



Contribution ID: 488

Type: **Oral Presentation**

Recent Advances in Modelling Reactive Interfaces in Pore-Scale Simulations

Thursday, 25 May 2023 14:30 (15 minutes)

Micro-continuum modeling enables the simulation of coupled multi-physics processes including multiphase flow and reactive transport at the pore scale. One key feature is the ability to move fluid-solid (e.g. mineral dissolution or precipitation) and fluid-fluid interfaces (e.g. dissolution of gaseous species in aqueous phase) using fixed-grids only, i.e without the need to remesh the grid when the mapping of phases evolves. The displacement of such interfaces relies on an accurate description of mass transfer between the two phases. Various approaches have been proposed to model, on the one hand, the reactive mass transfer at the solid surface, and on the other hand the transfer of species across the interface between two immiscible fluids. In this presentation, we discuss the recent progress made to simulate such processes under thermodynamic equilibrium and non-equilibrium. We review the Continuous Species Transfer techniques, the Volume of Solid approaches, and we introduce a new tentative to combine these two models into a unique framework.

Participation

In-Person

References

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Energy Transition Focused Abstracts

Primary authors: SOULAINÉ, Cyprien (CNRS Orleans, Univ Orleans); MAES, Julien (Heriot-Watt University)

Presenter: SOULAINÉ, Cyprien (CNRS Orleans, Univ Orleans)

Session Classification: MS06-B

Track Classification: (MS06-B) Interfacial phenomena across scales