume effect and also due to less dissolution.

Containment (Caprock) integrity under pressure: Higher pressure in the reservoir increases the stress on the caprock.

A key containment risk is if pressure approaches the fracture pressure of the seal or reactivates any faults. With impurities causing faster or greater pressure increase, careful pressure management is needed. Operators might inject more slowly or in multiple sites to compensate[34]. Additionally, if the CO_2 mixture has to be injected at higher wellhead pressure to remain dense (as noted in injectivity discussion), the bottomhole pressure could be closer to the fracturing limit. It is critical to monitor downhole pressures and stay within safe margins. Another aspect: pressure-induced brine displacement. Higher pressure can push brine upward through any available conduits; a more buoyant CO_2 plume (from impurities) can exacerbate this by lifting fluid columns[36]. However, buoyancy itself mainly affects the CO_2 migration, while pressure affects both CO_2 and brine. Ensuring the caprock's capillary entry pressure is not exceeded is another containment criterion – if impurities reduce CO_2 wettability or interfacial tension, it might actually raise the capillary entry threshold (slightly mitigating leakage risk), but if pressure is higher, that benefit could be negated[35].

Leakage and plume migration risks: Impurities that increase buoyancy (like N_2, CH_4) make the CO_2 plume more prone to rapid upward migration, potentially reaching the caprock faster and spreading out beneath it[34]. A fast, buoyant rise could find weaknesses (like thin cap sections or minor faults) sooner. If the caprock has heterogeneities, a lighter CO_2 might concentrate under a small area of caprock, increasing local pressure against it. Also, if any leakage were to occur (through an imperfect well or fault), the leaking fluid would contain those impurities[35]. Some impurities could increase the impact of a leak: e.g., H_2S leaking would be a significant health/environment hazard, so even if H_2S doesn't greatly change the likelihood of leakage, it elevates the consequences of any leak. Therefore, co-injecting toxic impurities demands stringent monitoring (e.g., downhole safety valves, enhanced leak detection at surface).

Wellbore containment and integrity: As mentioned, impurities like SO_2, NO_x, O_2 can be more corrosive to well materials than pure CO_2, especially once injection stops and water contacts the well[36]. Over decades, if well cements are degraded by acids, that could open a micro-annulus for CO_2 or brine to migrate upward outside the casing. Ensuring wells are completed with appropriate cement (e.g., acid-resistant cement formulations or epoxy coatings) and maybe adding corrosion inhibitors during injection can mitigate this[35]. From a containment perspective, it's often advised to dehydrate the CO_2 thoroughly so that no liquid water is present to drive corrosion during the operational phase. This works because a dry CO_2 stream will desiccate the formation around the well, keeping it dry and non-corrosive. After closure, however, eventually water will seep back – hence long-term well plug materials must withstand any acidic environment created then[34]. DNV and other standards usually require demonstrating that impurities will not compromise well integrity over the project life and post-closure.

Impact on trapping mechanisms and long-term containment: Non-condensable impurities reduce solubility trapping efficiency since they themselves do not dissolve much and they effectively reduce the partial pressure of CO_2 in the gas phase (so brine takes up less CO_2)[34]. This leaves more CO_2 in mobile free phase, which is a long-term containment disadvantage (dissolved CO_2 is effectively immobile and isolated). Residual trapping can also be reduced: a more buoyant, lower-viscosity CO_2 tends to bypass more pore volume and may leave behind less residual saturation (since it doesn't sweep pores as effectively and can more easily remobilize)[41]. The IEAGHG study noted that as a result, both solubility and residual trapping efficiencies decrease with the addition of non-condensable gases. This means after injection stops, a larger fraction of the CO_2 remains as a buoyant plume that could migrate until it finds a trapping structure. For containment, this is a negative because you prefer as much CO_2 as possible to be trapped immobile.

Example - Pressure and capacity in numbers: To illustrate, if a reservoir could store 50 million tonnes of pure CO_2 before pressure limits are hit, storing CO_2 containing 10% N_2 might reduce that capacity to, say, ~35 Mt (a 30% drop). The pressure in the reservoir at any given injected volume would be higher in the impure case [38]. This demonstrates why storage sites either limit impurities or adjust injection plans. In contrast, if 1% SO_2 were present, the capacity might be slightly higher than with pure CO_2 because that SO_2 makes the fluid denser (this is a more theoretical possibility; in practice SO_2 would likely be kept lower than 1% due to acid issues)[42]. Engineers use such calculations to decide if accepting impurities is feasible or if they must purify the CO_2.

Simulation insights from the Rio del rey basin case study

Context of the case study

The Rio del Rey Basin in the Gulf of Guinea (Cameroon) has been used as a model reservoir in this study to investigate CO_2 storage performance under various conditions. A compositional reservoir simulation (with geochemical reactions) was conducted[43], capturing the interplay of geological heterogeneity, aquifer properties and fluid composition on CO_2 storage efficiency. While Mwenketishi et al, 2025 focused on aquifer and rock property impacts (e.g., porosity, permeability, mineral composition, temperature, pressure), here we relate those findings to CO_2 stream composition.

Key findings relevant to impurities

In the simulations, it was observed that CO_2 in the supercritical state occupied roughly 70% of the total CO_2 in the reservoir after injection, with significant fractions dissolved (≈27%) and mineralized (≈17%) over time. These figures (from a base case with presumably pure CO_2) highlight the contributions of solubility and mineral trapping in a favorable scenario. If impurities were present, we can infer changes: for instance, a non-condensable impurity would likely reduce that 27% dissolved fraction (since less CO_2 partial pressure means less driving force for dissolution). Likewise, additional reactive impurities (like SO_2) might increase mineral trapping (by forming sulfates) but perhaps at the expense of some CO_2 staying in dissolved form or being used to form carbonate minerals. The net storage efficiency (sum of trapped forms) could thus shift.

Sensitivity analysis connections

Mwenketishi et al, 2025's sensitivity analysis showed how aquifer salinity significantly affected storage efficiency – an increase in salinity led to a ~52% reduction in dissolved CO_2 storage at the end of injection. This emphasises how fluid chemistry (in that case, brine salinity) can alter CO_2 solubility. By analogy, adding impurities like N_2 is somewhat akin to effectively increasing the "salinity" of the CO_2 phase (making it less CO_2-rich), which also diminishes CO_2 dissolution. Both high salinity and presence of inert impurities reduce CO_2 solubility in the aqueous phase, leading to lower dissolution trapping. This parallel validates that the model is capturing such thermodynamic sensitivity.

Injectivity and pressure in the model

While Mwenketishi, et al, primarily varied rock properties, one can interpret the results for hints of impurity effects[43]. For example, if a scenario with different injection rates or fluid compositions was run, any noted change in bottom-hole pressure or plume migration can inform us. Suppose the simulation included a case with a fraction of gas that does not dissolve (effectively simulating an impurity) - it likely showed higher final pressure or larger plume. Even if not explicitly done, the modeling results for pure CO_2 provide a baseline that we can qualitatively adjust: the presence of impurities would have likely required a higher injection pressure to achieve the same injectivity observed. If the base case had an injection well bottom-hole pressure of X to inject Y tonnes/year, an impure stream might have needed $(X + \Delta P)$ to inject the same mass.

