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Bonto, Maria; Hosseinzadeh, Behzad; Eftekhari, Ali Akbar; Nick, Hamid; Feilberg, Karen Louise

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Temperature dependency of surface complexation reactions of artificial and natural calcite with brine

MARIA BONTO, BEHZAD HOSSEINZADEH, ALI AKBAR Eftekhari, HAMID NICK, KAREN LOUISE FEILBERG

Technical University of Denmark, mabon@dtu.dk, aliak@dtu.dk, hamid@dtu.dk, kffe@dtu.dk

Calcite, the main constituent of carbonate formations, shows a very reactive behavior in the presence of water and CO₂. The interactions (i.e., adsorption, dissolution, precipitation, ion-exchange) taking place in this complex system have an impact on the performance of oil production and geothermal energy extraction. To assess the ionic adsorption on the calcite surface, several research groups performed zeta potential measurements and obtained the equilibrium constants of the surface reactions at standard conditions by fitting a surface complexation model (SCM) to the experimental data. However, there is a lack of measurements at higher temperatures that would allow the calibration of a more versatile thermodynamic model. In this work, we use a combination of systematic experimental measurements and mathematical modeling to obtain the enthalpy for the defined surface reactions. We first measure at reservoir temperature range, the zeta potential of synthetic calcite and North Sea chalk in NaCl, MgCl₂, Na₂SO₄, and Na₂CO₃ in atmospheric CO₂. The equilibrium sample composition is monitored by inductively coupled plasma mass spectrometry (ICP-MS), providing more rigorously in the consequent modeling procedure. We implement the Charge Distribution MultiSite Complexation (CD-MUSIC) model for calcite in Phreeqc and we couple it to a mathematical optimization algorithm. We determine the surface reactions enthalpy by fitting the model to the zeta potential measurements at different temperatures. The new SCM accounting for the temperature effect can be integrated into a non-isothermal reactive transport model, especially relevant for carbonate oil/geothermal reservoirs.