

EGU2020-5615

<https://doi.org/10.5194/egusphere-egu2020-5615>

EGU General Assembly 2020

© Author(s) 2021. This work is distributed under the Creative Commons Attribution 4.0 License.



A compositional formulation for multiphase multicomponent reactive transport modelling of highly coupled systems

Nicolas Seigneur^{1,2} and K. Ulrich Mayer²

¹Ecole des Mines de Paris, Geosciences, France (nicolas.seigneur@mines-paristech.fr)

²Department of Earth ocean and atmospheric Sciences, University of British Columbia, Vancouver, Canada

In certain reactive transport applications, strong coupling between geochemical reactions and hydrodynamics exists. Dissolution and precipitation of minerals, such as the conversion between gypsum and anhydrite [1] or the precipitation of nesquehonite during CO₂ sequestration [2], as well as gas bubble formation [3] are geochemical processes which modify the multiphase flow dynamics, with direct feedback on reactive transport processes. In addition, heat generation induced by sulphide mineral oxidation can lead to significant increases in temperature [4], impacting flow, transport and geochemical reactions. In these instances, commonly used reactive transport modelling approaches, which rely on decoupling flow and reactive transport processes, have limitations. For density dependent or two-phase flow problems in the presence of a gas phase, the coupling between flow and reactive transport can be accounted for through a Picard iterative approach [3,5,6]. However, this approach is computationally expensive, involving the solution of nonlinear problems multiple times during each timestep, and convergence properties are often poor. More recently, a weak explicit coupling approach was developed to capture the impact of chemistry on flow by integrating water as a component and perform a volume balance calculation [7]. In the current work, a compositional approach is implemented into MIN3P-THCm, in which the flow variables (pressure, density) are expressed based on mass variables. Hence, this global implicit approach does not require solving the flow problem, but instead integrates groundwater flow processes directly into the reactive transport equations. We show that this approach yields very similar results to the commonly used approaches for single and two-phase flow. Finally, we show that, in highly coupled systems, not considering these coupled effects may lead to significant errors in simulating system evolution, highlighting the benefits of the newly developed approach.

[1] Jowett, Cathles & Davis (1993). AAPG Bulletin, 77(3), 402-413.

[2] Harrison, Dipple, Power & Mayer (2015). Geochimica et cosmochimica Acta, 148, 477-495.

[3] Amos and Mayer (2006). Journal of contaminant hydrology, 87(1-2), 123-154.

[4] Lefebvre, Hockley, Smolensky & Gélinas (2001). Journal of contaminant hydrology, 52(1-4),

137-164.

[5] Henderson, Mayer, Parker, & Al (2009). *Journal of contaminant hydrology*, 106(3-4), 195-211.

[6] Sin, Lagneau and Corvisier (2017). *Advances in Water Resources*, 100, 62-77.

[7] Seigneur, Lagneau, Corvisier & Dautères (2018). *Advances in Water Resources* 122, 355-366.