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► To cite this version:

Mohamed Azaroual, Laurent André, Nicolas Devau, Arnault Lassin, Philippe Leroy, et al.. Numerical modeling of mineral dissolution – precipitation kinetics integrating interfacial processes. AGU Fall Meeting, Dec 2016, San Francisco, United States. 2016. hal-01381005

HAL Id: hal-01381005

<https://brgm.hal.science/hal-01381005v1>

Submitted on 13 Oct 2016

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Numerical modeling of mineral dissolution – precipitation kinetics integrating interfacial processes

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The controlling mechanisms of mineral dissolution/precipitation reactions are complex and interdependent. Their modelling may have to deal with strongly contrasted kinetic rates since, highly reactive minerals (i.e., carbonates, sulfate salts, etc.) and less reactive minerals (i.e., silica, alumino-silicates, etc.) generally coexist within a same rock. The kinetic ratios (high over low kinetic rates) can be greater than 10^{+6} and, thus, induce numerical instabilities for calculating mass and energy transfers between minerals and aqueous phases at the appropriate scales of time and space. The current scientific debate includes: i) changes (or not) of the mineral reactive surface area with the progress of the dissolution/precipitation reactions; ii) energy jumps (discontinuity) in the thermodynamic affinity function of some dissolution/precipitation reactions, as highlighted by some recent works; iii) integration of processes at the "mineral - aqueous solution" interfaces for alumino-silicates, silica and carbonates. In recent works dealing with the specific case of amorphous silica, measurements were performed on nanometric cross-sections indicating the presence of a surface layer between the bulk solution and the mineral. This thin layer is composed of amorphous silica and hydrated silica "permeable" to the transfer of water and ionic chemical constituents. The boundary/interface between the initial mineral and the silica layer is characterized by a high concentration jump of chemical products at the nanoscale and some interfacial dissolution/precipitation processes.

In this study, the results of numerical simulations dealing with different mechanisms of silicate and carbonate dissolution/precipitation reactions and integrating interfacial processes will be presented. The application of this approach to silica precipitation is based on laboratory experimental results and it highlights the significant role of the "titration" surface induced by surface complexation reactions on the precipitation.