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Perilaku Mol Komponen Mineral dan Akuatik dalam Penyimpanan Karbon (Carbon Capture Storage) dengan dan tanpa Sumur Injeksi Air

Behavior of Mineral and Aqueous Component Moles in Carbon Capture and Storage with and without Water Injection Wells

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Abstract. *This research aims to analyze the changes in mineral and aqueous component moles during Carbon Capture Storage (CCS) with and without water injection in a reservoir field. CCS is a key technology for mitigating climate change by capturing and storing CO_2 in geological formations, ensuring its long-term isolation from the atmosphere. However, understanding the geochemical interactions between CO_2, minerals, and aqueous components is critical for predicting reservoir behavior over time. Using GEM reservoir simulation software, the study models interactions between CO2, reservoir minerals (Anorthite, Calcite, Kaolinite), and aqueous components (Ca++, Al+++, SiO2(aq), HCO3-, CO3--, OH-) over 189 years a time period. The simulation reveals that water injection significantly accelerates mineral dissolution and precipitation, affecting reservoir porosity, permeability, and fluid chemistry. Key findings include enhanced Calcite stability and Kaolinite formation with water injection, alongside noticeable changes in aqueous chemistry. These results provide crucial insights for optimizing water injection strategies in CCS projects and improving reservoir management. The study concludes that water injection enhances mineral stability and impacts ionic concentration in the subsurface environment, aiding in more efficient carbon storage solutions.*
Keywords: *Carbon Capture Storage (CCS), Water Injection, Reservoir Minerals, Mineral Dissolution, Mineral Precipitation*

Abstrak. Penelitian ini bertujuan untuk menganalisis perubahan mol komponen mineral dan akueus selama proses Carbon Capture Storage (CCS) dengan dan tanpa injeksi air di lapangan reservoir. CCS merupakan teknologi kunci untuk mengurangi perubahan iklim dengan menangkap dan menyimpan CO_2 dalam formasi geologi, sehingga menjamin isolasinya dalam jangka panjang dari atmosfer. Pemahaman interaksi geokimia antara CO_2, mineral, dan komponen akueus menjadi penting untuk memprediksi perilaku reservoir dalam jangka panjang. Menggunakan perangkat lunak simulasi reservoir GEM, penelitian ini memodelkan interaksi antara CO2, mineral reservoir (Anorthite, Kalsit, Kaolinit), dan komponen akueus (Ca++, Al+++, SiO2(aq), HCO3-, CO3--, OH-) dalam periode waktu dari 189 tahun. Simulasi menunjukkan bahwa injeksi air secara signifikan mempercepat pelarutan dan presipitasi mineral, yang memengaruhi porositas, permeabilitas, dan kimia fluida dalam reservoir. Temuan utama mencakup peningkatan stabilitas Kalsit dan pembentukan Kaolinit dengan injeksi air, serta perubahan yang signifikan dalam kimia akueus. Hasil penelitian ini memberikan wawasan penting untuk mengoptimalkan strategi injeksi air dalam proyek CCS dan meningkatkan manajemen reservoir. Kesimpulannya, injeksi air meningkatkan stabilitas mineral dan memengaruhi konsentrasi ionik di lingkungan bawah permukaan, sehingga membantu solusi penyimpanan karbon yang lebih efisien.

Kata kunci: Carbon Capture Storage (CCS), Injeksi Air, Mineral Reservoir, Pelarutan Mineral, Presipitasi Mineral.

INTRODUCTION

Water injection is a common method used in the petroleum industry to enhance oil and gas recovery by maintaining reservoir pressure and improving hydrocarbon displacement. Besides boosting hydrocarbon recovery, water injection can trigger complex geochemical interactions between the injected water, reservoir minerals, and formation fluid components. These interactions affect mineral stability, porosity, permeability, and fluid chemistry, ultimately influencing the overall reservoir performance [1], [2], [3].

In the context of Carbon Capture Storage (CCS), the injection of CO_2 into deep geological formations is recognized as a key strategy for mitigating climate change, where CO_2 produced by industries is stored beneath the earth's surface. CCS aims to store CO_2 in geological formations through various mechanisms, including physical trapping, residual trapping, solubility trapping, and mineral trapping.

