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Analysis on the accuracy and efficiency of integration-point based reactive transport scheme

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Conventionally, when simulating reactive transport models with an operator-splitting finite element scheme, the chemical system calculations are placed on the node (the Nodal-OS scheme). This configuration typically results in a mixing of heterogeneous reactions on opposing sides in a multi-layer, chemically heterogamous domain, and it is thus not physically accurate. In this context, an adapted operator-splitting finite element scheme (IP-OS) is proposed in this presentation for reactive transport modeling in saturated porous media. In contrast to the conventional scheme, speciation calculations are performed on integration points rather than on nodes in the new scheme.

The implementation of the IP-OS scheme is verified through comparison with an analytical solution of a coupled diffusion–dissolution problem. On this basis, two representative benchmarks are used to examine the advantages and disadvantages of IP-OS. It is found that (1) IP-OS is more accurate in comparison to the Nodal-OS scheme; (2) IP-OS is less sensitive to grid resolution and is numerically more stable with coarser grid spacing; and (3) IP-OS is computationally more expensive. In light of the above pros and cons, we recommend to use Nodal-OS in cases where chemical reactions do not affect transport properties, while IP-OS scheme should be the better choice when multi-layer heterogeneous domains are present. Especially when the chemical reactions alter the transport properties of porous media, IP-OS should be applied to prevent the unphysical diffusion phenomenon at the interface between different layers. [1]

Reference

[1] Lu, Nagel, Poonoosamy, Naumov, Fischer, Montoya, Kolditz, Shao (2022), A new operator-splitting finite element scheme for reactive transport modeling in saturated porous media, Comput. Geosci. 163 , art. 105106