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Reactive Transport Modelling of carbon mineralization – a machine learning-based approach

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Carbon mineralisation is currently one of the most promising Carbon Capture and Storage (CSS) options for permanent gas sequestration since it ensures a rapid conversion of carbon from the gas phase to a carbonate mineral. Mafic and ultramafic rocks are the best geological options for mineral carbonation due to the relatively fast dissolution rates of the mineral components that can release carbonatable divalent cations such as Mg^{2+} , Sr^{2+} , Ba^{2+} , Mn^{2+} , Ca^{2+} and Fe^{2+} . Once in solution, these cations react with dissolved carbonate ions to form, under convenient pH and temperature conditions, carbonate minerals like calcite, magnesite, siderite, rhodochrosite, or dolomite.

The viability of carbon mineralization with injection of freshwater has been proven in the CarbFix project [1]. The main feature of the CarbFix method is that CO_2 (and other minor gases) is not injected under its gaseous form but already dissolved in an aqueous fluid, which greatly enhances the mineralisation rates. The methodology, however, requires vast amounts of water that can be a limited resource in many regions. Seawater may be the most viable water source for underground carbonation in many areas, but its use raises questions on the efficiency of the carbonation process. The high ionic strength of seawater makes the geochemical interactions between CO_2 -rock and seawater more complex and, so far, more unpredictable. Reactive transport modelling (RTM) based on experimental thermodynamic and kinetic data of seawater-basalt interaction [2, 3] can shed some light on the expected mineralisation progress in sites with different mineralogy and variable temperature conditions. Figure 1 shows the results obtained with a reactive transport model that simulates the injection of CO_2 -charged seawater in basaltic rock.

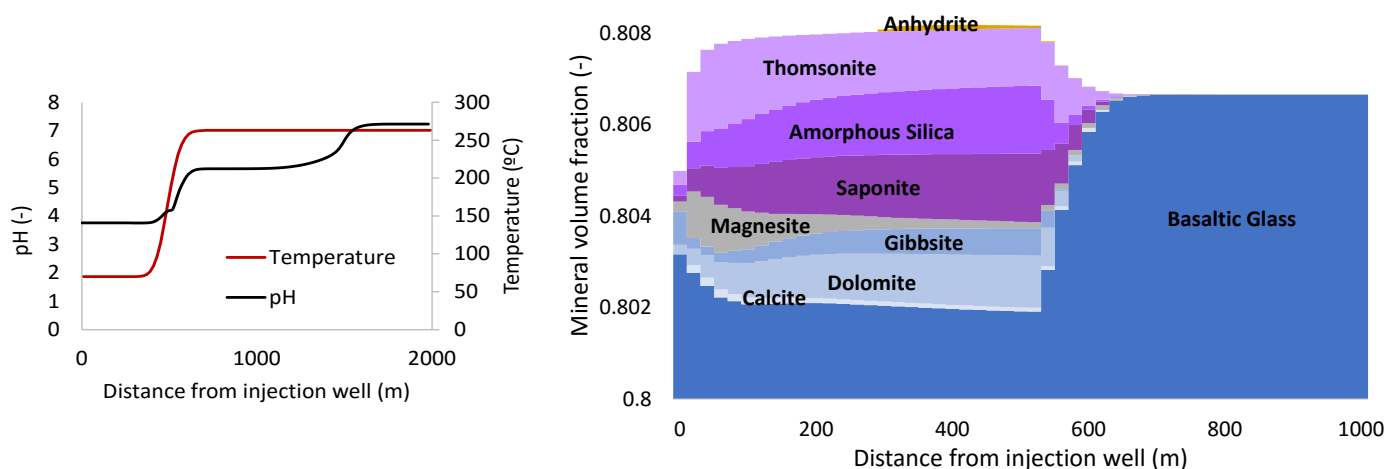


Figure 1: pH and temperature profile (left) and mineral volume distribution (right) obtained with a 1D axisymmetric reactive transport model of 4 years of CO_2 -charged seawater injection in a basaltic glass formation.

Reactive transport modelling (RTM) is a powerful predictive tool, but often requires large computational times [4] and increasing efforts are currently being made to improve the computational performance of available reactive transport codes. The

geochemical reaction calculations in particular might be considerably slow and are sometimes redundant as they might be based on a very similar set of input values. These challenges are usually faced by introducing a number of simplifications in the models to meet the objectives of the simulation studies. Thus, alternative ways to solving the full system are a priori a potential way to reduce the computational burden of numerical models.

One of such alternatives is Machine Learning (ML) and, more specifically, Artificial Neural Networks (ANN), which are inspired on biological neural networks as the ones found in the human brain. They contain several computational “neurons” arranged in different layers. Each of these neurons can be activated based on the response of the other connected neurons. The training process consists of feeding data into the ANN and fitting the connection weights between the neurons to reproduce and learn the hidden relationships of the data. Recently, the authors have coupled ANNs of a geochemical system into a reactive transport simulator [5]. In this approach, Supervised Machine Learning with ANNs is used to accurately predict the geochemical evolution in a reactive transport framework without the need of actually performing the (expensive) chemical equilibrium calculations in the reactive transport model.

The goal of this work is to apply and further develop the technology based on Supervised Machine Learning algorithms to drastically boost the efficiency of reactive transport models of carbon mineralization in the Carbfix system [6]. Firstly, a set of geochemical models of CCS are developed in batch systems (0D) as well as reactive transport models in 1D axisymmetric, 2D, and 3D RTM modelling with different degrees of complexity. Modelling focuses on the injection of CO₂-charged seawater into basaltic rocks. In this system, CO₂ is consumed via a two-step reaction: (1) Dissolution of Basaltic Glass and release of cations (Ca and Mg), and (2) precipitation of Ca-Mg carbonates and other secondary minerals. The RTM models consider a 1 km domain and a characteristic mineralization of 3-4 years. As a first step, these models are solved with the conventional (non ML-based) reactive transport simulator iCP [7]. Then, ANNs are trained and validated with the latest developments in setting up neural networks and used to solve these RTM systems with a Comsol-ML library. The resulting ANNs present good accuracies with coefficients of determination (R^2) above 0.95 for all outputs, and a batch calculation speedup of 30 as compared to traditional chemical equilibration with PhreeQC. Preliminary results of RTM using ML to predict the chemical step indicate a speedup of on order of magnitude and reasonable accuracy as compared to conventional RTM. Our results demonstrate that it is conceivable to replace a geochemical solver in a RTM environment with significantly faster surrogate-based models powered by a machine learning algorithm.

Contributor statement

All the authors equally contributed to this work.

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