The Figure 1 illustrates different mechanisms involved in trapping CO_2 within a geological reservoir for carbon sequestration. Each trapping mechanism plays a critical role in ensuring that the injected CO_2 remains securely stored over the long term. Here's an explanation of each component in the figure 1.

a). **CO_2 Injection and Initial Distribution**
The figure begins with CO_2 being injected into the reservoir. As CO_2 spreads within the rock formation, it encounters various geological and chemical environments that contribute to its immobilization through multiple trapping mechanisms.

b). **Structural Trapping:**
At the top of the formation, the CO_2 is confined by an impermeable layer, known as a caprock. This layer prevents the CO_2 from migrating upwards and escaping the reservoir. The structural trapping mechanism relies on the physical structure of the rock layers, with CO_2 accumulating beneath the caprock. This is typically the first layer of defense in CO_2 storage and relies heavily on the caprock integrity to contain CO_2 within the reservoir [4]

c). **Residual Trapping**
In the next section, CO_2 is shown moving through the pore spaces between rock grains. As CO_2 moves through the porous rock, some of the CO_2 becomes trapped as isolated bubbles in the pore spaces due to capillary forces. This immobilized CO_2, trapped within the pore network, cannot move further and becomes part of the **residual trapping** process. This CO_2 is immobilized as residual gas, providing a stable form of storage [5].

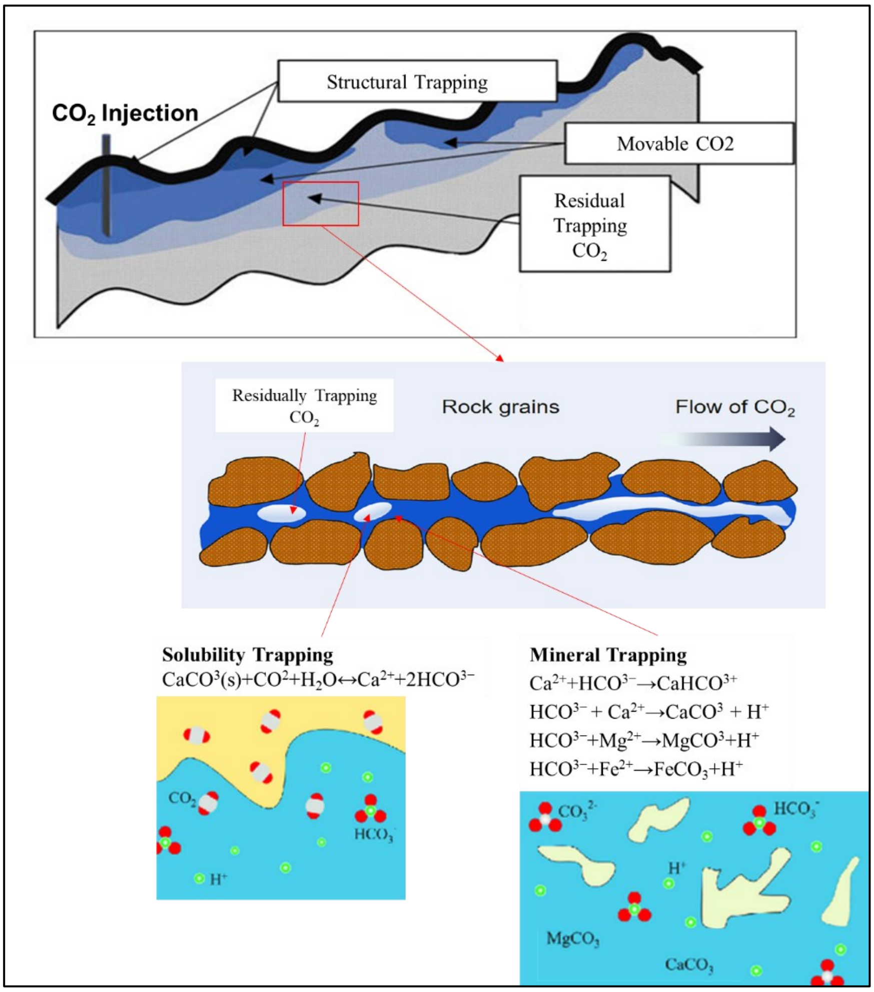


Figure 1. Mechanisms of CO_2 Trapping in Geological Carbon Sequestration: Structural, Residual, Solubility, and Mineral Trapping [20]

d). Solubility Trapping

In the lower left portion of the figure, **solubility trapping** is illustrated. CO_2 dissolves in the formation water (brine) within the reservoir, forming carbonic acid (HCO^{3-}), which then dissociates into bicarbonate ions (HCO^{3-}) and calcium ions (Ca^{2+}) according to the reaction:

$$CaCO^3(s)+CO^2+H_2O \leftrightarrow Ca^{2+}+2HCO^{3-}$$

Solubility trapping, therefore, plays a significant role in long-term CO_2 sequestration by securely storing CO_2 in a dissolved form within the brine, minimizing the risks of leakage or escape from the storage site. Solubility trapping, therefore, plays a significant role in long-term CO_2 sequestration by securely storing CO_2 in a dissolved form within the brine, minimizing the risks of leakage or escape from the storage site [6].