Geochemical outcomes

The case study's geochemical results indicated mineral precipitation of calcite and halite under certain conditions (one case saw 20% more calcite and 45% more halite precipitates). This precipitation was a result of interactions between injected CO_2, rock and brine composition. If we add impurities to this scenario, we'd expect additional mineral phases: e.g., with SO_2, gypsum might precipitate; with H_2S, pyrite might form. Each of these would modify porosity in different reservoir zones. The simulation framework from Mwenketishi, et al, could be extended to include these reactions – a recommendation going forward[43]. The model's demonstrated sensitivity to mineral reactions suggests it would capture impurity-driven reactions as well.

Applied understanding

The Rio del Rey simulations reinforce that understanding local geology is vital. For instance, a key result was that higher mineral content in the formation can increase mineral trapping but sometimes at the cost of porosity reduction (if too much precipitation). For an impurity-tolerant storage plan, this means one should seek formations that can accept some mineral alteration without losing seal or injectivity. If our case study formation showed good injectivity and only moderate porosity changes with pure CO_2, it's reasonable to expect it could handle small amounts of impurities without drastic issues, but higher impurity levels could push it into unfavorable regimes (like significant pore blocking or rapid pressure rise). By referencing the specific data from the model (such as percentages of trapping and sensitivity percentages), we underline how even baseline factors can swing storage efficiency by 50+%, which is comparable to or larger than many impurity effects. This puts in perspective that impurity impacts, while important, are one part of a bigger... picture. The Rio del Rey case confirms that multiple factors (salinity, mineralogy, etc.) drastically affect storage outcomes; thus, CO_2 stream impurities must be considered alongside those factors to fully evaluate storage efficiency in real projects. In essence, the simulations provide a baseline showing how sensitive CO_2 storage efficiency is to fluid and rock properties, implying that adding stream impurities would likewise have non-negligible impacts - which our outline above has detailed. These insights from the case study will inform practical decisions on CO_2 purity and injection strategies in the Gulf of Guinea context.

Key findings from simulation scenarios

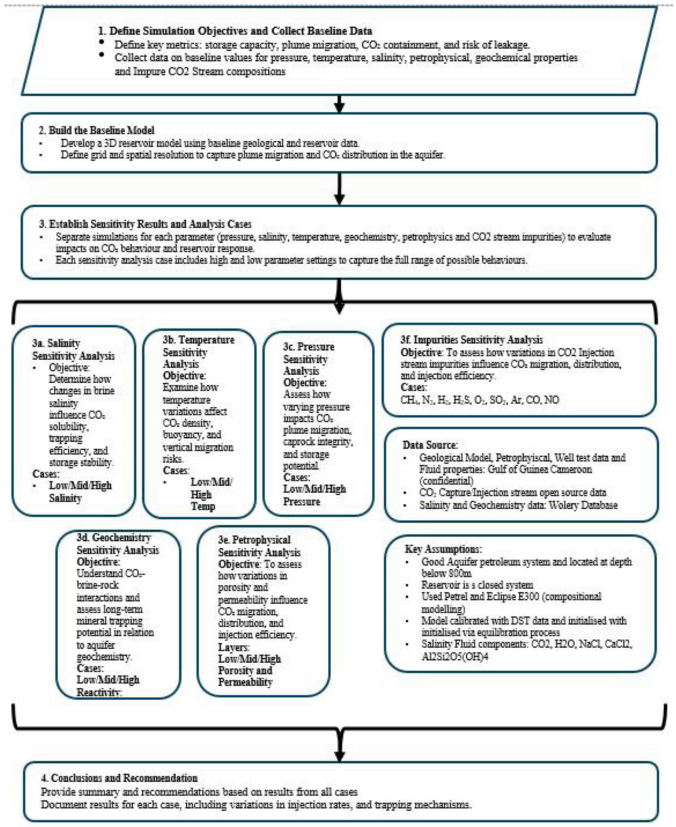


Figure 1: Methodology for Simulation.

Storage capacity and injectivity trends

Compositional reservoir simulations in Petrel/Eclipse E300 reveal that the presence of certain impurities can significantly influence the CO_2 storage capacity (as measured by gas volume stored) and injectivity in the Rio del Rey Basin aquifers **(Figure 2)**.

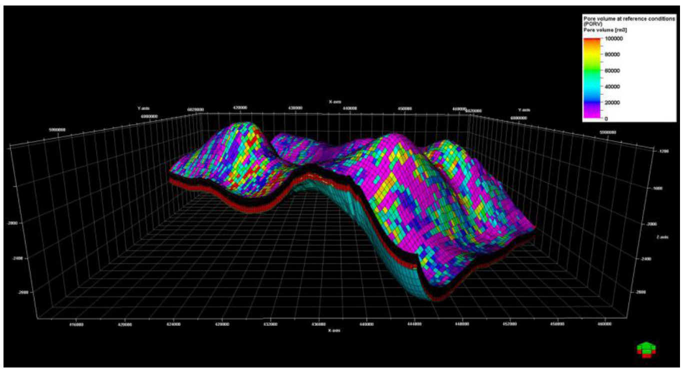


Figure 2: Geological Model.

Over a decade-long injection period (simulating continuous CO_2 injection), scenarios with light, low-solubility gases (CH_4, N_2, H_2) as co-injected impurities achieved higher cumulative gas storage volumes than scenarios with purer CO_2 streams. For example, the baseline mixed-impurity case (80% CO_2 with 5% each of CH_4, N_2, H_2S, H_2) stored about 1.27×10^5 m³ of gas in the reservoir after 10 years. Increasing the CH_4 content to 10% (with CO_2 reduced to 75%) raised the stored volume to ~1.32×10^5 m³, while a similar 10% N_2 case yielded ~1.35×10^5 m³. The highest storage was observed in the H_2-enriched scenario (10% H_2), reaching about 1.36×10^5 m³. By contrast, an almost-pure CO_2 case (98% CO_2 with only ~0.5% each of minor gases) stored substantially less, around 1.10×10^5 m³. These results indicate that adding light, less dense impurities can enhance the volumetric storage capacity by on the order of 5–25% compared to an ultra-pure CO_2 injection, under the same operational constraints.

The mechanism for this improvement is linked to injectivity. In simulations, injection well rates initially ramp up and then gradually decline as reservoir pressure builds and reactions progress. The cases with CH_4, N_2 or H_2 maintained slightly higher plateau injection rates (on the order of 30–31 m³/day) than the mostly-CO_2 cases (~28–29 m³/day), reflecting better injectivity with lighter gas mixtures. Physically, impurities like CH_4, N_2 and H_2 reduce the overall gas density and viscosity, making the fluid easier to inject and displace into the formation. All scenarios were injection-pressure-limited in this closed aquifer model, so improved injectivity translated directly into more volume injected before reaching pressure limits. Notably, the simulations showed that the bottom-hole pressure requirements varied with prior gas saturation: if residual gas was present in the aquifer, the required injection pressure was higher to continue the injection. This suggests that in multi-step injection or re-injection scenarios, leftover free gas (including less soluble components from earlier injections) could increase operational pressures. Overall, the presence of non-condensable, insoluble impurities tends to lower resistance to flow, allowing greater CO_2 (and co-gas) throughput, whereas a pure CO_2 stream, being denser and more viscous, reached pressure constraints sooner and stored less total volume.

