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Artificial Intelligence for Predicting and Accelerating Reactive Contaminant Transport in Porous Media

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Porous media, such as soils and aquifers, play a crucial role in various environmental and industrial processes, including groundwater management, pollution control, and resource extraction. Modeling the transport of reactive contaminants within these media involves complex interactions between physical properties (e.g., porosity and permeability) and chemical reactions. Traditional numerical simulation methods, though effective, are often computationally expensive and face difficulties in efficiently resolving the nonlinear, coupled interactions that characterize these processes.

This study addresses these challenges by applying Artificial Intelligence (AI) techniques to enhance the simulation of reactive contaminant transport in porous media. The underlying problem is modeled by a system of nonlinear partial differential equations describing diffusion-convection processes, coupled with algebraic equations representing chemical equilibria. A key computational bottleneck arises from the chemical reaction calculations, which require significantly more computational resources than the transport simulations.

To mitigate this, the study integrates machine learning and AI algorithms to predict and accelerate these simulations, achieving both high accuracy and reduced computational costs. Deep learning models, trained on pre-computed numerical solutions, are employed to efficiently predict species concentrations and fluxes. Data preprocessing techniques, such as smoothing and feature scaling, further enhance the quality of the predictions. These AI models serve as surrogates for traditional numerical methods, providing a more efficient solution, particularly in cases where chemical reaction calculations dominate computational resources.

The performance of the proposed framework is validated through comparisons with conventional numerical methods, considering various chemical species and heterogeneous porous media. Results demonstrate substantial reductions in computational time while maintaining high accuracy. This approach underscores the potential of AI to accelerate and optimize reactive transport modeling, offering scalable and reliable predictions for applications in environmental management, groundwater contamination, carbon sequestration, and soil remediation.

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References

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