A compositional model for the reactive transport modelling of strongly coupled processes

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In certain reactive transport applications, strong coupling between geochemical reactions, solute transport and water/gas flows can be encountered. For these problems, such as the precipitation of hydrated minerals, in particular under relatively dry conditions, the typical approach involving the decoupling flow and reactive transport can lead to difficulties. Similarly, the modelling of density-dependent flow and reactive transport requires consideration of feedback mechanisms,. Coupling between flow and reactive transport can be considered through a Picard iterative approach (Henderson et al. 2009). However, this approach requires solving two nonlinear problems multiple times at each timestep, which is computationnally expensive. Seigneur et al. (2018) described a weak coupling approach where the impact of chemistry on flow is considered through a water/volume balance calculation. However the latter coupling method is explicit, limiting the timestep of the simulation. Our current research focuses on the development of a compositional model, in which the flow variables (pressure, density) are expressed based directly on the reactive transport variables. The advantage of this approach is that it simultanueously solves the flow and reactive transport problems and intrinsically accounts for feedback processes. The method further provides an accurate treatment of water as both a reactant and a mobile fluid phase. First, we show the agreement between the compositional and commonly used approaches and compare their respective numerical performances. Second, we show simulation results of typical cases in which these couplings play a significant role.

[1] Henderson, Mayer, Parker & Al (2009), Journal of Contaminant Hydrology 106, 195-211.

[2] Seigneur, Lagneau, Corvisier & Dauzères (2018), Advances in Water Resources 122, 355-366.