e). Mineral Trapping

In the lower right portion of the figure, **mineral trapping** is depicted. Mineral trapping is a slow process but provides the most permanent form of CO_2 storage [7]. This process occurs when bicarbonate ions (HCO^{3-}) react with minerals in the reservoir, forming stable carbonate minerals such as calcite ($CaCO_3$), magnesite ($MgCO_3$), and siderite ($FeCO_3$). The reactions shown include:

$$Ca^{2+}+HCO^{3-}\rightarrow CaHCO^{3+}$$
$$HCO^{3-}+Ca^{2+}\rightarrow CaCO^{3}+H^{+}$$
$$HCO^{3-}+Mg^{2+}\rightarrow MgCO^{3}+H^{+}$$
$$HCO^{3-}+Fe^{2+}\rightarrow FeCO_3+H^{+}$$

The connection between water injection and CCS lies in the fact that water injection can influence the chemical reactions between the injected CO_2 and reservoir minerals. In CCS processes, water injection can facilitate solubility and mineral trapping by increasing the availability of water molecules, which enhances CO_2 dissolution into formation water and promotes the precipitation of carbonate minerals like calcite [8]. These processes are crucial in ensuring that CO_2 can be stored safely and efficiently over the long term. For example, calcite precipitation can enhance reservoir rock stability, but on the other hand, the dissolution of silicate minerals can reduce rock integrity [9].

Water injection can accelerate the dissolution and precipitation of certain minerals. For instance, Zhang et al. [1] show that the dissolution rate of feldspar significantly increases when water is injected into the formation, which is relevant to CCS, where minerals like feldspar play a critical role in determining chemical reactions between CO_2 and reservoir minerals. Recent studies by Xiao et al. (2018) have also confirmed that water injection enhances carbonate precipitation, particularly calcite, which is crucial for CO_2 trapping in solid form over long periods [10].

Understanding geochemical changes caused by water injection becomes critical in the context of CCS. A detailed analysis of how water injection affects the moles of mineral components (such as Anorthite, Calcite, and Kaolinite) and aqueous components (such as Ca^{2+}, Al^{3+}, $SiO_2(aq)$, HCO_3^-, CO_3^{2-}, and OH^-) is necessary to predict long-term geochemical changes. These changes will impact reservoir stability and CO_2 storage capacity, which are key to the success of CCS projects [11]. In this study, we compare scenarios with and without water injection to understand the impact of water injection on mineral stability and aqueous chemistry over a long period, from the year 2000 to 2189. The aims of this research are to determine how water injection influences mineral dissolution and precipitation, improves mineral stability, and alters ionic concentrations in the reservoir system. Furthermore, this study seeks to assess the resulting changes in reservoir porosity, permeability, and CO_2 storage capacity, providing valuable insights for optimizing water injection strategies and ensuring more efficient and stable long-term carbon storage.

METHODOLOGY

This simulation is designed to model the process of CO_2 injection into a geological reservoir using GEM (**Figure** *2*), an advanced reservoir simulator capable of handling multiphase fluids and integrating geochemical and geomechanical processes. The model accounts for factors like hysteresis, CO_2 solubility in water, and interactions between CO_2 and reservoir minerals such as Anorthite, Calcite, and Kaolinite. These mineral interactions are crucial as they can alter the reservoir's porosity and permeability, impacting both the storage capacity and injectivity of the reservoir [12], [13].

