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Hidden reactive transport neural network: A physics- and chemistry-informed accelerator for pyrite oxidation modeling

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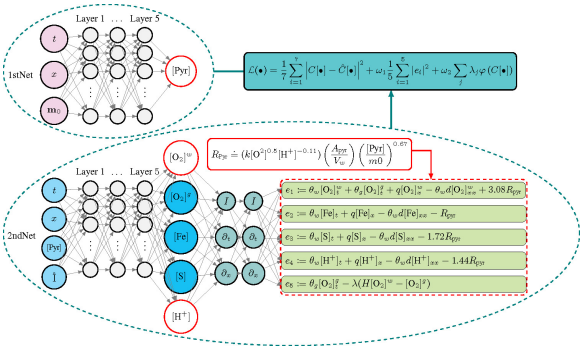

Reactive transport models (RTMs) are instrumental in integrating partial differential equations (PDEs) describing physical transport processes and chemical reactions occurring in natural and engineered porous media. The most challenging aspect of RTMs is the heavy computational burden associated with the solution of coupled system of PDEs in single- and multiphase systems [1]. In this study, we propose a hidden reactive transport neural network (HRTNet) to speed up and mitigate the expensive computing cost yielded by the traditional reactive transport simulations. We consider pyrite oxidation as a model example to demonstrate the capability as well as to analyze the performance of the developed surrogate modeling approach. Based on a physics-informed deep learning model [2], we developed a two-network architecture that shares a common loss function for HRTNet (Fig. 1). The output of the first neural network is used as one of the inputs of the second network. The predictions of the data-driven part are in the calculation of pyrite reaction rates, whereas the physics- and chemistry- part explicitly encodes the reactive transport equations, allowing both a physics- and chemistry-informed learning. To this end, HRTNet is evaluated on a 1-D pyrite oxidation example inspired by an earlier study [3], and the performance has been analyzed in terms of simulation time, prediction accuracy, and generalization. The predictions obtained by HRTNet agree well with those from the process-based RTM simulations in a considerably reduced computational time. Furthermore, HRTNet could predict the desired outcomes for a wide range of pyrite initial concentrations beyond the training dataset. These results are very promising for generalization the capability of the HRTNet approach proposed and tested in this study.

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[2] Raissi, et al. (2020) *Science* **367**, 1026–1030.

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