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Optimizing Carbon Storage in Mafic Rocks: From Empirical Data to Dynamic Reactive Models and Uncertainty Analysis

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In-situ geological CO_2 mineralization is a promising method for long-term carbon storage due to its potential large storage capacity and its inferred long-term chemical integrity ensuring short time monitoring. The CarbonStone R&D TotalEnergies project aims to implement this technology in offshore mafic structures using CO_2 dissolved in seawater in low temperature environment (<100°C). Industrial upscaling requires predicting the fluid and reservoir's chemical and physical changes over time.

When static and dynamic parameters are diagnosed using field data or analogues, the reactivity models use empirical kinetic parameters derived from laboratory experiments, typically conducted at temperatures above 80°C and under far-from-equilibrium conditions. Validating low-temperature models requires integrating with long-term and slow kinetics lab experiments. Various additional biases may arise without thorough evaluation of their impact on predictive models: the absence of kinetics data for secondary minerals precipitation, reactive surface areas, selection of representative secondary mineralogy, reaction pathways, and the evolution of associated flow properties over time. The implementation of these parameters is also limited by computational capacities, where overly complex models may fail to converge or require impractically long computation times. This raises several methodological and fit-to-purpose issues for mineralization:

- How do we ensure accurate calibration of reactive transport models in seawater and low-temperature systems?
- How can we reduce the uncertainty of mineralized volumes estimated over time while factoring in variations in reactive parameters?
- What impact does model simplification have during upscaling?
- Using toy-models, what do we learn about mineralization efficiency and reaction paths under various temperature, flow, and mineralogical conditions?

The study was sequentially performed from (1) thermodynamic database review and assessment, (2) 0D-batch modelling coupled with laboratory experiments, (3) upscaling in linear multi-1D toy models, (4) upscaling in linear and radial 2D-toy models, and (5) develop and perform an automatized sensitivity analysis within given range of uncertainties for reactive parameter. This study's preliminary findings from toy models and sensitivity analyses show that low-temperature environments diffuse the reaction path while preserving reservoir properties. High-temperature conditions cause localized mineralization, significantly impacting the reservoir near the injection point. This contribution illustrates how mineralization and transport kinetics influence development strategies.