Contribution ID: **375** Type: **Oral Presentation**

Higher-Order Finite Element Multiphase Multicomponent Reactive Transport Model for Unstructured and Fractured Grids

Wednesday, 2 June 2021 15:00 (15 minutes)

We present a higher-order finite element (FE) reactive transport model for unstructured and fractured grids. We use an advanced research simulator (Osures) for flow and transport in subsurface fractured porous media, which models the convection, gravity, mechanical dispersion, Fickian diffusion, Nernst-Planck (electrochemical) diffusion, and capillarity as driving forces. Fluid flow is modeled with the Mixed Hybrid FE method, which provides smooth velocity fields even in highly heterogenous formations with discrete fractures. Multicomponent species transport is updated with a Discontinuous Galerkin (DG) FE method, which offers strict local mass conservation and low numerical dispersion. The Cubic Plus Association (CPA) equation of state is adopted to compute thermodynamic properties of all fluid phases. CPA considers the self-association of polar molecules and polar-induced cross-association. To incorporate the broadest range of reactions (equilibrium and kinetic, aqueous and rock-fluid, electrokinetics etc.), we leverage the PHREEQC geochemistry engine, which has been widely used for (ground)water / hydrogeology applications and thoroughly validated against a wide array of experimental data. PHREEQC provides interfaces, such as PhreeqcRM, which supports implementation as a geochemistry module within any flow and transport simulation framework. We integrate the PhreeqcRM interface and flow simulator Osures in a sequential iterative operator splitting scheme and utilize OpenMP to enable parallel computations for the pressure solver, phase-splits, DG transport updates, geochemistry, and more. This state-of-the-art higher-order FE reactive transport model is capable of simulating geochemical reactions in the aqueous phase (e.g. cation exchange, electrochemical migration), the interdependence of soluble gas components (e.g., carbon dioxide and light hydrocarbons such as methane) and aqueous-rock geochemistry. It allows for any type of unstructured grids, can incorporate discrete fractures, has low numerical dispersion, and can therefore provide more accurate simulation results on relatively coarse grids and low computational cost. The application domains range from lab to field scales and allow highly heterogeneous and fractured rocks.

Model validations are performed to demonstrate the accuracy and robustness of this model for single-phase and two-phase multicomponent subsurface flow. Scaling analyses are presented to quantify the computational efficiency. Reactive transport problems with increasing levels of complexity are investigated, including the effect of dissolved chemical species on CO2 solubilities, competitive dissolution/exsolution between CO2 and light hydrocarbons, and CO2 injection in a field-scale domain with highly heterogeneous formation properties and discrete fractures [2].

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Time Block Preference

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

References

[1] Moortgat, J., Li, M., Amooie, M.A. and Zhu, D., 2020. A higher-order finite element reactive transport model for unstructured and fractured grids. Scientific Reports, 10(1), pp.1-14.
[2] Soltanian, Mohamad Reza, et al. "Simulating the Cranfield geological carbon sequestration project with high-resolution static models and an accurate equation of state." International Journal of Greenhouse Gas Control 54 (2016): 282-296

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