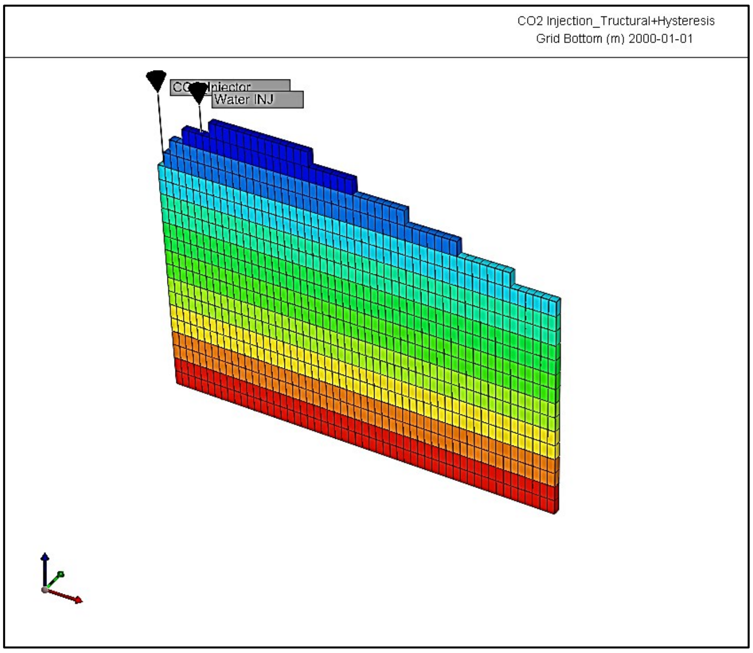


Figure 2. 3D Grid Model of CO_2 and Water Injection for Structural Trapping with Hysteresis Analysis

Key fluid properties, including gas density (DENG) and water density (DENW), are incorporated to track the distribution of CO_2 and water within the reservoir during injection. Modified mineral porosity (DPORMNR) captures changes in porosity from chemical reactions between CO_2 and surrounding minerals, reflecting mineral dissolution or precipitation's effects. While oil is not involved in this simulation, relative permeability factors for gas (KRG) and oil (KRO) are included, anticipating possible future modifications that might introduce oil into the model [14].

Geochemically, the simulation monitors the molality (mol/kg) of ions in the water phase, such as Al^{3+}, CO_2, CO_3^{2-}, and Ca^{2+}, to capture crucial chemical reactions during CO_2 injection. The dissociation of CO_2 in water, leading to carbonic acid formation, may react with minerals like Calcite, causing dissolution or structural changes in the mineral. The simulation also tracks pH, a critical factor in mineral reactivity. For example, a decrease in pH can accelerate the dissolution of minerals like Calcite, increasing porosity but potentially destabilizing reservoir rock integrity [15, 21].

Geomechanical responses are modeled using variables such as Young's modulus (YOUNGI, YOUNGJ), which measures the rock stiffness to account for the mechanical response to pressure changes induced by CO_2 injection, thus anticipating potential fracturing or deformation. Gas saturation (SG) and water saturation (SW) help assess the CO_2 concentration in the gas phase and water distribution within the pore space. Stress components (STRESSI, STRESJ, STRESK, STRESNORM) aid in predicting reservoir deformation under injection pressures. Additionally, porosity (POR) and permeability directionality (PRMXDIR, PRMNDIR) provide insights into fluid flow anisotropy and reservoir heterogeneity [16].

Reaction rate variables (REACTION) control the speed of chemical interactions between CO_2 and minerals like Anorthite, Calcite, and Kaolinite, which are vital for predicting long-term CO_2 behavior within the reservoir. Chemical equilibrium coefficients (LOG-CHEM-EQUIL-COEFS) estimate the deviation from chemical equilibrium, allowing the model to anticipate final mineral and fluid compositions accurately [17].

Overall, this model offers a comprehensive framework for understanding CO_2 injection into geological reservoirs by integrating fluid dynamics, geomechanics, and geochemical reactions. The detailed variables ensure accurate predictions of both immediate injection behaviors and long-term reservoir changes. This level of detail is essential for optimizing CO_2 injection strategies, ultimately supporting the success of long-term carbon capture and storage (CCS) projects [18].

The analysis is based on data obtained from simulations conducted using reservoir simulation software. Two distinct scenarios were modeled:

- Scenario 1: Reservoir conditions without water injection.
- Scenario 2: Reservoir conditions with water injection.

The simulations were run over an extended period, from the year 2000 to 2189, to capture both short-term and long-term geochemical changes. The primary focus was on the following minerals and aqueous components : Minerals (Anorthite, Calcite, Kaolinite) and Aqueous Components (Ca++, Al+++, SiO2(aq), HCO3-, CO3--, OH-). For each scenario, the simulations tracked the moles of these minerals and aqueous components at regular intervals. The results were plotted to visualize the changes over time, providing insights into the impact of water injection on mineral stability and aqueous chemistry.

