MULTIPHASE CHEMICAL KINETICS MODELING FOR AQUEOUS-MINERALS REACTIVE SYSTEMS

Anthony Michel, Bastien Hamlat, Jocelyne Erhel and Thibault Faney

Keywords: Multiphase reactions, chemical kinetics, discontinuous differential equations.

During the last few years, there has been a growing interest in global formulations of multiphase reactive transport models with a special focus on the complete dissolution of minerals by kinetic reactions involving aqueous species and minerals.

In the specific case of one mineral by reaction and one reaction by mineral, we can introduce a modified model which consists in limiting the dissolution rate when the mineral amount is equal to zero. However, such a discontinuous switching may induce failures in standard implicit solvers and is not compatible with classical mathematical theories. These issues have been solved, by N. Bouillard et al. [1] and J.Hoffman et al. [2], by translating discontinuous switching in complementarity conditions and by using a differential inclusion approach.

In this talk, we will present and justify the "limited kinetics model" introduced by B. Hamlat et al. [3, 4] to extend the range of applications to general systems including any type and number of kinetic reactions. Then we will discuss the mathematical and numerical results obtained and the remaining issues in light of our recent advances.

References

[1] N. Bouillard, R. Eymard, R. Herbin and P. Montarnal, *Diffusion with dissolution and precipitation in a porous medium: Mathematical analysis and numerical approximation of a simplied model*, ESAIM: M2AN, 41, 975-1000, 2007.

[2] J. Hoffman, S. Krautle and P. Knabner, *Existence and uniqueness of a global solution for reactive transport with mineral precipitation-dissolution and aquatic reactions in porous media*, SIAM Journal of Numerical Analysis, 49, 4812-4837, 2017.

[3] B. Hamlat, J. Erhel, A. Michel and T. Faney, *Modélisation des systêmes cinétiques limités*, SMAI 2017 Congress.

[4] B. Hamlat, J. Erhel, A. Michel and T. Faney, *Discontinuous kinetics models for reactive transport problems*, CMWR 2018 Congress.

A. Michel, B. Hamlat, T. Faney
IFPEN Rueil Malmaison
anthony.michel@ifpen.fr, bastien.hamlat@ifpen.fr, thibault.faney@ifpen.fr

J. Erhel, B. HamaltT
INRIA Rennes
jocelyne.erhel@inria.fr, bastien.hamlat@inria.fr