PS A Numerical Simulation of CO_2 Mineralization in the Serra Geral Formation Basalts

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Abstract

Basalt provinces offer promising opportunities as geological carbon storage sites due to their high reactivity with CO_2, leading to a significant capacity for rapid and permanent trapping, one of the main challenges which Carbon Capture and Storage (CCS) techniques need to address in order to become a viable tool for fighting GHG emissions on a large scale. Despite the topic being still relatively understudied, projects developed in Iceland and the USA have demonstrated in situ CO_2 mineralization rates of up to 95% and 60%, respectively. In Brazil, basalts from the Serra Geral Formation present similar potential for carbon dioxide mineralization, highlighting a wide array of previously uncharted locations as suitable for CCS hubs. Such hubs could be of strategic importance in the national context, as the Serra Geral Formation overlaps with highly industrialized areas of the country, in which multiple major stationary emission sources are present. Laboratory experiments indicate that basaltic rocks from the Serra Geral Formation are able to rapidly mineralize up to 75% of the injected CO_2 in a controlled environment, yet studies simulating rock-fluid interactions in large scale at reservoir conditions are still in a preliminary stage for basalt provinces. Therefore, numerical simulations reproducing real life conditions are of great importance as a next step in fostering further understanding on the viability of this CCS method. This study proposes a methodology to simulate CO_2 rock fluid interaction and trapping using the GEM software, developed by CMG. Results show most of the injected CO_2 was trapped in a timespan compatible with industrial operations, most of which through carbonate precipitation. Mineralization rates were then compared with laboratory results, providing valuable insight into the key bottlenecks regarding integrated reservoir modelling for CO_2 storage and mineralization. These findings provide significant motivation for further studies, which could lead the way to considerably reducing the carbon footprint of the Brazilian industrial and energy sectors.

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Theme 8: CCUS Mineralization

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Relevance

Carbon Capture and Storage (CCS) is widely recognized as a key strategy for achieving a net-zero emissions scenario by 2050. However, it faces several challenges, among which permanent storage assurance is a major concern, as leakages would not only render the technology ineffective but also pose significant safety and environmental risks.

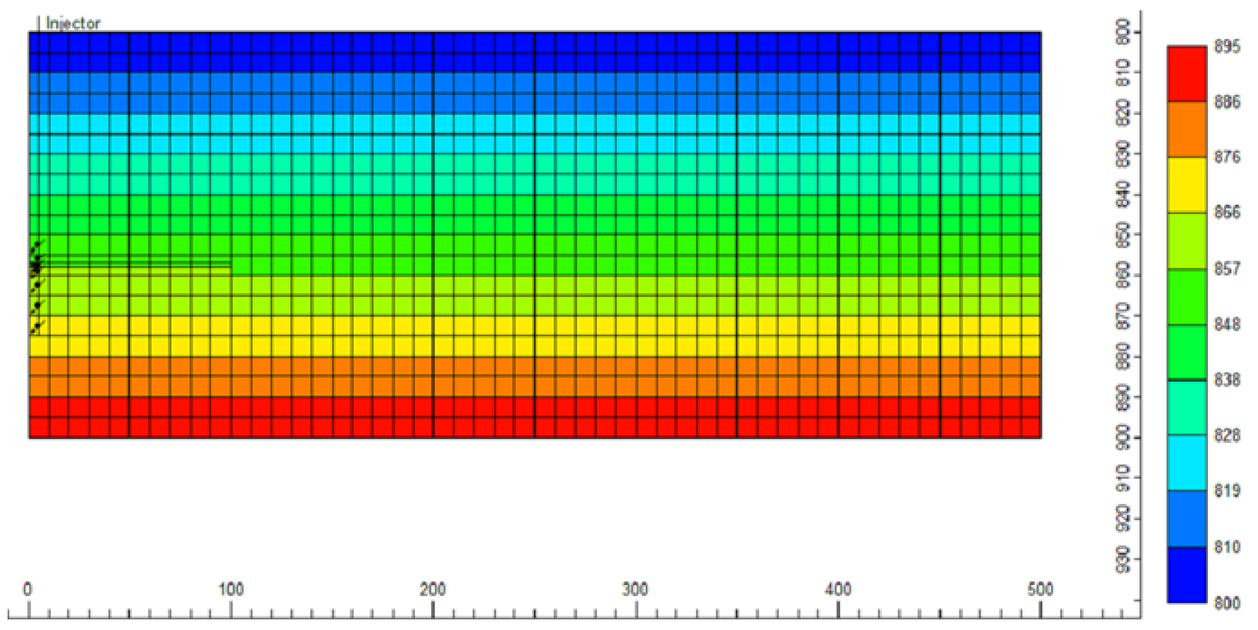
In this context, CO_2 mineral carbonation in mafic rocks is an innovative and field-tested solution to ensure the permanent and secure storage of a significant amount of injected CO_2 in the form of stable carbonates within a few years. This study models a two-phase simulation to predict the behavior of supercritical CO_2 injected into a water-saturated basaltic reservoir, with properties based on those of the Serra Geral Group.