The simulation results were analyzed to identify trends and differences between the two scenarios. Specific attention was given to:

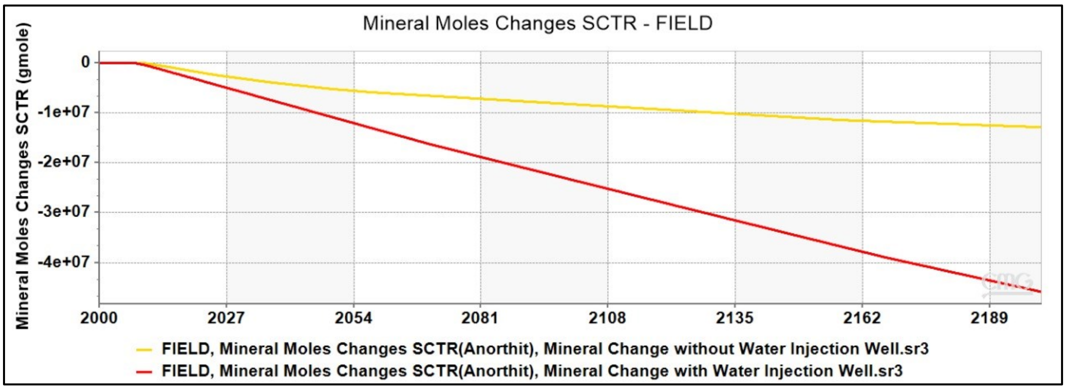
- Dissolution and precipitation patterns: To understand how water injection affects mineral stability.
- Ionic concentration changes: To determine the impact on aqueous chemistry and potential buffering effects.

These analyses were then compared with findings from previous studies to validate the results and provide a comprehensive understanding of the geochemical processes at play.

RESULTS AND DISCUSSION

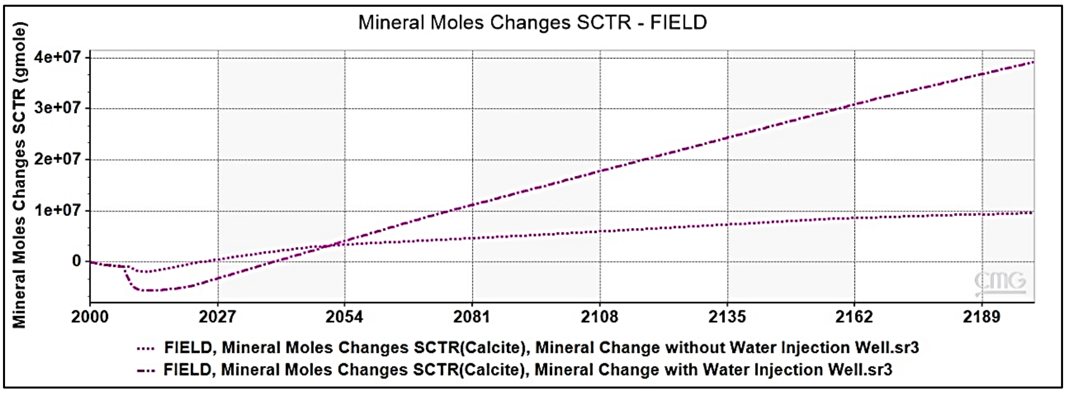
A. Mineral Moles Changes

The data for Anorthite shows a gradual decrease in moles in both scenarios, with a more pronounced decline observed in the water injection scenario. This suggests that water injection accelerates the dissolution of Anorthite, likely due to increased water-rock interactions. This observation aligns with recent studies, such as Xiao et al. [19], who reported that water injection enhances the dissolution rates of feldspar minerals under similar conditions. This accelerated dissolution could impact the reservoir's mineral composition and porosity over time, affecting its suitability for long-term CO_2 storage.



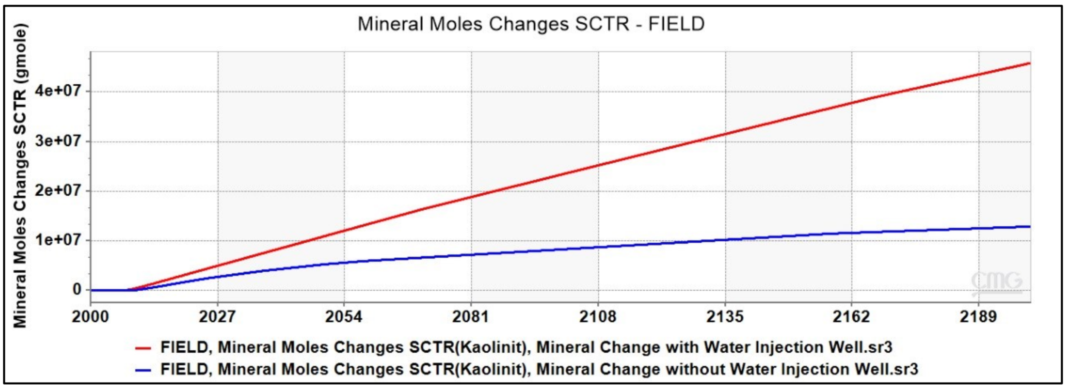
Gambar 1. Impact of Water Injection on Anorthite Mineral Mole Changes in the Field Over Time

The data for Calcite shows an increase in moles under water injection, while a slight decrease is observed without it. This suggests that water injection promotes the precipitation of Calcite, likely due to increased carbonate ion concentration in the presence of water. This observation is consistent with findings from recent studies, such as Marty et al. [20] that found enhanced calcite stability in the presence of water injection due to increased carbonate ion concentration.



