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Thermodynamics of solutions $NaCl–H_2SO_4–H_2O$

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Abstract

The method of thermodynamic modeling is used to estimate equilibrium and the compositions of the gas phase and water solutions of the system $NaCl–H_2SO_4–H_2O$ at atmospheric pressure and temperatures of 25-100 °C in the range of total reagent concentrations from 0 to 3.6 mol/l. The results of the modeling indicate the probability of interactions with the formation of solutions containing mainly cations H_3O^+, Na^+, anions Cl^-, HSO_4^- and in a very low concentration of anion SO_4^{2-}. The gas phase is characterized by the presence of variable amounts of water vapor and hydrogen chloride with a proportionally varying contents of nitrogen and oxygen in a ratio that meets the air. The increase in the total reagent concentrations and temperature must be accompanied by an increase in the content of HCl in solution and the gas phase. Changing the ratio of reagents $NaCl/H_2SO_4$ in the range from 0 to 19 indicating the possibility of the presence of the regions of the maximum concentration of HCl in the gas phase close to the ratio of reagents equal to 0.5, and concentrations in solution of about ratio of 0.4. Estimated interphase distribution of HCl, which showed a predominant concentration of HCl in aqueous solution (99%). Simulation result indicate promising solutions of the system $NaCl–H_2SO_4–H_2O$ in chemical engineering.

References

[1] M.I. Levinsky, A.F. Mazanko, I.N. Novikov. Chloride hydrogen and hydrochloric acid. *Moscow: Chemistry.* **1985**. 160p. (russian)
[2] A.T. Chanysheva, A.M. Syrkin. Properties of solutions of electrolytes and nonelectrolytes: studies. manual. *Ufa: UGNTU publishing house.* **2009**. 65p. (russian)
[3] Electrolytes and their properties. http://mirznanii.com/a/325073/elektrolity-i-ikh-svoystva. (russian)
[4] The "strong" acids. http://org3215.chem.msu.ru/rus/books/robinson/part 3.pdf. (russian)
[5] V.M. Andreyev, A.S. Kuznetsov, G.I. Petrov, L.N. Shigina. Production of germanium. *Moscow: Metallurgy.* **1969**. 96p. (russian)
[6] V.F. Borbat, Yu.L. Mikhaylov, L.N. Adeeva, O.A. Golovanova, T.N. Filatova. Investigation of a possibility of enrichment of ashes ablation of combined heat and power plant on rare and non-ferrous metals for their subsequent extraction. *Chemistry and Chemical Technology*. **1999**. Vol.42. Iss.5. P.86-90. (russian)
[7] S.O. Potapov, M.N. Sviridova, I.N. Tanutrov, D.A. Toloknov. Physical and chemical properties of ashes ablation from burning the ekibastuzskikh of coals. *Butlerov Communications.* **2016**. Vol.45. No.3. P.36-39. (russian)
[8] S.O. Potapov, M.N. Sviridova, I.N. Tanutrov. The behaviorof gallium and aluminum during sulfuric acid processing of fly-ash from reftinskaya hydroelectric power plant. *Butlerov Communications.* **2016**. Vol.45. No.3. P.40-43. (russian)
[9] N.G. Ageev, S.S. Naboychenko. Metallurgical calculations with use of an application program package of HSC Chemistry: studies. manual. *Yekaterinburg: UFU publishing house.* **2016**. 124p. (russian)
[10] T.V. Kulikova, A.V. Mayorov, K.Yu. Shunyaev, T.I. Gorbunova, V.I. Saloutin, O.N. Chupakhin. Thermodynamic modeling of the interaction of polychlorinated biphenyls with potassium hydroxide. *Ecology and industry of Russia.* **2013**. No.11. P.23-27. (russian)
[11] S.N. Tushnakov, E.N. Selivanov. Thermodynamic simulation of phase formation during cooling zinc-copper smelting slag. *Butlerov Communications.* **2015**. Vol.43. No.9. P.102-107. (russian)