Methodology

A two-dimensional reservoir section was modeled to allow the analysis of the two-phase interaction between injected supercritical CO_2 and connate water within a typical basaltic reservoir from the Serra Geral Basin.

Solubilization, hysteresis and mineralization trapping were accounted for in the simulations. The Land model was used for hysteresis gas trapping and a maximum residual gas saturation of 28.5% was adopted. Relative permeability curves based on experimental data were obtained from Gierzynski and Pollyea (2017).

The simulation employed a 50 x 1 x 20 grid with cell dimensions of 10 m x 10 m x 5 m, and an injection rate of 100 m³/day was considered for a period of four years. Average porosity and horizontal permeability were assumed at 16.5% and 0.1 mD respectively (Rosseti et al., 2019), while vertical permeability was set to 10% of the horizontal value across all regions. A volume multiplier of 100 was applied to the cells farthest from the injection well to account for additional storage capacity and avoid artificial pressure build-up. At depths of 855-860 m, a simplified fractured zone was introduced. Within this region, an effective horizontal permeability of 100 mD was assigned between 857 m to 858 m, while 10 mD was considered for the intervals from 855 m and 857 m and from 858 m to 860 m.



Reference temperature and pressure conditions of 46.7°C and 7.8 Mpa were applied for the reservoir, while rock compressibility for basalt was assumed as 2.1 x 10^{-8} /kPa.

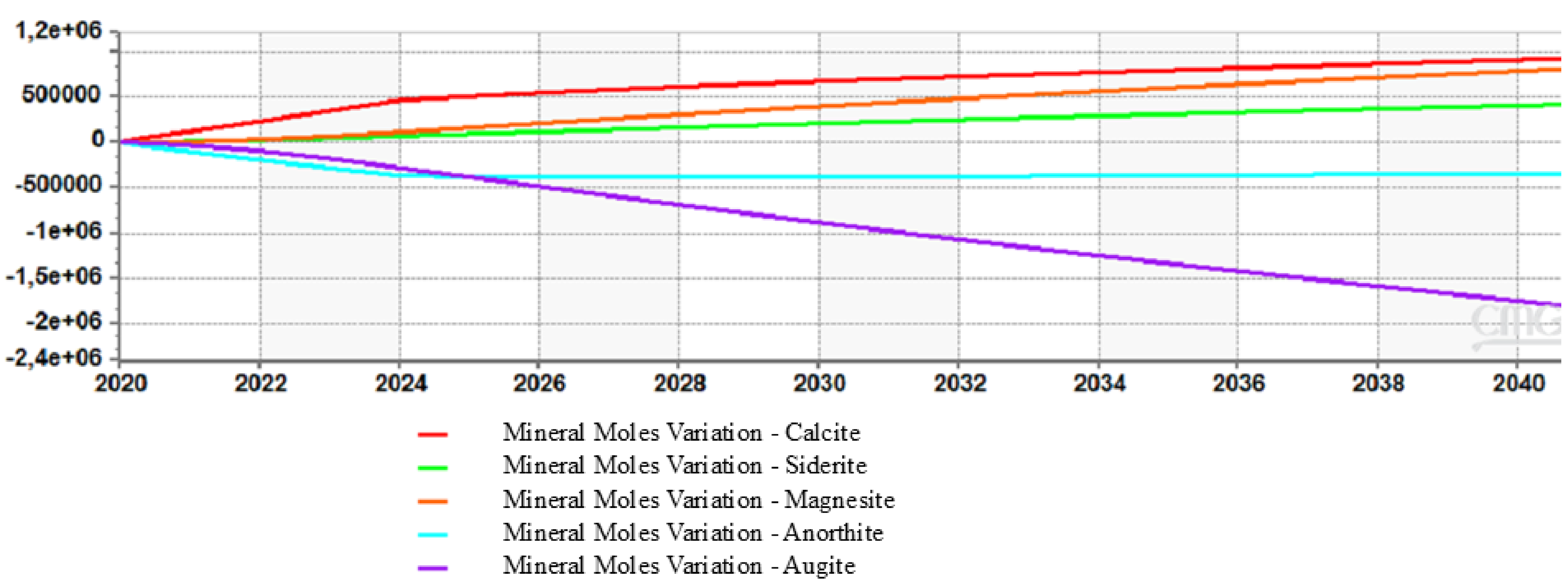
Geochemical modelling was based on a representative mineralogical composition of 29% anorthite and 25% pyroxene, which constitute the main reactive minerals in the Serra Geral basalts. These minerals release Ca^{2+}, Mg^{2+} and Fe^{2+} cations when in contact with CO_2 under acidic conditions (Rosseti et al., 2018).