CO_2 plume migration and distribution

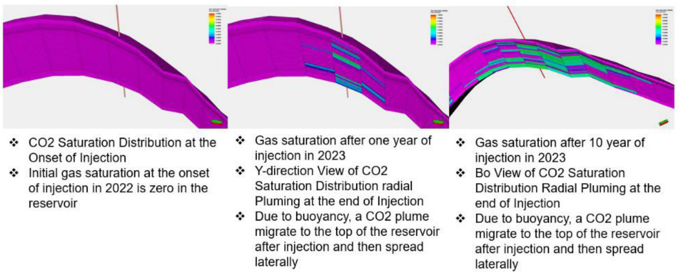


Figure 3: CO_2 Injection Philosophy.

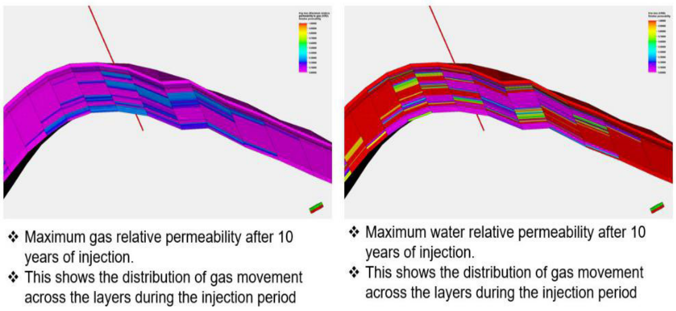


Figure 4: Rock Property Concept.

The CO_2 and H2O activity were computed following Spycher and Pruess (2005) (2009) analyses and fluid properties are assigned internally in the model data. The gas density was obtained by a cubic equation of state and a modified Redlich-Kwong equation of state was used:

Where V is the molar volume, P is the pressure, TK is the temperature in Kelvin, R is the universal gas constant and amix and bmix is the attraction and repulsion parameters. The model applies a maximum NaCl concentration for the CO_2 solubility model, corresponding to the value of salting out while other salts are limited to a fixed value in the CO_2 solubility model.

$$P = \left(\frac{RT_k}{V - b_{mix}}\right) - \left(\frac{a_{mix}}{T_{K^{1/2}} V \left(V + b_{mix}\right)}\right)$$

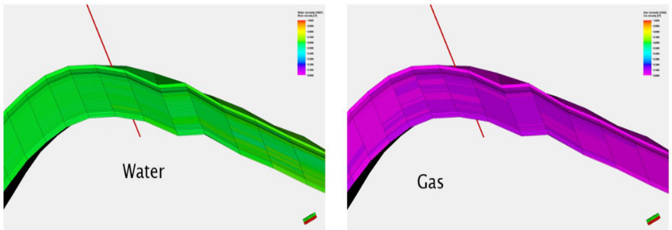


Figure 5: Gas and Water Viscosity Distribution

As per figure above, gas viscosity stand at about 0.300cP after 10 years of injection - EOS

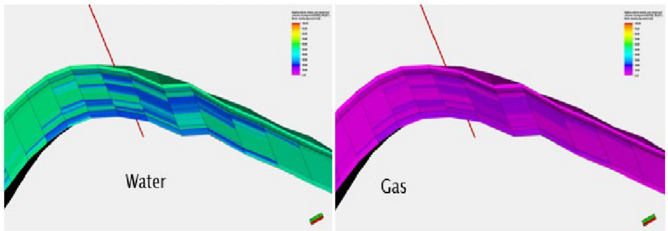


Figure 6: Gas and Water Molar Density Distribution

As shown in above figure, gas moles per reservoir volumes increases throughout the injection zones as water molar density drops following chemo-physical reaction between CO2, brine and salt concentration.

The spread and migration of the CO_2 plume in the reservoir were also strongly affected by the impurity composition. Plume extent was observed to increase in scenarios with lighter, less water-soluble gases. In the CH_4-rich case, the CO_2–CH_4 plume migrated further upward and outward; higher CH_4 content caused the plume to rise more due to increased buoyancy. Simulations showed CH_4 preferentially accumulating at the leading edge of the plume (a result of CH_4's low solubility in brine), effectively enlarging the plume footprint and extent. A similar effect was noted for N_2 and H_2: like CH_4, these low-solubility gases do not readily dissolve into formation water and thus partition preferentially into the gas phase, riding at the plume top. In fact, compositional fractionation occurs whereby the plume's fringe becomes enriched in the most insoluble components (including any initially dissolved gases exsolving into the CO_2 stream). This chromatographic separation means the non-reactive impurities travel with the CO_2 front, reaching farther distances at slightly higher concentrations than their initial average. Quantitatively, literature and simulation results indicate that even an inert gas like Ar (argon, also insoluble) can expand the plume radius measurably – on the order of an additional 1.5–6% in areal extent per 1% Ar added – purely due to physical effects on the plume buoyancy and mobility. Thus, impurities such as CH_4, N_2, H_2 or Ar chiefly exert a physical influence, enlarging the plume and potentially accelerating its advance under buoyancy forces.

In contrast, more soluble impurities like H_2S and SO_2 tend to reduce the plume size and slow its advance. CO_2–H_2S

co-injection simulations showed that H_2S, being more soluble in water than CO_2, lags behind the plume front – it dissolves into the brine more readily and thus does not migrate as far in the gas phase. The aquifer effectively strips some H_2S out of the mobile gas plume. This results in a smaller overall gas plume volume and a shorter migration distance compared to an equivalent case without H_2S. In fact, due to H_2S dissolving into formation water, the net gas-phase volume in an H_2S-rich scenario can be lower than in a pure CO_2 case, all else equal. The simulations are consistent with findings by Bachu and Bennion (2009) that co-injected H_2S will form a trailing "H_2S-rich bank" behind the CO_2 front, given the right aquifer capacity to dissolve H_2S. Similarly, SO_2, which reacts with water to form acidic solutions, would not travel as far as an inert gas – it gets consumed and dissolved, limiting its presence in the free CO_2 plume. The cases with these reactive, water-soluble gases essentially showed the opposite of the CH_4/N_2 effect: plume contraction and delayed arrival of the impurity at observation points. In practical terms, non-reactive impurities will arrive at monitoring wells concurrently with the CO_2, whereas reactive impurities may exhibit a delayed breakthrough **(Table 1)**. The greater the chemical "incompatibility" or solubility of a component in the aquifer, the larger the lag time before it appears in the gas phase at a distant location. This has important monitoring implications, as discussed later **(Figure 7)**.