Gambar 2. Impact of Water Injection on Calcite Mineral Mole Changes in the Field Over Time

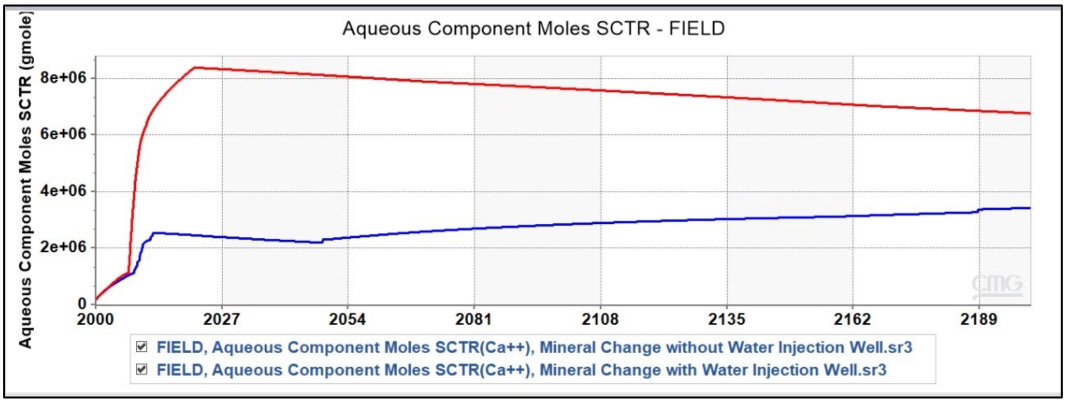
The data for Kaolinite shows a consistent increase in moles in both scenarios, with a greater increase observed under water injection. This trend suggests that water injection enhances the formation of Kaolinite, possibly due to the increased fluid flow promoting secondary mineral formation. This observation aligns with the findings of Xu et al. [14], who reported that Kaolinite formation is favored in environments with increased fluid flow, as it provides the necessary conditions for secondary mineral growth.



Gambar 3. Impact of Water Injection on Kaolinit Mineral Mole Changes in the Field Over Time

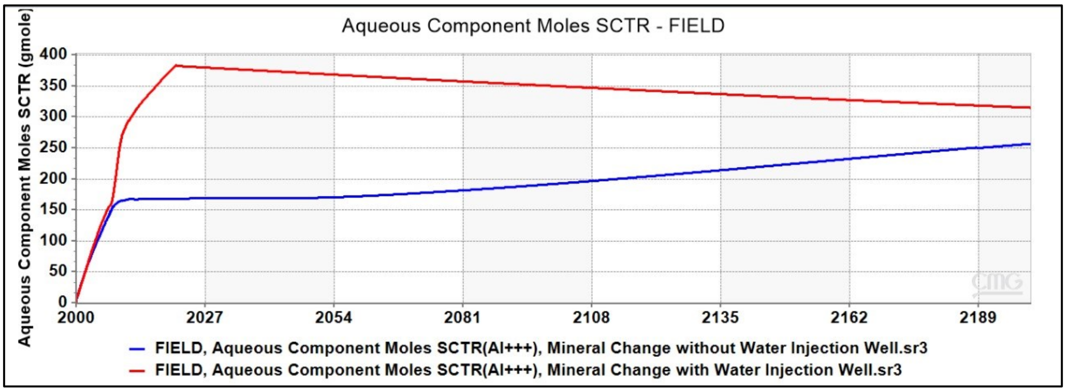
B. Aqueous Component Moles Changes

The data for Ca^{2+} (Calcium ions) shows a sharp initial increase in moles, followed by stabilization with minor fluctuations, with higher concentrations observed in the no-injection scenario. This trend suggests significant dissolution of calcium-bearing minerals in the absence of water injection. In the water injection scenario, however, the increase in calcium ions is less pronounced, potentially due to the re-precipitation of Calcite facilitated by the higher availability of carbonate ions. This observation aligns with studies such as those by Smith et al. [22], who found that water injection promotes Calcite precipitation, which can limit calcium ion concentration in the fluid phase.