Pyroxene composition was considered as 0.32Ca 0.45Mg 0.23Fe augite, and diopside was used as reference for the thermodynamical parameters, all of which were sourced from the Wolery database. Calcite, magnesite and siderite were considered as mineralization products.

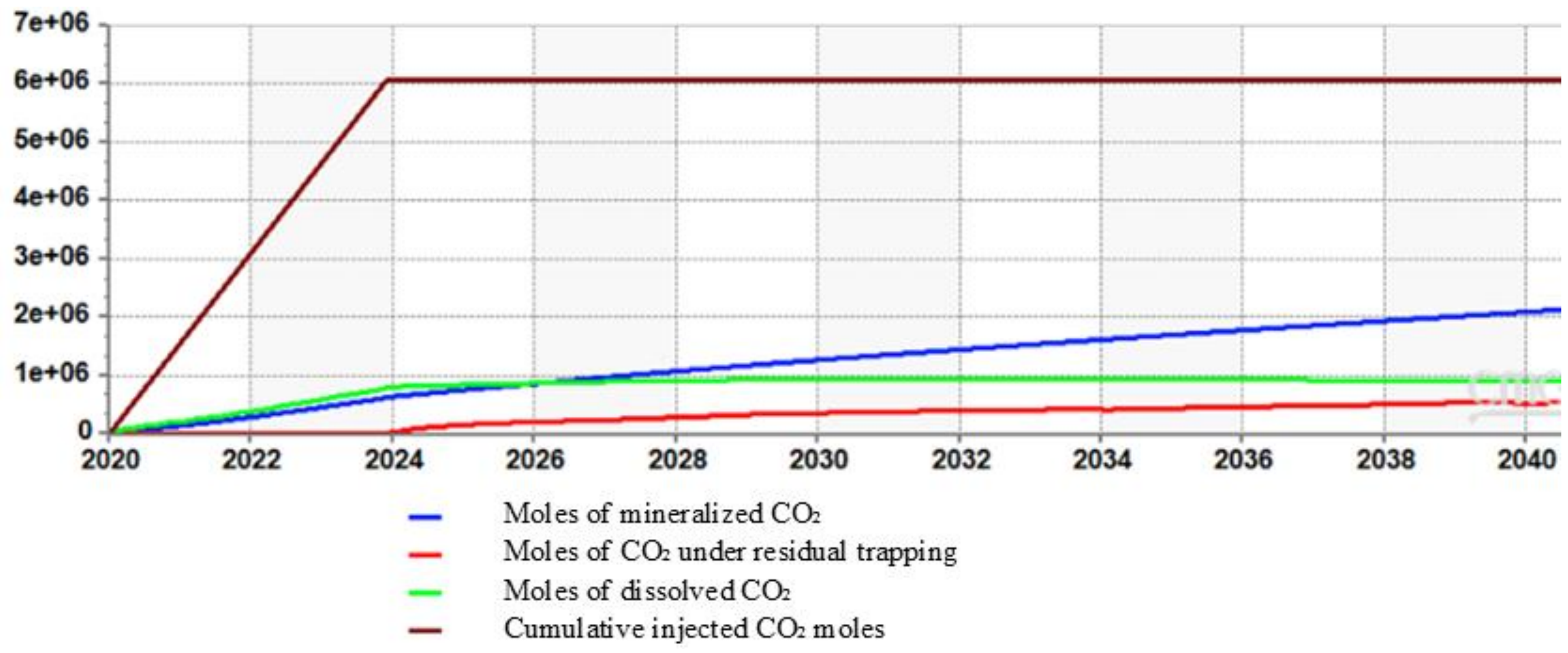
Mineral Reaction	$logk_{25}$ (mol/m²s)	Ea (kJ/mol)	Initial composition	RSA (m²/m³)
Anorthite	-5.17	58.0	29.0 %	4265.0
Augite	-8.20	81.8	25.0 %	3676.8
Calcite	-5.8	14.4	-	2007.8
Siderite	-7.7	48.0	-	2007.8
Magnesite	-11.80	159.0	-	2007.8