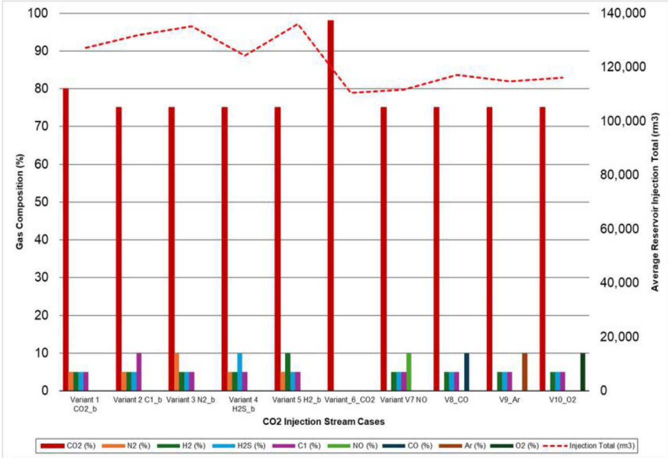


Figure 7: Results Summary for Quantifying the Impact of Contaminants on CO_2 Aquifer Storage.

Table 1: Results Summary for Quantifying the Impact of Contaminants on CO_2 Aquifer Storage cont.

Component	Variant 1 CO2_b	Variant 2 C1_b	Variant 3 N2_b	Variant 4 H2S_b	Variant 5 H2_b	Variant_6_CO_2	Variant V7 NO	V8_CO	V9_Ar	V10_O2
CO_2 (%)	80	75	75	75	75	98	75	75	75	75
N_2 (%)	5	5	10	5	5	0.005	0	0	0	0
H_2 (%)	5	5	5	5	10	0.005	5	5	5	5
H_2S (%)	5	5	5	10	5	0.005	5	5	5	5
C1 (%)	5	10	5	5	5	0.005	5	5	5	5
NO (%)	0	0	0	0	0	0	10		0	0
CO (%)	0	0	0	0	0	0	0	10	0	0
Ar (%)	0	0	0	0	0	0	0	0	10	0
O_2 (%)	0	0	0	0	0	0	0	0	0	10
Total (rm^3)	127,251	131,898	135,164	124,291	136,041	110,487	111,719	117,069	114,785	116,195

Physical versus chemical impacts of impurities

These simulation scenarios highlight a clear distinction between physical effects and chemical (geochemical) effects of co-injected impurities on CO_2 storage behavior. The physical effects are primarily due to changes in fluid properties: gas phase density, viscosity and interfacial tension, as well as differences in dissolution behavior. All the non-condensable, sparingly soluble gases (N_2, CH_4, H_2, Ar) cause a reduction in the CO_2-rich phase density and viscosity, which increases buoyancy and mobility of the plume. This is why such impurities expanded the plume and improved injectivity, as described above. However, a trade-off is that increased buoyancy can potentially reduce storage security; the simulations and literature note that a lighter plume may have a greater tendency to rise toward the caprock and could increase the risk of migration out of the target zone if not properly contained. Additionally, some impurities can lower the CO_2–brine interfacial tension (IFT), further influencing plume behavior. Notably, H_2S was identified as causing significant IFT reductionfile-blpq8a1wunzohpdwt7zjae. A lower IFT can diminish capillary trapping of CO_2 (since the CO_2 will not occupy pore spaces as residually if it can overcome capillary forces more easily), potentially reducing residual trapping efficiency. It also means the caprock's entry pressure for the gas may be lowered, which is a negative impact on containment security. In these simulations, co-injected H_2S was indeed seen as a detrimental impurity from a physical standpoint, tending to reduce stored gas volume and potentially easing the gas movement through the reservoirfile-blpq8a1wunzohpdwt7zjae. On the other hand, H_2 was mildly beneficial physically (despite being reactive) because H_2 has an extremely low molecular weight and is essentially insoluble; it provided a strong buoyancy boost and mobility increase to the CO_2 stream, similar to N_2. Likewise, N_2 and Ar being inert do not partake in reactions; their impacts were purely via physics – e.g., Ar's inclusion leads to a slight drop in mixture density and viscosity (and a likely slight increase in IFT), influencing plume spread but not chemistry.

The chemical effects of impurities were found to be secondary in most cases, except for certain reactive components that can alter the geochemistry of the aquifer. The simulation results and supporting experimental evidence suggest that impurities like SO_2, NO_2 (NO_x), O_2, H_2S and CO can engage in geochemical reactions upon injection. When present, these impurities acidify the formation fluids or alter redox conditions, which can lead to mineral dissolution or precipitation. For instance, co-injected SO_2 will oxidize (especially if O_2 is also present) to form sulfuric acid (H_2SO_4) in the subsurface. This causes a pronounced drop in pH and has been shown to aggressively dissolve carbonate minerals like calcite and to a lesser extent dolomite. In the simulations, any scenario including SO_2 (even at trace levels) would be expected to produce localized acidification and enhanced mineral dissolution around the plume front. O_2 itself, often present in oxy-fuel derived CO_2 streams, is reactive in a different way: it can be consumed by reduced minerals (like pyrite or siderite) in the formation, further oxidizing those minerals and producing acidity. Oxygen also has the effect of promoting the oxidation of other impurities – for example, facilitating the conversion of SO_2 to sulfate or of NO to NO_2. The simulations noted that in an O_2-rich environment, more SO_2 will convert to sulfuric acid (with O_2 to spare), exacerbating aquifer acidification. NO_x (NO_2/NO), which might be present in post-combustion CO_2 at ppm levels, likewise forms strong acids (nitric/nitrous acid) upon hydration, though NO_x gases are relatively insoluble and tend to distribute more diffusely in the reservoir. Importantly, no solid nitrate precipitates are expected, so the net effect of NO_x is continued presence in the fluid phase until oxidized to acid.

In contrast to the acid-generating impurities, CO and H_2 are reactive in a reductive sense. Both are highly reducing gases and tend to get oxidized by the rock formation. Chemical reactions (such as with Fe(III)-bearing minerals) can consume H_2 and CO, producing in situ alkalinity (OH^-) and in the case of CO, additional CO_2. For example, one modeled reaction is $2Fe(OH)_3 + H_2 \rightarrow 2Fe^{2+} + 4OH^- + 2H_2O$. Such reactions raise the pH locally (counteracting some acidity) and can even generate secondary CO_2 from CO, effectively increasing the moles of CO_2 in the formation slightly. However, the concentrations of CO and H_2 in typical captured streams are low (≈1% or less), so these chemical effects are limited in magnitude and were not a dominant factor in the overall storage performance. Indeed, across all scenarios studied, the chemical impacts were generally minor relative to physical impacts – a conclusion echoed by prior assessments. The notable exceptions are the sulfur and nitrogen oxides, which, even in small amounts, can locally alter water–rock reactions and thus must be considered in geochemical risk assessments. Overall, the simulations indicate that an injected impure CO_2 stream will primarily be governed by physical processes (migration and trapping influenced by density/viscosity/IFT changes), with geochemical reactions playing a secondary role that becomes important only for specific reactive impurities (e.g. causing acidification or mineral changes in the near-well region or along the plume path) **(Table 2)**.

Table 2: Impact of contaminants on CO2 aquifer storage - Control case: Variant_1_CO2_b_80%.

