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CO_2 geological storage: impact of minero-chemical heterogeneities on thermodynamic and geochemical modelling

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The complexity of CO_2-rocks-fluids interactions is influenced, among others, by the mineralogical composition of the reservoir, and thus requires an integrated approach combining minero-chemical analyses, thermodynamics, and numerical modelling. The goal is to evaluate how compositional heterogeneity of site-specific minerals impacts reactive processes taking place upon CO_2 injection.

The investigation targets sandstones and marly sandstones characterized by significant fractions of illite-smectite micas, chlorites, feldspars and carbonates. These mineral assemblages control pH fluctuations and dissolution–precipitation reactions.

The adopted workflow integrates experimental data, commercial codes (Geochemist's Workbench-GWB) and Eni proprietary software tools (e-gwok and e-muflot/TOUGHREACT) for data management, processing, and numerical modelling.

Based on experimental SEM dataset, site-specific stoichiometries are recalculated and standard thermodynamic parameters – $\Delta G°$, $\Delta H°$, $S°$, $V°$, $Cp°$ – are determined following Vieillard [1] approach to augment SUPCRT [2] thermodynamic database. Log K's vs T are then computed to update the GWB/TOUGHREACT geochemical databases. In this step attention must be paid to the simplification of the experimental stoichiometric formula (characterized by minor elements such as Ti, Mn, Cr, Li) used in numerical models. 2D activity diagrams are then used to check the consistency of estimated parameters for site-specific minerals.

0D static models, combining different site-specific minerals and logKs, serve to explore different scenarios aimed at reproducing the diagenetic evolution of the system in a 2My timeframe, while 0D flush models are used to investigate the system's reactivity over 100 kyr under increasing content of CO_2.

Results show that differences in chemical composition, $\Delta G°$ and logK values have a significant impact on the inter-conversion of aluminosilicates and carbonates either with or without CO2. A preliminary analysis of the minero-chemical heterogeneity must be carried out before initializing complex reactive models.

References

[1] Vieillard P. (1994). Prediction of enthalpy of formation based on refined crystal structures of multisite compounds. Theories and examples. *Geochimica Cosmochimica Acta* 58, 4049-4063.

[2] Johnson J. W., Oelkers E. H., and Helgeson H. C. (1992). SUPCRT92: A software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species and reactions from 1 to 5000 bars and 0 to 1000 °C. *Computers and Geosciences* 18, 889–947.