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From Direct Numerical Simulation to Uncertainty Quantification in reactive microscale flows for CO2 mineral storage applications

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SUMMARY

Reactive microscale flows play a crucial role in understanding the effects of geochemical processes and fluid-rock interactions in CO2 storage applications. The geochemical mechanisms involve precipitation and crystallization, resulting in mineral trapping of the injected CO2, and carbonate dissolution due to the acidification of the medium. Quantifying their impact at the larger scale through upscaling approaches is essential to inform storage capacities and reservoir integrity for risk management of CO2 storage facilities. Studying reactive flows at the pore scale involves complex geometries of real porous samples, extracted from X-ray microtomography (X-ray μCT), and requires developing efficient mathematical models and Direct Numerical Simulation (DNS) tools [1]. This talk focuses on a Semi-Lagrangian formulation of CO2 mineral trapping and introduces a two-step crystallization model involving a probabilistic aggregation rate for crystal growth. This model accounts for geometrical dependency in the crystallization and enables the investigation of flow path restructuring due to partial or complete clogging of pore throats. We identify different clogging/non-clogging regimes and highlight the need to introduce a new dimensionless number for identifying clogging patterns. Modeling and imaging uncertainties, however, arise in pore-scale modeling due to discrepancies in estimating mineral reactivities and kinetic parameters, as well as from image artifacts such as noise and unresolved features in μCT [2]. To enhance the reliability of DNS of micrometric reactive processes, we address the challenge of quantifying these two types of uncertainty by developing a new deep learning strategy applied to reactive inverse problems at the pore scale [3]. We quantify morphological uncertainties and provide reliability ranges on reactive parameters in the context of calcite core dissolution.

Keywords: Pore-scale modeling, Reactive flows, Uncertainty Quantification, AI

AMS Classification: 76-10, 65M22, 68T37

References

[1] S. Molins, C. Soulaine, N. I. Prasianakis et al., Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: review of approaches and benchmark problem set, *Computational Geosciences* **25**, pp. 12851318, 2021.

[2] S. Perez, P. Moonen, P. Poncet, On the deviation of computed permeability induced by unresolved morphological features at the pore scale, *Transport in Porous Media* **141**, pp. 151-184, 2022.

[3] S. Perez, S. Maddu, I.F. Sbalzarini, P. Poncet, Adaptive weighting of Bayesian Physics Informed Neural Networks for multitask and multiscale forward and inverse problems, *Journal of Computational Physics* **491**, pp. 112342, 2023.

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