DATE	Average Reservoir Volume Injection Rate (rm³/day)	Average Reservoir Volume Injection Total (rm³)
Jan-22	27	9,841
Jan-23	29	20,561
Jan-24	29	31,274
Jan-25	29	41,982
Jan-26	29	52,680
Jan-27	29	63,366
Jan-28	29	74,041
Jan-29	29	84,704
Jan-30	29	95,357
Jan-31	29	105,999
Jan-32	29	116,630
Jan-33	29	127,251

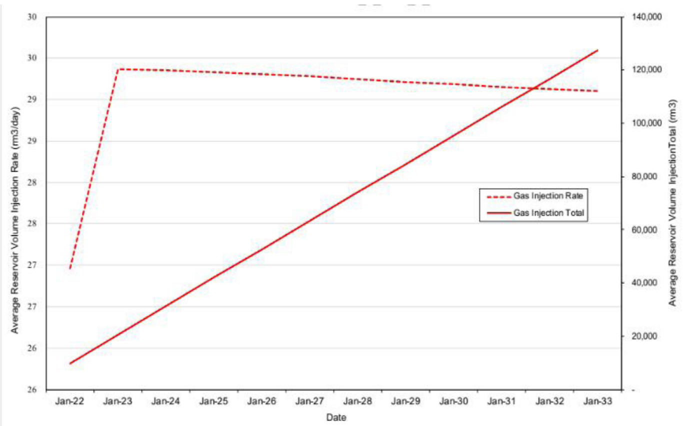


Figure 8:

In the control simulation (Variant_1_CO2_b_80%), a fixed composition of 80% CO_2 and 5% each of CH_4, N_2, Ar and other trace impurities was considered to evaluate baseline storage behavior in a Gulf of Guinea deep saline aquifer. The reservoir injection rate exhibited exponential growth until 2023, after which it began a gradual decline due to chemo-physical interactions between the injection stream and the formation matrix. Over a ten-year injection period, a cumulative volumetric gas storage of approximately 127,251 m³ was achieved. Notably, the presence of CH_4 significantly influenced plume dynamics due to its lower solubility in water compared to CO_2, resulting in CH_4 enrichment at the leading edge of the gas plume. This effect was compounded by N_2, which displayed even lower solubility and Ar, contributing to an expanded plume extent and vertical rise. The displacement of formation water by CO_2 further induced exsolution of dissolved methane into the gas phase, leading to an approximate 1% increase in CH_4 concentration within the plume. Simulation outputs also indicated that the presence of residual gas phases within the aquifer increased the bottom-hole injection pressure, highlighting operational implications for long-term injection strategies. These findings underline the critical role of impurity profiles in determining plume morphology, injection efficiency and overall storage performance in deep aquifer systems.

This case was considered to have fix values/composition of 5% each for all the contaminant gas components **(Table 3)**.

Table 3: Impact of Contaminants on CO2 Aquifer Storage - Scenario Case: Variant_2_C1_b_10%.

DATE	Average Reservoir Volume Injection Rate (rm³/day)	Average Reservoir Volume Injection Total (rm³)
Jan-22	28	10,203
Jan-23	30	21,316
Jan-24	30	32,422
Jan-25	30	43,522
Jan-26	30	54,611
Jan-27	30	65,688
Jan-28	30	76,753
Jan-29	30	87,805
Jan-30	30	98,846
Jan-31	30	109,875
Jan-32	30	120,892
Jan-33	30	131,898

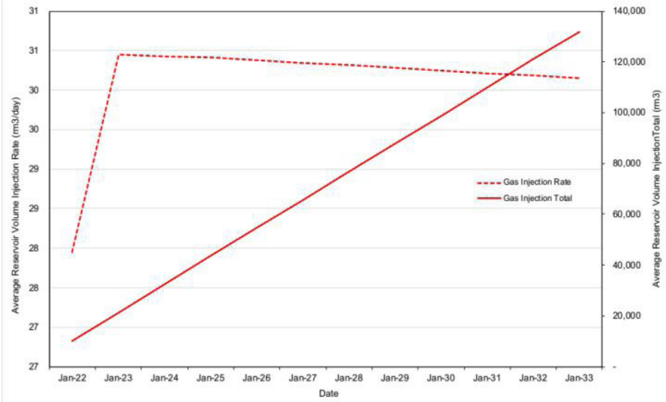


Figure 9:

In the scenario case Variant_2_C1_b_10%, the injection stream was composed of 75% CO_2, 10% CH_4 (C1) and 5% each of N_2, H_2S and H_2. This configuration was designed to assess the impact of a higher CH_4 concentration on CO_2 storage dynamics. The reservoir experienced an exponential increase in injection rate until 2023, followed by a gradual decline driven by chemo-physical interactions within the aquifer matrix. After a decade of continuous injection, a total of 131,898.00 m³ of gas was stored in the reservoir **(Table 4)**. The elevated CH_4 concentration in this scenario likely influenced plume behavior and solubility dynamics, contributing to storage variation compared to the control case. These results emphasize the significance of gas composition variability in determining injection efficiency and long-term storage performance in deep aquifer systems **(Figure 10)**.

Table 4: Impact of Contaminants on CO_2 Aquifer Storage - Scenario Case: Variant_3_N2_b_10%.

DATE	Average Reservoir Volume Injection Rate (rm³/day)	Average Reservoir Volume Injection Total (rm³)
Jan-22	29	10,457
Jan-23	31	21,847
Jan-24	31	33,230
Jan-25	31	44,606
Jan-26	31	55,971
Jan-27	31	67,322
Jan-28	31	78,661
Jan-29	31	89,986
Jan-30	31	101,299
Jan-31	31	112,600
Jan-32	31	123,888
Jan-33	33	135,164

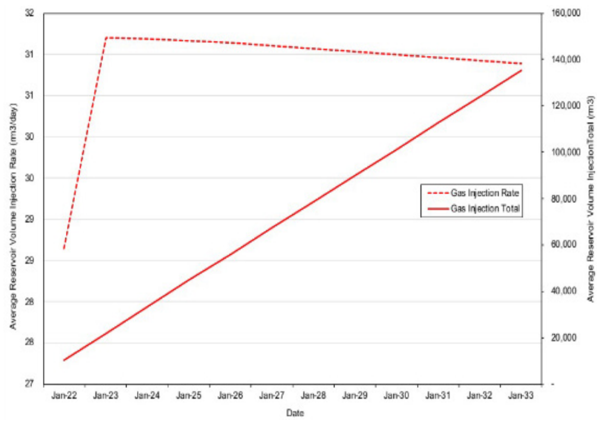


Figure 10:

In the scenario case variant_3_N2_b_10%, the injection stream consisted of 75% CO_2, 10% H_2 and 5% each of CH_4 (C1), N_2 and H_2S. This case was designed to assess the influence of a higher hydrogen concentration on CO_2 storage behavior in the Gulf of Guinea deep saline aquifer. The reservoir demonstrated an exponential increase in injection rate until 2023, followed by a gradual decline, primarily driven by physical interactions within the formation. After ten years of injection **(Table 5)**, the simulation recorded a total stored gas volume of 132,642.00 m³. Hydrogen's small molecular size and high diffusivity may have contributed to enhanced plume dispersion, potentially influencing overall injectivity and storage uniformity. These findings highlight the sensitivity of CO_2 storage systems to the presence of lighter, more mobile contaminants such as hydrogen, which can significantly affect plume migration and containment dynamics **(Figure 11)**.