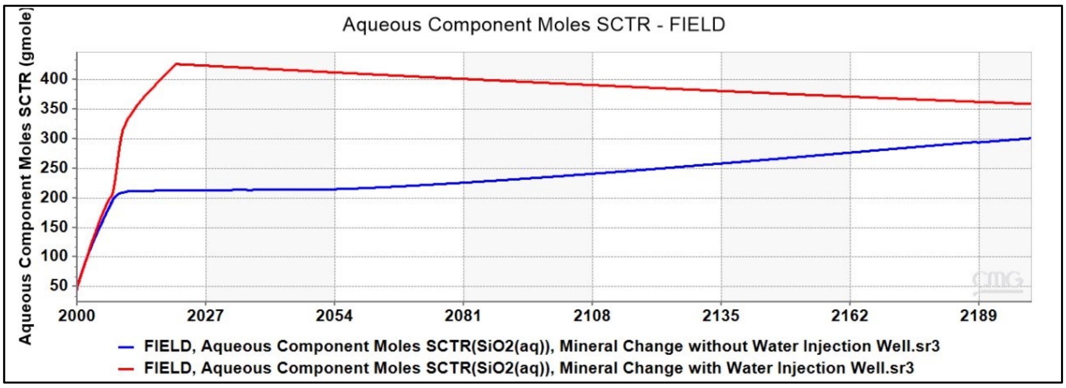
Gambar 4. Impact of Water Injection on Ca^{++} Mineral Mole Changes in the Field Over Time

The data for Al^{3+} (Aluminum ions) shows a trend similar to that of Ca^{2+}, with an initial increase followed by stabilization. However, lower concentrations of aluminum are observed in the water injection scenario. This trend suggests that water injection may reduce the dissolution of aluminum-bearing minerals or enhance the precipitation of aluminum hydroxides. This observation is consistent with findings by Carroll et al. [23], who reported that water injection can reduce aluminum dissolution and promote the formation of stable aluminum hydroxides under certain conditions.



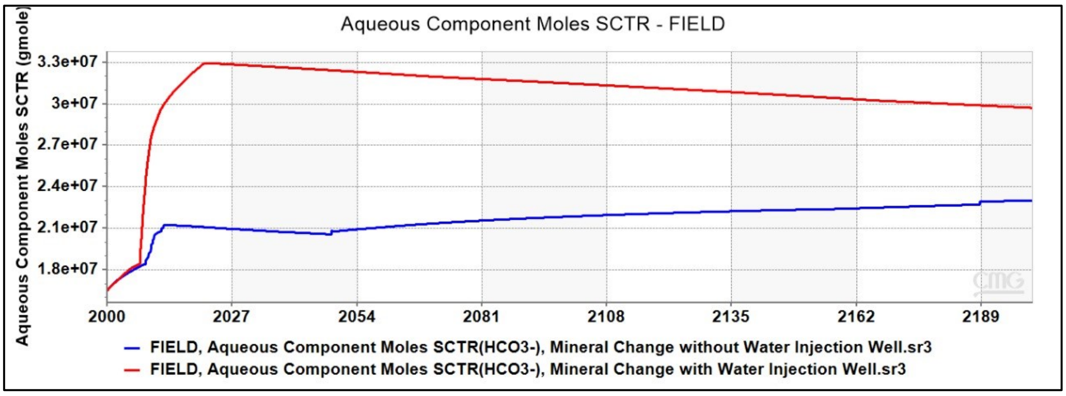
Gambar 5. Impact of Water Injection on Al^{++} Mineral Mole Changes in the Field Over Time

The data for SiO_2 (dissolved silica) shows a significant initial increase in moles, followed by a gradual decrease, with higher concentrations observed in the water injection scenario. This trend likely results from the enhanced dissolution of silicate minerals in the presence of water injection. This observation is in line with findings from Gysi and Stefánsson [24], who reported that water injection accelerates the dissolution of silicate minerals, thereby increasing dissolved silica concentrations in similar conditions.

