Considerations for saturation calculations of concentrated non-equimolar calcium carbonate precipitation

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Microbially induced precipitation is a multi-disciplinary field combining biology, chemistry and geotechnology. An example of such a process is biogrout, where high concentrations of calcium ions together with biological carbonate production is used to precipitate calcium carbonate in soils. To be able to describe the precipitation rate, the chemical saturation, which is needed for the driving force of precipitation, must be calculated properly. A small deviation in the saturation can lead to large deviations in crystal growth and nucleation rates.

Calculating the saturation in a carbonate system requires ion speciation and activity corrections to be taken into account. There are many activity correction methods available, most of which are only valid up to a moderate ionic strength of the solution (< 0.1 mol kg^{-1}). Some of these methods are also developed for equimolar electrolytes. This is in contrast with the biogrout process which involves solutions with high ionic strengths and calcium and carbonate concentrations which are initially strongly non-equimolar.

Additionally, the calculation of saturation can be simplified by ignoring several ion complexes and water self-ionization. However, simplifications must be made with care as the speciation is strongly non-linear. This means that any simplification may have a significant impact on the saturation.

This research aimed to compare several softwares using different activity correction methods, e.g. PhreeqC, as well as a full speciation scheme coupled with an activity correction method suitable for solutions with a high ionic strength. Their performance for solutions with ionic strength and non-equimolar concentrations are tested. Additionally, this research aims to provide a speciation scheme for such solutions that is simplified as much as possible without significant accuracy loss for the chemical saturation.