Thermodynamic model for $\text{H}_2$-$\text{H}_2\text{O}$-$\text{NaCl}$ system

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The knowledge of hydrogen ($\text{H}_2$) properties in hydrothermal fluids under high T-P is indispensible for estimations of $\text{H}_2$ reservoirs in the middle and lower crust of the Earth [1]. These data can also help in the development of new $\text{H}_2$-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-$\text{xH}_2$ 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 $\text{H}_2$-$\text{H}_2\text{O}$-$\text{NaCl}$ system up to 600°C and 3 kbar. Under vapor-liquid immiscibility (near $\text{H}_2\text{O}$ saturated vapor pressure and under high pressures and high $\text{H}_2$ 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, $\text{H}_2$-$\text{H}_2\text{O}$ system, our model is based on highly precise data for pure $\text{H}_2$ and pure $\text{H}_2\text{O}$, Henry’s law constants, and the vapor-liquid partitioning for $\text{H}_2$, our estimations of Setchenov coefficients of $\text{H}_2$ 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-$\text{H}_2\text{O}$-$\text{H}_2$ systems calculated using our model are in good agreement with data of Seward and Franck [3], Kishima [4], and Ding and Seyfried [5].

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