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A neural-network-based hydrothermal dolomitization model for future coupling with basin modeling in the energy transition context

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In the context of energy transition, basin modeling, initially dedicated to the understanding of oil and gas systems, can address several challenges that the sustainable energy sector faces, such as identifying large storage volumes for carbon sequestration, determining the thermal recharge sources for geothermal exploration, or characterizing the generation, migration, sink, and accumulation of critical element resources. In this regard, there is a need for spatio-temporal information on the mineral reactions that control the petrophysical properties of the rocks in order to map the best locations in the basin for capturing geothermal energy or storing carbon in basin-wide reservoirs for CO_2 mitigation. Hydrothermal dolomitization is one of these well-known diagenetic reactions that can enhance or destroy reservoir porosity and permeability [1, 2]. It has been extensively characterized by static reactive transport models [e.g., 3] but not kinematic ones. In this study, we replace the CPU-intensive geochemical solver with a hydrothermal dolomitization metamodel using a machine-learning (ML) approach to capture the spatiotemporal diagenetic control on reservoir quality with high computational efficiency for the coupling with thermo-hydro-mechanical simulation of the basin model.

With this aim, we train and test several regression algorithms upon a synthetic dataset to predict the dissolved/precipitated amount of calcite and dolomite. The dataset contains six inputs (T, pH, NaCl, Ca, Mg, C) generated by a Latin Hypercube Sampling and two target values, i.e. dissolved/precipitated mole number of calcite and dolomite, obtained by performing thermodynamic equilibrium calculations. Our results show that the neural network model best generalizes with a root mean square error of 10^{-3} mol on the predictions and a speedup factor of around 1000. This contribution demonstrates the great potential of ML methods in emulating computationally intensive components of numerical simulations to reduce computational costs.

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