Table 5: Impact of Contaminants on CO_2 Aquifer Storage - Scenario Case: Variant_4_H2S_b_10%.

DATE	Average Reservoir Volume Injection Rate (rm³/day)	Average Reservoir Volume Injection Total (rm³)
Jan-22	26	9,615
Jan-23	29	20,089
Jan-24	29	30,557
Jan-25	29	41,020
Jan-26	29	51,473
Jan-27	29	61,916
Jan-28	29	72,348
Jan-29	28	82,748
Jan-30	28	93,143
Jan-31	28	103,531
Jan-32	28	113,914
Jan-33	28	124,291

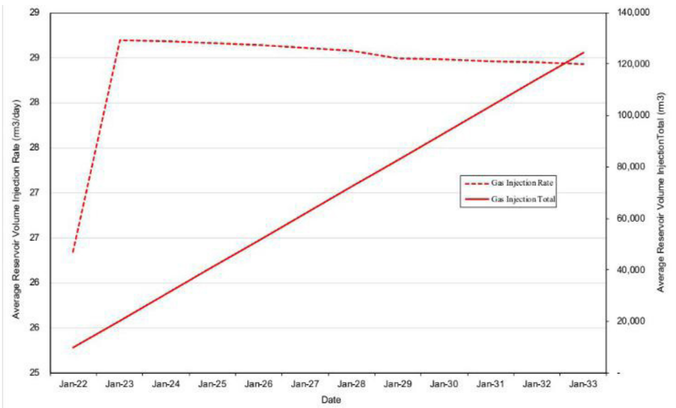


Figure 11:

In Scenario Case Variant_4_H_2S_b_10%, the injection composition included 75% CO_2, 10% H_2S and 5% each of CH_4 (C1), N_2 and H_2. This scenario was developed to investigate the effects of increased hydrogen sulfide concentration on CO_2 storage efficiency and reservoir behavior. The reservoir exhibited a rising injection rate until 2023, followed by a gradual decline due to chemo-physical reactions occurring between the injection stream and reservoir rock-fluid system. After a decade of continuous injection, the total gas stored was 124,291.00 m³. Compared to other variants, the lower storage volume in this case suggests that higher H_2S content may influence reactivity and reduce overall storage efficiency **(Table 6)**. H_2S, being chemically reactive, may engage in mineral interactions or influence wettability, potentially altering pore-scale displacement dynamics. These results underscore the critical role of reactive impurities in shaping long-term CO_2 storage outcomes in deep aquifer environments **(Figure 12)**.

Table 6: Impact of Contaminants on CO2 Aquifer Storage - Scenario Case: Variant_5_H2_b_10%.

DATE	Average Reservoir Volume Injection Rate (rm³/day)	Average Reservoir Volume Injection Total (rm³)
Jan-22	29	10,531
Jan-23	31	22,001
Jan-24	31	33,465
Jan-25	31	44,921
Jan-26	31	56,365
Jan-27	31	67,796
Jan-28	31	79,214
Jan-29	31	90,618
Jan-30	31	101,989
Jan-31	31	113,346
Jan-32	31	124,697
Jan-33	31	136,041

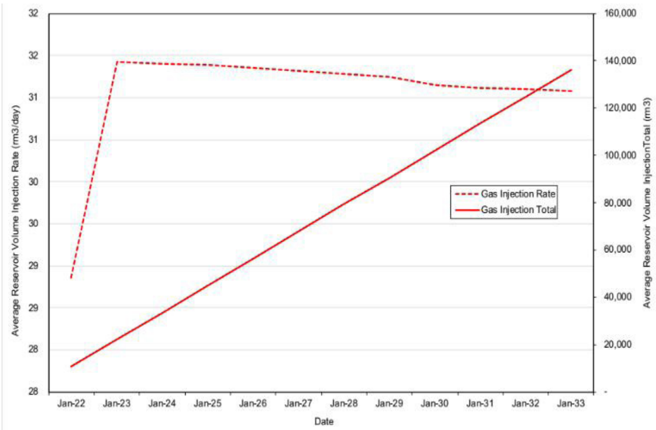


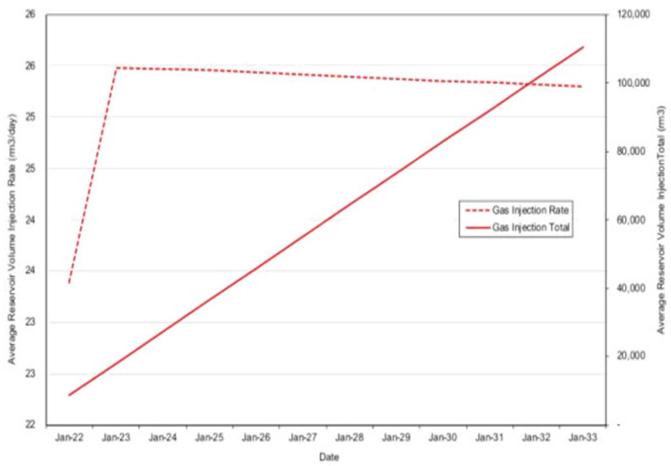
Figure 12:

In Scenario Case Variant_5_H_2_b_10%, the injection stream consisted of 75% CO_2, 10% hydrogen (H_2) and 5% each of CH_4 (C1), N_2 and H_2S. This case was intended to evaluate the effects of elevated hydrogen concentration on storage behavior in deep aquifer conditions. The reservoir injection rate increased exponentially until 2023, after which it gradually declined due to chemo-physical interactions. After ten years of injection, the model indicated a total gas storage volume of 136,041.00 m³-the highest among all scenarios **(Table 7)**. The high mobility and diffusivity of H_2 likely contributed to broader plume dispersion and improved injectivity, although these properties also pose containment challenges. The results emphasize that hydrogen's presence, while potentially beneficial for injection performance, may also influence the spatial distribution and long-term migration behavior of the injected plume **(Figure 13)**.

Scenario Case Variant_6_CO_2_98% was configured to simulate near-pure CO_2 injection, with a stream composition of 98% CO_2 and only trace amounts (0.005% each) of CH_4, N_2, H_2S and H_2. This high-purity case serves as a benchmark for evaluating the effect of minimal impurities on storage efficiency. The reservoir exhibited the typical injection pattern, with exponential growth in injection rates until 2023, followed by a progressive decline attributed to chemo-physical processes. After a decade, the total volume of stored gas was 110,487.00 m³—the lowest among all studied cases. Despite the streamlined chemical profile, the relatively reduced injectivity and plume mobility may be linked to the absence of less soluble or more mobile components that enhance pore space displacement. These findings highlight that while purity improves predictability, small concentrations of impurities can enhance storage dynamics under specific reservoir conditions.

Table 7: Impact of Contaminants on CO2 Aquifer Storage - Scenario Case: Variant_6_CO2_98%.

