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Adaptive physics- and chemistry-informed neural network for multi-dimensional reactive transport modeling

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Reactive transport modeling (RTM) can effectively describe physical transport processes and chemical reactions in various geochemical systems. It serves as an interpretive tool to uncover the complex interactions between coupled processes at multiple spatial and temporal scales within Earth systems [1]. However, the solution of PDEs describing such coupled single- and multiphase systems leads to intense computational burden and limits its practical applications. In this study, we develop a dual-network surrogate model with an adaptive mode based on physics-informed neural networks (PINNs) [2] to accelerate the computing process of multi-dimensional reactive transport systems. The adaptive mechanism is used to improve the accuracy of predictions for different chemical reaction occurring in different phases. We consider 2-D pyrite oxidation from an earlier study [3] as a model example to demonstrate the capability as well as to analyze the performance of the proposed physics- and chemistry-informed deep learning model. The dual-network structure uses the intermediate outputs, which is used to calculate the chemical reaction rates, and the PDE residuals of the loss function ensure that the model learns the governing physical laws. The developed model allows both physics- and chemistry-informed learning. The predictions are consistent with those from process-based RTM simulations in a considerably reduced computational time. Furthermore, our model could predict the desired outcomes for a variety of pyrite initial concentrations outside the training dataset, which verifies the potential for excellent generalization capability.

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[3]. Battistel, et al. (2019) *Applied Geochemistry* **100**, 77-89.