Surrogate Model In COMSOL Multiphysics For Reactive Transport Modelling Of Calcite-Dolomite System

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Abstract

Reactive transport modelling in subsurface environments, such as geological disposal of radioactive waste, often requires complex coupling between transport phenomena and geochemical reactions. Traditionally, this coupling requires third-party tools such as iCP to link multiphysics simulators like COMSOL Multiphysics with geochemical solvers such as PHREEQC. However, recent advances in COMSOL Multiphysics Surrogate Model Training capabilities now allow direct integration of trained machine learning models into coupled processes simulations, enabling a streamlined and more computationally efficient workflow.

This study demonstrates the application of COMSOL's built-in surrogate modelling tools to represent complex geochemical reactions involving calcite dissolution and dolomite precipitation, without relying on external coupling interfaces. The benchmark problem, based on Kolditz et al. (2012), involves a one-dimensional reactive column initially filled with calcite. The column is subjected to a continuous inflow of magnesium chloride solution. As the fluid front propagates, calcite dissolves and dolomite forms temporarily due to the reaction with magnesium ions.

IPhreeqc API for C++ is employed offline to generate high-fidelity training and validation datasets covering a wide range of relevant geochemical states and reaction conditions. These datasets capture the dynamic evolution of species concentrations and mineral saturations. A deep neural network (DNN) is then trained using COMSOL Multiphysics Surrogate Model interface to reproduce the essential outputs of PHREEQC with high accuracy. The trained surrogate model is then embedded into the COMSOL Multiphysics model as a replacement for the direct geochemical calculations.

Results show that the surrogate-based COMSOL Multiphysics model accurately reproduces the key geochemical trends observed in PHREEQC simulations, including the timing and extent of calcite dissolution and dolomite precipitation. Moreover, this approach reduces simulation time and removes the dependency on external coupling interfaces. The integration of machine learning within COMSOL Multiphysics not only simplifies the modelling workflow but also opens new possibilities for multiscale and multiphysics simulations in geosciences.

This work highlights the potential of COMSOL Multiphysics Surrogate Model Training functionality to serve as a bridge between high-fidelity geochemical solvers and flexible multiphysics simulation platforms. The approach is particularly promising for modelling systems where direct reactive transport is computationally intensive or where real-time performance is required, such as in large-scale environmental simulations or digital twin applications.

Reference

O. Kolditz et al., OpenGeoSys: an open-source initiative for numerical simulation of thermo-hydro-mechanical/chemical (THM/C) processes in porous media, Environmental Earth Sciences, 67, 589–599 (2012)

Figures used in the abstract

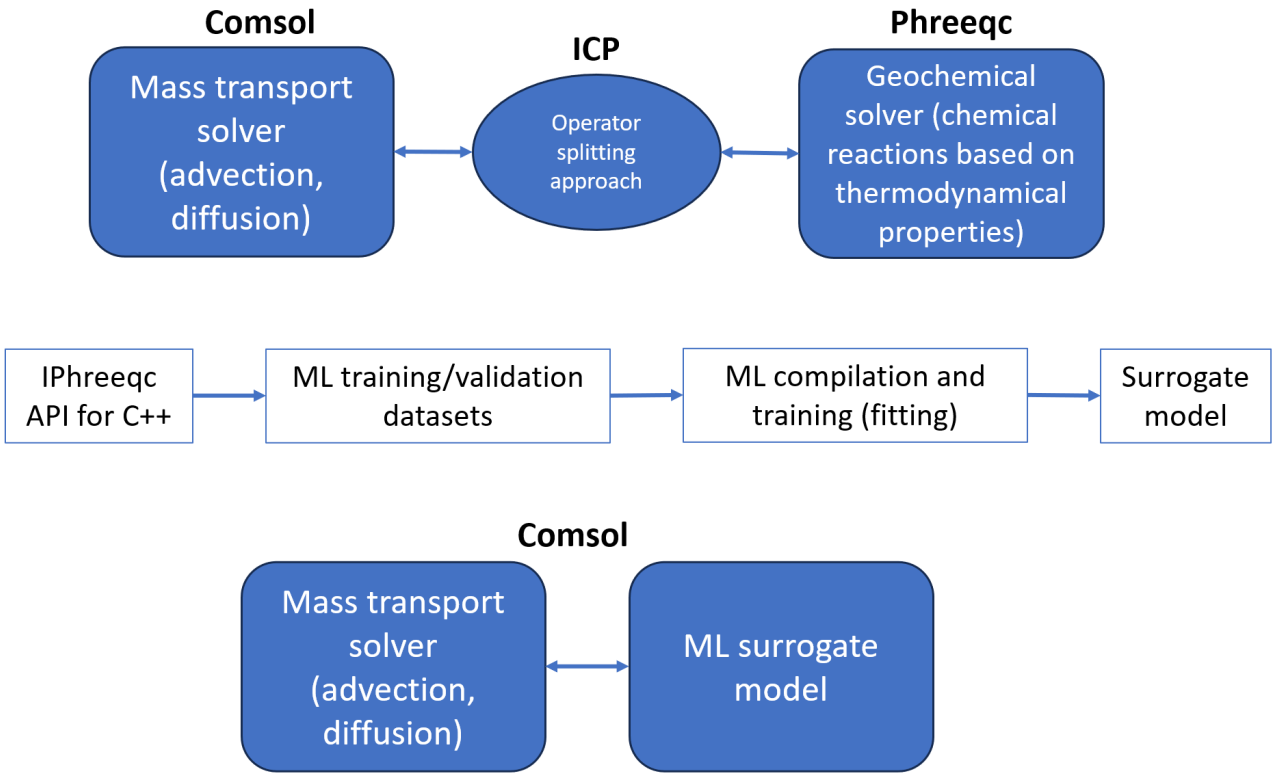

Figure 1 : Workflow and program architecture for surrogate model training: initially integrating a geochemistry solver, followed by the use of the trained surrogate model