DATE	Average Reservoir Volume Injection Rate (rm³/day)	Average Reservoir Volume Injection Total (rm³)
Jan-22	23	8,536
Jan-23	25	17,834
Jan-24	25	27,129
Jan-25	25	36,419
Jan-26	25	45,704
Jan-27	25	54,980
Jan-28	25	64,250
Jan-29	25	73,511
Jan-30	25	82,766
Jan-31	25	92,013
Jan-32	25	101,254
Jan-33	25	110,487



Practical implications and real-world relevance

These findings carry important practical implications for CO_2 storage project planning in the Gulf of Guinea region. First, the results suggest that allowing certain benign impurities (like N_2 or CH_4) in the CO_2 stream could be advantageous from an injectivity and capacity standpoint – more gas can be injected and stored without exceeding pressure limits. In a real project, this could translate to cost savings by tolerating a less stringent purification of CO_2. However, planners must weigh this against the fact that those impurities do not contribute to climate mitigation (they occupy pore space but are not climatically active CO_2) and they expand the plume footprint, potentially requiring a larger monitoring area and careful site selection to ensure the plume remains contained within secure boundaries. Increased plume buoyancy might demand stronger emphasis on caprock integrity and trapping mechanisms, since a more buoyant plume can reach the top seal faster. In the Gulf of Guinea context (Rio del Rey Basin), where reservoirs are deep saline aquifers with likely high salinity, the relative effect of plume expansion may be somewhat dampened (as higher salinity water dissolves less CO_2 and provides slightly higher fluid density), but it is still a critical factor. The simulations also indicate that co-injection of highly soluble or reactive gases (H_2S, SO_2) should be approached with caution. These components can reduce effective storage capacity and pose risks of souring the formation fluids and corroding well materials (due to acid formation). For instance, H_2S, which might be co-captured from industrial streams, should ideally be kept below a few percent in the injectate to avoid excessive dissolution losses and IFT reduction that could compromise caprock sealing capacity. It may be beneficial to separately handle or remove H_2S and SO_2 prior to injection when feasible or else ensure the reservoir has sufficient buffering capacity (e.g. carbonate minerals to neutralize acids) if they are injected. Geochemical modeling of the specific Gulf of Guinea formation rocks (which may contain carbonates, silicates and iron-bearing minerals) is recommended to predict the extent of mineral dissolution or precipitation from impurities like SO_2, O_2 and NO_2. This can inform monitoring plans – for example, tracking pH changes, ionic concentrations or mineral tracers in observation wells. Another practical consideration is the use of monitoring wells to distinguish impurity breakthrough times. The simulations demonstrate that non-reactive tracers (e.g. N_2) will migrate with the CO_2 plume, whereas reactive ones like SO_2 or H_2S may be delayed. Thus, by sampling gas composition in monitoring wells, operators could detect a lag in the arrival of certain impurities as a diagnostic of how much is being retained or reacted in the formation. For example, if an injected CO_2 stream contains a small amount of SO_2 and that SO_2 is not observed in a monitoring well that already detects the CO_2 plume, it implies the SO_2 is being sequestered by dissolution or reactions along the way. This information is valuable for risk assessment and model validation. It is recommended that any CCS project in the region with impure CO_2 include dedicated tracers or impurity monitoring to validate the behavior predicted by these simulations.

CO_2 stream purity standards and guidelines

Current guidelines set by industry and regulatory bodies ensure CO_2 streams are within certain purity limits for safe transport and storage. For instance, ISO 27914:2017 (an international standard for geological storage of CO_2) emphasizes that the injected CO_2 stream should consist "overwhelmingly" of CO_2, with impurities limited to incidental amounts that do not compromise safety or containment. It requires operators to characterize impurities and assess their potential impacts as part of the storage site development. DNV's Recommended Practice (DNV-RP-J203) on CO_2 storage similarly provides criteria for acceptable impurity levels. Typical recommendations include a minimum CO_2 purity ~95–98% in most cases. Some specific limits commonly cited are: total non-condensable gases (N_2 + O_2 + Ar) ≤ 4% vol to avoid excessive capacity loss, O_2 kept to very low concentrations (on the order of 100 ppm or below) due to risks of microbial growth and material oxidation, H_2O content limited to a dew point of about -40 °C (often <500 ppm) to prevent corrosion/hydrate formation and sulfur species (H_2S, SO_2) kept low (100s of ppm to a few percent at most) depending on tolerances. For example, one guideline recommends $SO_2 \leq 100$ ppmv based on health hazard levels and $NO_x \leq 100$ ppmv due to acid formation and toxicity. In enhanced oil recovery (EOR) scenarios, standards can be even stricter (O_2 virtually zero, H_2S limited to avoid souring the oil, etc.), but for dedicated saline storage, slightly higher impurities might be allowable if justified. The key point here is: regulations (like the EU CCS Directive) also forbid using the CO_2 stream to dispose of unrelated waste; only substances derived from the capture process itself are permissible and they must not impede safe containment. These standards set the framework that Chapter 5's analysis feeds into – by understanding the effects of each impurity, one can interpret what levels are acceptable in line with such standards.

Trade-offs: Purification costs vs. Storage performance

There is an inherent economic trade-off between producing a high-purity CO_2 stream and the performance of storage. Achieving 99%+ CO_2 purity can significantly increase capture cost and energy use (due to additional separation steps or polishing units). On the other hand, a less pure stream might reduce how much CO_2 can be stored per injection well or require more monitoring and risk management. It's important to evaluate the cost per ton of CO_2 avoided holistically. It has been shown that allowing small amounts of impurities can be economically beneficial: for example, one analysis found that with 10 mol% N_2 in the CO_2, the storage efficiency in the reservoir fell by about one-third, but the overall storage cost increased by less than \$0.01 per ton (virtually negligible) because the same formation could still be used with minor adjustments. In contrast, removing that 10% N_2 at the capture plant might cost several dollars per ton of CO_2. This indicates that, from a cost perspective, it can be optimal to accept some impurities and compensate by slightly larger storage operations. However, not all impurities are equal: safety-critical impurities like H_2S or NO_x might impose costs in monitoring or require special permits, which could offset savings from not removing them. Another consideration is transport: a CO_2 stream with high impurities might require a thicker pipeline or special materials (for corrosive components), which has its own cost. For instance, pipelines transporting CO_2 with >1% H_2S must use expensive corrosion-resistant alloys or inhibitors. These added costs can sometimes outweigh the savings of not purifying the CO_2. Thus, project developers often perform a techno-economic optimization: they evaluate the "sweet spot" where the marginal cost of purifying an impurity equals the marginal benefit in storage capacity or risk reduction. Generally, impurities that drastically reduce storage capacity (like large fractions of N_2) or pose risks tend to be limited unless capture systems inherently produce them. On the other hand, impurities that are costly to remove but have mild storage impacts (like a bit of Argon or 1–2% CH_4) are often accepted. The literature also discusses the carbon credit or emissions accounting angle: if CO_2 is being stored for climate benefit, impurities like CH_4 have global warming potential – a small amount might leak or not be stored, slightly detracting from the net greenhouse gas reduction. These factors also play into the cost-benefit analysis of CO_2 purity.

