Contribution ID: **629** Type: **Oral Presentation**

Benchmark of different coupling schemes for reactive transport in saturated porous media

Tuesday, 1 June 2021 15:10 (15 minutes)

The development of continuum reactive transport models in porous media traces back to mid-80's when the theoretical framework to consider reactions in mass transport equations was outlined. Since their establishment, the operator-splitting (OS) approach has been frequently used due to its easy implementation and computational efficiency in large scale simulations including complex chemical processes. Existing and widely used OS-finite element framework in reactive transport normally adopts different collocation schemes for spatially discretizing the transport (i.e. advection and diffusion) and the reaction term of the advection-diffusion-reaction equation. While this numerical approach in general works well in homogeneous systems, it may fail if the field variables (i.e. concentration, hydraulic pressure) vary rapidly, for example, close to the domain boundaries or in the interfaces between different materials. In these cases sharp gradients exist and standard numerical schemes normally lead to inaccurate and unstable numerical results.
A novel OS-finite element framework adopting a consistent collocation scheme of all the field variables in the integration points has been recently developed in our group, validated and implemented in OpenGeoSys-6 (Lu et al. (2021). Contrary to previous finite element OS-schemes, the reaction term was calculated at the integration point level, instead of the nodes where a chemical solver (i.e. Phreeqc) was called for the chemical speciation calculation. Verification of the new implementation was done by comparing the results with different analytical solutions including a first order bio-degradation reaction and a coupled transport-dissolution processes and feedback on porosity changes. In this study, we extend the validation of the method by benchmarking different numerical coupling schemes and comparing the results to experimental observations obtained in a) a well-controlled laboratory scale column experiment including a dissolution reaction with feedback on porosity changes and b) through diffusion experiments of sorbing cations in clay.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

Lu et al. (2021) Water Resources Research (submitted)

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Session Classification: MS7

Track Classification: (MS7) Mathematical and numerical methods for multi-scale multi-physics, non-linear coupled processes