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KAN-based Surrogate Model of Chemical Calculations for Subsurface Reactive Transport

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Computational methods are central to geoscience research, with reactive transport modelling (RTM) enabling the simulation of coupled physical, chemical, and biological processes across diverse applications. These include, e.g., CO_2 sequestration, geothermal reservoirs, and electrokinetic desalination. Our driving application consists of deep geological repositories for radioactive waste, where RTM simulations predict the evolution of pH, porosity, and radionuclide migration under experimentally inaccessible conditions. The repeated solution of chemical reactions, which is required up to billions of times per simulation, constitutes the main computational bottleneck in RTM.

Data-driven models are employed as surrogates to speed up chemical calculations, with multilayer perceptrons (MLPs) being one of the most accurate options [1]; however, recent advancements in deep learning should also be investigated. In particular, Kolmogorov-Arnold Networks (KANs) replace fixed activation functions with spline-based trainable ones, achieving higher accuracy than MLPs in function fitting tasks [2]. Their ability to capture complex relationships makes them a strong candidate for chemical calculation emulators.

In this contribution, we propose data-driven and physics-based KAN-based surrogate models for chemical equilibrium calculations. First, we show the performance of the surrogate on an existing cement system benchmark [1]. Then, we consider an application case for the determination of radionuclide-bearing solids solubilities, including solid solutions of binary $(Ba,Ra)SO_4$ and ternary $(Sr,Ba,Ra)SO_4$ systems. In the final case, we move to a calcite-dolomite reactive transport benchmark [3] and investigate a physics-based KAN formulation that includes the Gibbs energy minimization problem in the training process to mitigate error accumulation over time.

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