Impurity-tolerant storage strategies

To enable use of less-pure CO_2 streams while maintaining safety and efficiency, several strategies can be employed:

Personalized site selection: Choose geological storage sites that can handle impurities. For example, a formation with high calcite content can buffer acid gases by dissolving calcite (neutralizing acid) – effectively self-mitigating the low pH from SO_2 or H_2S. A thick, ductile caprock might better withstand any perturbations from impurities (like slight mineral dissolution) compared to a thin brittle one. If one plans to inject CO_2 with, say, 5% H_2S, a site that already contains natural H_2S or has been used for acid gas injection would be ideal, as it indicates compatibility. In the Gulf of Guinea context, this might mean selecting a saline aquifer that underlies a gas reservoir that contained H_2S – proving the seal held sour gas for geologic time.

Adaptive engineering controls: Implement injection strategies that mitigate impurity effects. One idea is co-injection of CO_2 with water ("water-alternating-gas" WAG) or chase water after CO_2 injection[44]. This can help trap CO_2 and also push reactive impurities to mix more with formation water (enhancing their consumption by reactions, thus protecting farther regions). Another approach is partitioned injection: if a significant amount of, say, H_2S is present, an operator might inject that stream into a separate, smaller compartment of the reservoir (compartmentalization) or at a different well, effectively isolating the more hazardous component. Using corrosion inhibitors and biocides can counteract O_2 and acid effects in wells – allowing a bit more O_2 if the well casing is continuously protected. Furthermore, controlling the injection temperature can be important (to avoid thermal stresses that, combined with chemical effects, could crack rock or cement).

Monitoring and dynamic management: An impurity-tolerant operation would involve robust monitoring to ensure things are proceeding as expected. For instance, if more impurities might lead to more rapid pressure rise, one could install additional pressure gauges and set thresholds to cut back injection if needed[45]. Geochemical monitoring (sampling reservoir fluids or using observation wells) can detect if impurities like SO_4^{2-} (from SO_2) or H_2S are propagating – if they move faster or cause unexpected reactions, the injection plan can be adjusted [46]. The use of reactive transport models (as developed in Chapter 4 simulations) is crucial here: by updating the model with field data, operators can refine predictions of how impurities behave and tweak injection accordingly (adaptive management). This reduces uncertainty and allows pushing the boundaries a bit more safely than a static operation.

Leverage co-optimization opportunities: In some cases, allowing impurities can add value. For example, co-sequestering CO_2 with H_2S solves two problems (climate and local pollution) and may attract incentives for acid gas disposal[47]. If the site can mineralize sulfur as pyrite, that's a stable form of trapping. By framing the project as co-storage of CO_2 and pollutants, one might access additional funding (environmental cleanup funds) or carbon credits for avoided sulfur emissions. This strategy is being considered in some regions where gas processing produces acid gas – instead of separate sulfur recovery, they co-inject with CO_2, saving cost and securely storing sulfur [48]. The key is that the storage site must be suitable and the regulatory regime must allow it.

Real-world case studies and relevance to gulf of guinea

Around the world, there are precedents of CO_2 storage involving impurities:

Sleipner (North Sea): Stores nearly pure CO_2 (>98%) in a saline aquifer, but even Sleipner's CO_2 (from natural gas processing) contains a few percent methane[49]. It has demonstrated that a bit of CH_4 doesn't hinder large-scale injection, though it slightly reduces the net greenhouse benefit.

Snøhvit (Norway): Injects CO_2 from LNG processing (contains some hydrocarbons and I believe minor nitrogen). The operation had challenges with pressure buildup, which underscores the importance of understanding impurity effects (though impurities were not the main cause – rather, the reservoir's properties were)[50].

Acid gas injection (Canada): Over 40 small-scale sites in Canada inject mixtures of CO_2 and H_2S into deep formations as a disposal method. These projects, while smaller in scale than CCS, have provided valuable lessons: e.g., H_2S/CO_2 mixtures can be safely contained long-term with proper site selection (usually a depleted gas zone or saline formation with good seal) and that monitoring of pressure and plume is effective[51]. They report minimal issues with injectivity decline, suggesting that concerns like sulfur deposition can be managed. This experience directly supports the idea that the Gulf of Guinea could handle co-injection of CO_2 with H_2S (relevant if gas fields in the region contain CO_2/H_2S).

Kansas and Illinois (USA) projects: Some CO_2-EOR projects, such as in Cranfield or Illinois Basin, have allowed a bit higher impurity CO_2 from ethanol plants or gas processing[52]. They generally found performance acceptable, but note that when CO_2 is used for EOR, operators often try to remove oxygen completely to avoid degrading oil and corroding equipment.

Gulf of guinea context

Countries in the Gulf of Guinea, like Nigeria, Equatorial Guinea, Cameroon, Angola (further south), are exploring CCS mainly linked to gas production and refining. The CO_2 source here often comes with hydrocarbons or H_2S. For example, LNG projects in West Africa might separate CO_2 from natural gas (to meet pipeline specs) – that CO_2 could be 85–95% pure with methane and ethane as the rest. Re-injecting it offshore could enhance oil recovery or just sequester it. The strategies discussed are highly pertinent: instead of building expensive onshore CO_2 purification, operators might directly inject offshore if the reservoir can accept it. This reduces infrastructure needs in regions where capital is a constraint. Moreover, aligning with developing country needs, an impurity-tolerant approach can lower the entry barrier for CCS projects (cheaper, easier to retrofit onto existing plants). The case study we have (Cameroon's Rio del Rey) demonstrates that with careful study, even a developing region can assess its geology to make such decisions. The results showing sensitivity to salinity and mineralization provide a template: a region can evaluate its aquifer's buffering capacity and then decide how pure the CO_2 needs to be. In practice, a Gulf of Guinea project might negotiate a slightly lower purity requirement in exchange for thorough monitoring and risk mitigation as outlined. International partnerships (with organizations like the IEAGHG or the World Bank's CCS trust funds) could help set appropriate impurity limits tailored to local geology, rather than strictly imposing perhaps overly conservative standards that would make projects unviable.

Conclusion and Recommendations

The findings highlight a need for refining reservoir simulation tools and data for impure CO_2 streams. The Gulf of

Guinea case study underscores that equations of state (EoS) and reactive transport models must be accurate for multi-component CO_2 mixtures. Improving the EoS for mixtures like CO_2–SO_2 and CO_2–H_2S, as well as better kinetic data for reactions of SO_2/NO_x in brines, will reduce uncertainties. Future research and field pilot projects in the region should aim to collect data on how impurities partition and react in real subsurface conditions, feeding back into model calibration. In summary, project planners should leverage these simulation insights by optimizing the CO_2 stream purity for maximum storage efficiency while ensuring that any included impurities do not jeopardize long-term storage security. Balancing physical injection benefits against chemical risks is key. The recommendation is to permit and even utilize non-reactive impurities to improve injection performance (within safe limits), but to minimize highly reactive components or at least incorporate robust monitoring and mitigation strategies for them. By doing so, carbon storage operations in the Gulf of Guinea can be designed to be both efficient and secure, aligning with the region's carbon management goals.

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