Thermodynamic properties and crystallization behaviour of $(Mg,Fe)CO_3$ solid solution

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This work aims to improve our understanding of the crystallization behaviour and the thermodynamic properties of $(Mg,Fe)CO_3$ solid solution. Knowledge about this particular solid solution is particularly needed in relation with Geological Carbon Storage, in particular for projects as the CarbFix [1] that aims to *in situ* carbonation of basaltic rocks (especially rich in both these cations).

Precipitation experiments with different initial amounts of the constituting ions are performed in high-pressure stainless steel reactors inside a Teflon lining. Two operative temperatures are used: 150 and 180ºC. The evolution of the closed SS-AS system is monitored after specific reaction time by analysing, filtered and dried solids, through powder-XRD, SEM-EDX and EMPA; the reaction solution is analysed with ICP-MS and Alkalimetry.

The analysis of solids through powder X-Ray Diffraction allows us to refine the cell parameters and to calculate the molar volumes of excess, a qualitative measure of the ideality of the system; complementary information could be also deduced from an accurate peak shape analysis [2].

The analytical concentration of the elements is the input for Phreeqc [3] simulations that allow to calculate the final activity of the ions in the different solutions. From the values obtained for the activity of the elements we can calculate the partition coefficients ($D_{Mg/Fe}$), doing so, we obtained direct information on the influence of aging process in crystallization behaviour of $(Mg,Fe)CO_3$. From the equilibrium partition coefficients, through Phreeqc models, is possible to get information on the excess mixing properties of the system, the obtained values can be compared with literature data obtained in different systems with different temperatures.

[1] Matter, J.M. *et al* (2011) *Energy Procedia*, **4**, 5579-5585. [2] Katsikopoulos, D. *et al* (2008) *Chemical Geology*, **254**, 87-100. [3] Parkhurst, D.L. and Appelo, C.A.J. (2013) U.S. Geological Survey Techniques and Methods, **6**, A43, 497 p.