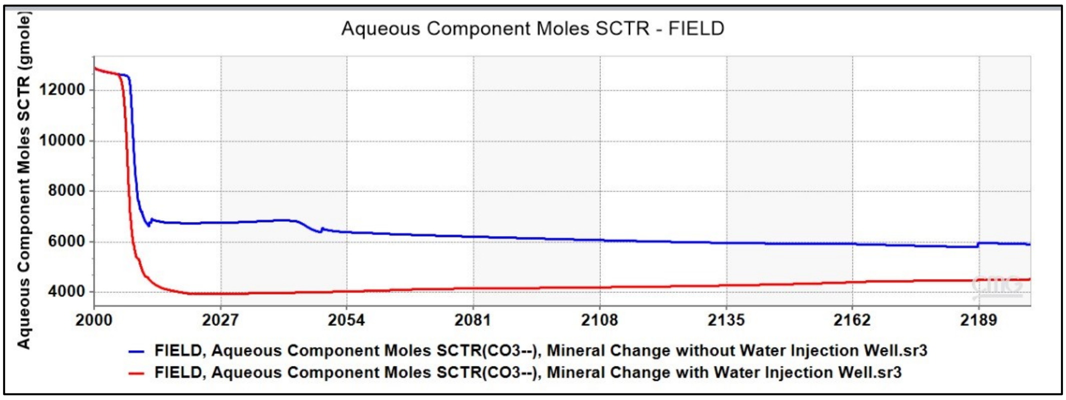


Gambar 6. Impact of Water Injection on SiO_2 Mineral Mole Changes in the Field Over Time

The data for HCO^{3-} (bicarbonate) and CO_3^{2-} (carbonate) shows distinct patterns, with a sharp initial decrease followed by stabilization at lower concentrations in the water injection scenario. This trend suggests that water injection may enhance the system's buffering capacity, which promotes carbonate precipitation and reduces bicarbonate and carbonate ion concentrations in the fluid phase. This observation aligns with findings by Parkhurst and Appelo [25], who noted that increased buffering from water injection can lead to enhanced carbonate precipitation in similar environments.

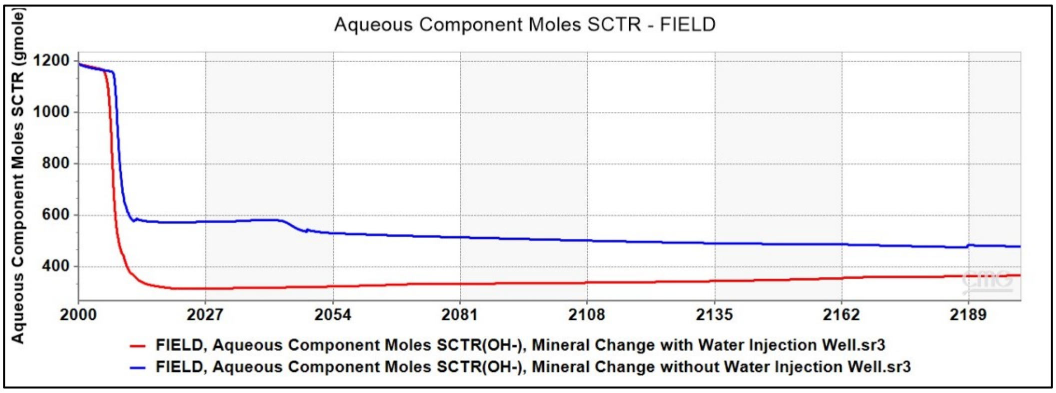


Gambar 7. Impact of Water Injection on HCO_{3-} Mineral Mole Changes in the Field Over Time



Gambar 8. Impact of Water Injection on CO_{3--} Mineral Mole Changes in the Field Over Time

The data for OH^- (hydroxide ions) exhibits a trend similar to that of HCO3−\text{HCO}_3^-HCO_3^-, with higher concentrations observed in the no-injection scenario. This pattern could be attributed to pH dynamics affected by water injection, which may alter the acid-base balance in the reservoir. The lower OH^- concentrations in the water injection scenario suggest that injected water might buffer the system, leading to reduced hydroxide levels. This observation aligns with findings by Zhu et al. [26], who noted that water injection can significantly impact pH and hydroxide concentrations in CO_2 sequestration environments.



Gambar 9. Impact of Water Injection on OH. Mineral Mole Changes in the Field Over Time

CONCLUSION

Water injection plays a crucial role in altering the chemical environment of a reservoir, significantly impacting the behavior of both minerals and aqueous components. In particular, the injection of water into subsurface formations influences the dissolution and precipitation rates of various minerals, leading to changes in their stability. For instance, minerals like calcite and kaolinite tend to exhibit increased stability under water injection conditions due to shifts in the pH and ionic balance of the reservoir fluids. The process of water injection also leads to changes in the concentration of key ions such as calcium (Ca++), bicarbonate (HCO3-), carbonate (CO3--), and hydroxide (OH-), which in turn affect mineral equilibria and reactions within the reservoir. Furthermore, the interaction between injected water and existing reservoir fluids can influence porosity and permeability, with potential implications for fluid flow and overall reservoir performance. By understanding these geochemical reactions and their effects on the mineral composition and fluid chemistry, this study offers valuable insights into optimizing reservoir management strategies.

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