Kinetic reaction parameters, including rate constants and activation energy, were adopted from Heřmanská et al. (2022) and Awolayo et al. (2022), while values for reactive surface area were adapted from Berrezueta et al. (2023).

Results and discussion



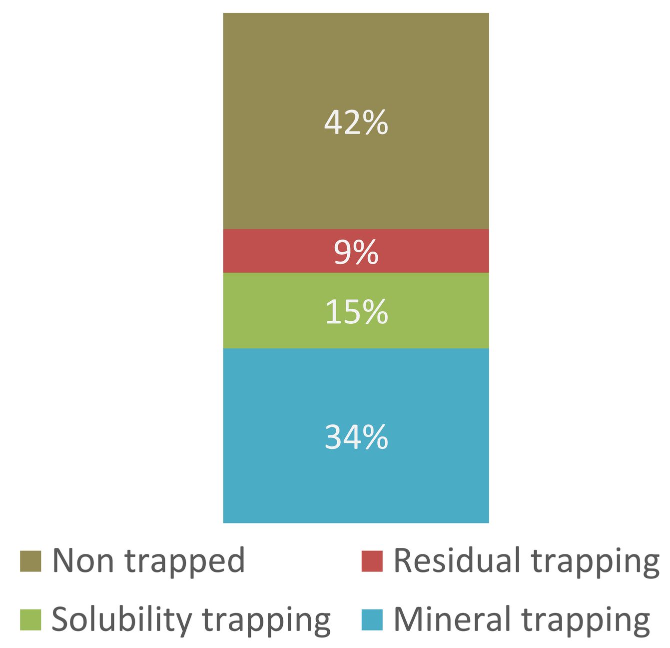
The simulations indicate significant dissolution of both anorthite and augite during the injection phase, occurring concurrently with rapid calcite precipitation, primarily responsible for storing injected CO_2 upon contact with dissolved Ca^{2+} cations during injection. However, plagioclase dissolution stalls as the injection is interrupted, significantly hindering further calcite formation. In contrast, augite dissolution does not suffer any significant drawbacks once injection ceases.



Siderite and magnesite precipitate in a much slower manner due to their more sluggish reaction kinetics, which causes them to become significantly more relevant during the observation phase, as opposed to calcite.

The difference in behaviors observed between both minerals after the injection is interrupted is likely related to Al^{3+} saturation in the formation water, which favors the precipitation of a wide range of aluminosilicate minerals, in a complex "multi-sources, multi-sink" scenario with outcomes which are often difficult to predict (Lu et al., 2024).

Overall, the simulation indicate that a significant amount of CO_2 was trapped over a 21 years timespan, corresponding to 58% of the total injected moles. Among the trapping mechanisms, carbonate mineralization was the most significant, representing around one third of the injected CO_2 (34%), followed by solubility trapping (15%) and hysteresis trapping (9%).



Conclusion

While these values are inferior to the mineralization rates reported in the Carbfix and Wallula experiments, they provide valuable insight into the significant amount of CO_2 which can be securely retained in a reservoir section. It is worth noting that this study does not consider any stratigraphic trapping. Moreover, the inclusion of aluminosilicate minerals as secondary mineralization phases could significantly enhance anorthite dissolution by shifting the equilibrium conditions.

Additionally, different reservoir conditions, as well as the presence of olivine, Fe-Ti oxides or higher augite concentrations, could promote significant improvements in mineralization efficiency.

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