

Phase equilibria in the $\text{Na}^+ - \text{K}^+ - \text{Ca}^{2+} - \text{Mg}^{2+} - \text{Cl}^- - \text{H}_2\text{O}$ system

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The problem of the separation of different electrolytes is not new but still relevant. Traditional separation techniques are based on crystallization or extraction processes, these operations are usually carried out at room or higher temperatures. Modern industrial solutions make it possible to conduct separation not only due to different distribution of components between phases. At some stages of the technological process it may be quite effective to separate the crystals of various compounds in aqueous suspension due to different size, density, and other physical properties. For the development of new technologies information about the phase equilibria in the systems under investigation in a wide temperature range and in a concentration range up to saturation is required. In this regard, the thermodynamic model of the $\text{Na}^+ - \text{K}^+ - \text{Ca}^{2+} - \text{Mg}^{2+} - \text{Cl}^- - \text{H}_2\text{O}$ system in the temperature range from 218 to 373 K can be useful.

For the description of the liquid phase in the multicomponent system under investigation Pitzer-Simonson-Clegg [1] expression for the Gibbs energy was applied. The gas phase was regarded as ideal. Modelling of the system was begun with binary subsystems, whereupon a number of the components was increased gradually. If necessary, in addition to the binary parameters, parameters of higher dimension were added. Parametrization of the model was carried out by the method of least squares. The minimized objective function was the sum of squared residuals of calculated and experimental values. Vapor-liquid equilibrium data, osmotic coefficients and solid-liquid equilibrium data in a wide temperature and concentration ranges were used for estimation of parameters. In addition to parameters 95 % confidence intervals were calculated. Thereby, only statistically significant parameters were obtained.

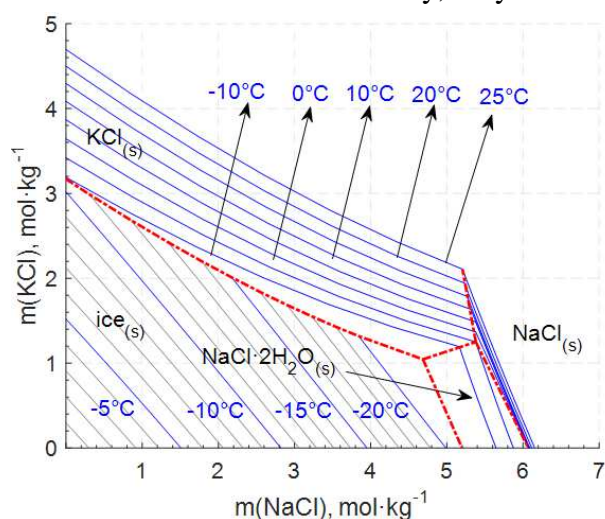


Fig. 1. Isothermal sections (blue solid line) and liquidus projection (red dashed line) in the NaCl – KCl – H_2O system

On the basis of the obtained thermodynamic model and the calculated phase diagrams, the most favorable conditions for the separation of sodium chloride from an aqueous solution of halides were determined and the process design was created. For the verification of the proposed technological scheme a pilot plant which corresponds to the stage of production of sodium chloride was constructed. Results of calculation were compared with obtained experimental results.