Contribution ID: **404** Type: **Oral Presentation**

Improved micro-continuum formulations for pore-scale simulation of mineral dissolution

Monday, 31 May 2021 18:15 (15 minutes)

Mineral dissolution is relevant to most subsurface processes, including CO2 storage, geothermal systems and enhanced oil recovery. Pore-scale simulation can be a useful tools to decipher the reactive transport within the pore-space and estimate upscaled parameters such as permeability and reaction constants. These simulations may be challenging though as they involve the tracking of multiple solid interfaces. The micro-continuum method is an efficient approach as it does not involve complex algorithms for explicit reconstruction of the interface, but use volume-averaging of the fluid and solid properties. However, there are two fundamental issues with the current formulation: the need of an interface localisation function to avoid local negative porosity, and concentration bleeding into the solid phase. These two issues lead to significant underprediction of the reaction rate, especially in the diffusion-limited regime, and the reaction constant usually needs to be fitted. To solve these issues, we propose new formulations using a mass conservative localisation function based on the divergence and using the Continuous Species Transfer (CST) method to insure a zero concentration in the solid phase. Our improved formulations are validated by comparison with experimental results and with numerical simulations using a direct method and using the standard micro-continuum approach. We then performed numerical simulations in porous media images and we show that our novel method is as accurate as direct methods and orders of magnitude faster.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

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Session Classification: MS9

Track Classification: (MS9) Pore-scale modelling