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Sequential coupling for reactive transport modeling using PHREEQC

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SUMMARY

This study tackles the challenges of reactive transport modeling in environmental contexts, including nuclear waste disposal and geological CO_2 sequestration. Given the lack of extensive long-term experimental data in these applications, numerical simulation is essential. A detailed review of existing codes reveals two primary numerical approaches for reactive flows: global implicit methods and sequential (or operator splitting) approaches. Sequential methods are advantageous as they allow for specific programming of hydrological and chemical processes. The aim of this work is to create a reactive transport package that integrates PHREEQC [1] for chemical processes and DuMu^X [2] for hydrological processes. An operator splitting method is employed in a non-iterative sequential manner. Chemical processes are handled using an element-based approach to facilitate direct coupling with PHREEQC. The spatial discretization is achieved using a cell-centered finite volume method, and time discretization is performed with an implicit Euler scheme. The model is first validated for single-phase flow, demonstrating efficiency through numerical experiments. The method is then expanded to address reactive two-phase flow, undergoing validation through a comparison with an implicit strategy on a recently introduced benchmark [3].

References

[1] D.L. Parkhurst, C.A.J Appelo . Description of input and examples for PHREEQC version 3a computer program for speciation, batch-reaction, one-dimensional transport, and inverse geochemical calculations. Technical report, US Geological Survey, 2013.

[2] T. Koch *et al.*. DuMu^{x}3 - an open-source simulator for solving flow and transport problems in porous media with a focus on model coupling. *Computers and Mathematics with Applications* **81**, 423-443, 2021.

[3] S. DeHoop, D. Voskov , E. Ahusborde, B. Amaziane, M. Kern. Reactive multiphase flow in porous media at the Darcy scale : Part I Benchmark description. *Computational Geosciences*, DOI : 10.1007/s10596-024-10268-z, 2024.

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