

Thermodynamic model for H₂-H₂O- NaCl system

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The knowledge of hydrogen (H₂) properties in hydrothermal fluids under high T-P is indispensable for estimations of H₂ reservoirs in the middle and lower crust of the Earth [1]. These data can also help in the development of new H₂-based sources of energy. However, our knowledge of water-hydrogen solubilities, the effect of electrolytes (e.g., NaCl, KCl), and phase relations at high T-P-xH₂ remains poor, the robust models are missing. Based on available experimental data, we propose a new thermodynamic model which attempts to describe phase boundaries, solubilities, and fugacities in an H₂-H₂O-NaCl system up to 600°C and 3 kbar. Under vapor-liquid immiscibility (near H₂O saturated vapor pressure and under high pressures and high H₂ concentrations, as well as in the wide T-P range in the presence of NaCl), two separate equations of state for the liquid and the vapor phases are proposed. For the liquid phase, H₂-H₂O system, our model is based on highly precise data for pure H₂ and pure H₂O, Henry's law constants, and the vapor-liquid partitioning for H₂, our estimations of Setchenov coefficients of H₂, and Akinfiev and Diamond approach [2]. For the vapor phase, the improved Peng-Robinson approach was employed.

Compositions of vapor and liquid phases in NaCl-H₂O-H₂ systems calculated using our model are in good agreement with data of Seward and Franck [3], Kishima [4], and Ding and Seyfred [5].

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