THERMODYNAMIC MODELING OF MULTICOMPONENT LITHIUM INDUSTRIAL BRINES

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The sedimentary cover of the Siberian Platform contains chloride brines with a high content of lithium and other valuable components (Rb, Cs, Br). Such brines are thermodynamically nonequilibrium systems with a complex composition. They are characterized by high mineralization and density, which makes them similar in properties to melts. The study of salt crystallization processes under changes in temperature and pressure is an important practical task.

Crystallization in the temperature range of 0... -22 °C and a pressure of 1 bar was simulated using the Selector software package based on minimizing Gibbs energy [1]. Cambrian brines from the Siberian Platform (Nepsky Dome). Brines are acidic - pH (3.8), the content of the main components (in g/l): Ca 153.9; Mg 13.2; Na 2.9; K 15.7; Li 0.2; Cl 334.0. The model contains about 500 probable components (components of the aqueous phase, minerals, gases).

As a result of the modeling, it was found that the beginning of stable ice formation (freezing of brines) occurs at a temperature of -12 °C. At a temperature of -10 °C, chlorides begin to crystallize, their composition and quantity are shown in the table.

Properties of brine and mineral phases during brine crystallization, in g per 1 kg of brine

T, °C	pH	TDS (g/kg)	$KMgCl_3(H_2O)_6$	KCl	$NaCl(H_2O)_2$	NaCl	$CaCl_2(H_2O)_6$	$MgCl_2(H_2O)_6$
-10	3.6	524.9	15.91	1.01	0.16	0.07	0.03	0.01
-12	3.6	548.4	37.07	1.89	0.38	0.17	0.07	0.02
-14	3.7	663.9	66.47	2.49	0.84	0.38	0.14	0.03
-16	3.8	779.0	83.81	2.24	1.27	0.56	0.18	0.03
-22	4.2	1116.2	105.08	0.90	2.39	1.04	0.23	0.03

The first generalized model of strong Cambrian brines has been obtained, which can be used to study phase transitions in the Ca-Mg-Na-K-Li-Cl-H_2O system as the basis for the well production cycle of this type of raw material.

1. Chudnenko, K. V. Thermodynamic modeling in geochemistry: theory, algorithms, software, applications. Novosibirsk: Geo, 2010. – 287 p.