

# About Some Numerical Models for Geochemistry

T. Migot <sup>1</sup> and J. Erhel <sup>2</sup>

**Abstract:** Reactive transport models are very useful to study the fate of contaminants in groundwater. These models couple transport equations with geochemistry equations. In this talk, we focus on precipitation and dissolution chemical reactions, because they induce numerical difficulties.

We consider a set of solute species and minerals, with precipitation occurring when a saturation threshold is reached. A challenge is to detect which minerals are dissolved and which minerals are precipitated. This depends on the total quantities of chemical species. We propose an analytical approach to build a phase diagram, which provides the interfaces between the different possible cases. We illustrate our method with three examples arising from brine media and acid mine drainage.

---

<sup>1,2</sup> Inria: French Institute for Research in Computer Science, Control and Applied Mathematics  
Campus de Beaulieu, 35042 Rennes, France  
*tangi.migot@gmail.com, jocelyne.erhel@inria.fr*