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Uncertainty Aware CO_2 Mineralization Modeling

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In-situ CO_2 mineralization offers a robust pathway for permanent carbon storage, combining high storage capacity with chemical stability that minimizes long-term monitoring needs. This project focuses on deploying this approach in offshore mafic formations using seawater under low-temperature conditions (<120 °C). Scaling this technology to industrial levels requires anticipating how reservoir properties evolve over time. While static and dynamic parameters can be inferred from field data or analogues, predictive models often rely on kinetic constants derived from laboratory experiments conducted at elevated temperatures (>80 °C) and far-from-equilibrium conditions. Validating these models for low-temperature regimes therefore requires integration with long-duration experiments capable of capturing slow reaction kinetics.

Several uncertainties complicate the modeling process, including incomplete kinetic data for secondary mineral precipitation, poorly constrained reactive surface areas and scaling factors, evolving mineralogical assemblages, and changes in flow properties. Computational constraints further limit model complexity, as highly detailed simulations may fail to converge or become impractical. These challenges highlight the need to reduce uncertainty in predicted mineralized volumes, assess the impact of model simplification during upscaling, and evaluate how simplified models influence mineralization efficiency and reaction pathways under varying thermal and hydrological conditions.

To address these issues, we present a workflow coupling DAKOTA, an iterative analysis framework, with PHREEQC, a geochemical modeling tool. This integration, implemented through a Python driver, streamlines the design of complex numerical experiments and enables systematic sensitivity analyses and uncertainty quantification. In this workflow, DAKOTA drives the geochemical model and efficiently explores its response across the relevant parameter space. Simulation outputs are subsequently post-processed using machine learning techniques to identify variable interactions and quantify prediction losses associated with model simplification.

Deployed on the TotalEnergies proprietary Pangea4 HPC platform, this workflow leverages massive parallelization to efficiently explore parameter uncertainty. Initial results show that reducing the parameter space from 16 to 6 variables yields a 62% reduction in computation time with a prediction loss of only 3.94%. Future developments will integrate numerical and experimental data to further refine predictive models and accelerate offshore deployment of CO_2 mineralization.