Thermodynamics of saline aqueous solutions

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Choisissez un élément.**Methodology: Thermophysical Properties (experiment &modeling)** **Oral**

THERMODYNAMICS OF SALINE AQUEOUS SOLUTIONS

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Natural brines are of major interest for industrial developments, because of their valuable properties and/or because of the technical problems they cause in the georessource production processes. Valorization concerns the extraction of valuable dissolved species (lithium of the salars, potassium, boron, magnesium, …), the recovery of chemical reactants from industrial waste, the exploitation of water resources (desalination) and of deep saline aquifers (CO_2 storage, geothermal energy, oil and gas exploration …). The industrial problems caused by brines are in relation with the management of deposits, the scaling/corrosion in tubings during the exploitation of geothermal fluids and oil brines and the reservoir management especially the near wellbore domains.

Optimizing these applications implies a better control of the electrolyte solution properties, which means a better knowledge of activity of the dissolved species, salt solubility, heat capacity (heat exchanges), interfacial tension and wettability (flow, scalings), density, refractive index, speed of sound, etc. However, because of the high ionic strengths of these solutions, the description and the modelling of their physicochemical properties still remain a scientific challenge.

The Pitzer formalism(1) uses the derivative of the Gibbs excess energy (G^{ex}) to reach the excess properties of brines like (i) the osmotic coefficient (ϕ), (ii) the apparent relative molar enthalpy (L_ϕ), (iii) the apparent molar heat capacity ($C_{p,\phi}$) and (iv) the apparent molar volume (V_ϕ). From the last three expressions, we can calculate the dilution enthalpy (ΔH^D), the heat capacity (C_p) and the density (ρ) of a solution, respectively. A numerical code, derived from PhreeqC(2) and called PhreeSCALE(3), has been developed to address all these sensitive thermodynamic properties of brine solutions (Figure 1).

The software is used with success to simulate various applications. The presentation will include application cases, the state-of-the-art but also the remaining scientific locks that need to be addressed to accurately characterize and predict the behavior of such brines in environmental and industrial processes. One of the most challenging issue is the characterization and the numerical description of systems of highly contrasted solubility, like aluminosilicate minerals in brines.

References:

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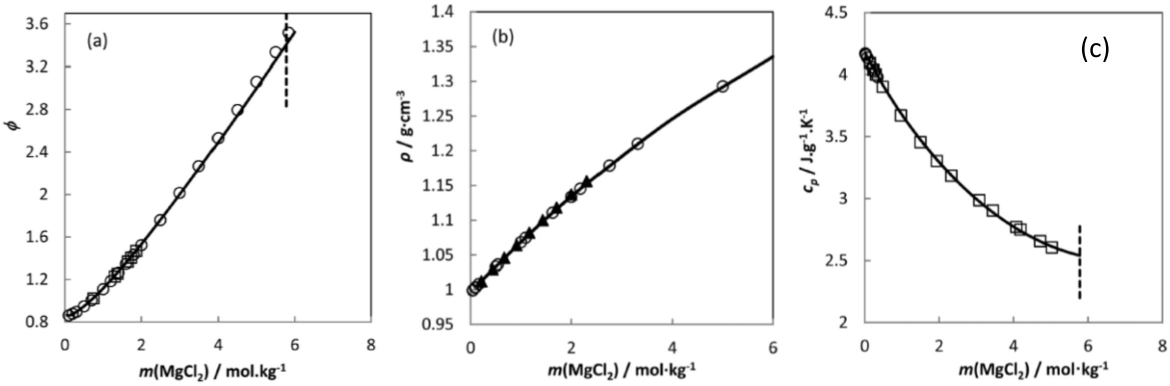

Figure 1: The Mg-Cl-H_2O system at 298.15 K. (a) osmotic coefficient ; (b) brine density; (c) heat capacity. Symbols are experimental data, full lines are model results (4).