

LIU Yuanhui, GUO Yafei, YU Xiaoping, WANG Shiqiang and DENG Tianlong. 2014. Predictive phase equilibria for the aqueous ternary system ($\text{Li}_2\text{SO}_4 + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$) from 273.15 to 373.15 K. *Acta Geologica Sinica* (English Edition), 88 (supp. 1): 352-353.

Predictive Phase Equilibria for the Aqueous Ternary System ($\text{Li}_2\text{SO}_4 + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$) from 273.15 to 373.15 K

LIU Yuanhui, GUO Yafei, YU Xiaoping, WANG Shiqiang and DENG Tianlong *

Tianjin Key Laboratory of Marine Resources and Chemistry, College of Marine Science and Engineering at Tianjin University of Science and Technology, Tianjin, 300457, P.R. of China

1 Introduction

Many variable temperature chemical models were developed to predict mineral solubility in the natural waters (Na^+ , K^+ , Ca^{2+} , Mg^{2+} // Cl^- , $\text{SO}_4^{2-} - \text{H}_2\text{O}$) in the temperature range below 298.15 K (to near 213.15 K) and (Na^+ , K^+ , Ca^{2+} // Cl^- , $\text{SO}_4^{2-} - \text{H}_2\text{O}$) and calcium acid-base system (H^+ , Na^+ , K^+ , Ca^{2+} // OH^- , Cl^- , HSO_4^- , $\text{SO}_4^{2-} - \text{H}_2\text{O}$) within 273.15 ~ 473.15 K to high solution concentration.

In this paper, The variable temperature chemical model of salt-water system containing lithium was constructed. The Pitzer salt parameters of LiCl and Li_2SO_4 at different temperatures were gained by fitting osmotic coefficients of two aqueous binary systems. The mixed Pitzer parameters $\theta_{\text{Li}, \text{K}}$ and $\Psi_{\text{Li}, \text{K}, \text{SO}_4}$ were obtained through fitting solubilities of the ternary systems ($\text{LiCl} + \text{KCl} + \text{H}_2\text{O}$) and ($\text{Li}_2\text{SO}_4 + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$) in the temperature range 273.15 ~ 373.15 K according to available salt parameters. Furthermore, the

equilibrium dissolution constants of solid phases $\text{Li}_2\text{SO}_4 \cdot \text{H}_2\text{O}$ and $\text{Li}_2\text{SO}_4 \cdot \text{K}_2\text{SO}_4$ were calculated with solubilities of the systems ($\text{Li}_2\text{SO}_4 - \text{H}_2\text{O}$) and ($\text{Li}_2\text{SO}_4 + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$) at different temperatures.

The stable phase diagram of the aqueous ternary system ($\text{Li}_2\text{SO}_4 + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$) in the temperature range 273.15 ~ 373.15 K was predicted on the basis of Pitzer theory and variable temperature chemical model. The results were shown in Figure 1. The predictive and experimental phase equilibria are compared as shown in Figure 2(a-d). In Figure 2(a-d), the calculated phase diagrams using Pitzer model agree well with experimental phase diagrams of this system.

2 Conclusion

The variable temperature chemical model can be used to obtain reliable Pitzer parameters containing lithium and the equilibrium solubility of complex brine containing lithium can be accurately predicted by using Pitzer ion-interaction model in broader temperature range from 243.15 to 423.15K.

Key words: solubility prediction, lithium salt, Pitzer parameters, chemical model

Acknowledgments

Financial support from the National Natural Science Foundation of China (21276194 and 21306136), the Training Program for Changjiang Scholars and Innovative Research Team in University ([2013]373), the Innovative Research Team of Tianjin Municipal Education Commission (TD12-5004) and Tianjin Key Laboratory of Marine Resources and Chemistry (201201) is

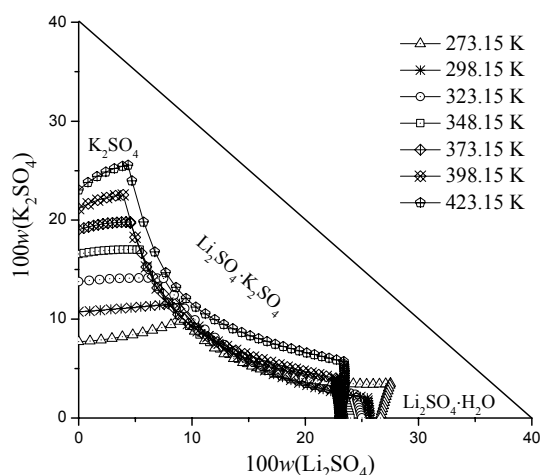


Fig. 1. The calculated phase diagram of the system ($\text{Li}_2\text{SO}_4 + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$) from 273.15 K to 423.15 K

* Corresponding author. E-mail: tldeng@tust.edu.cn

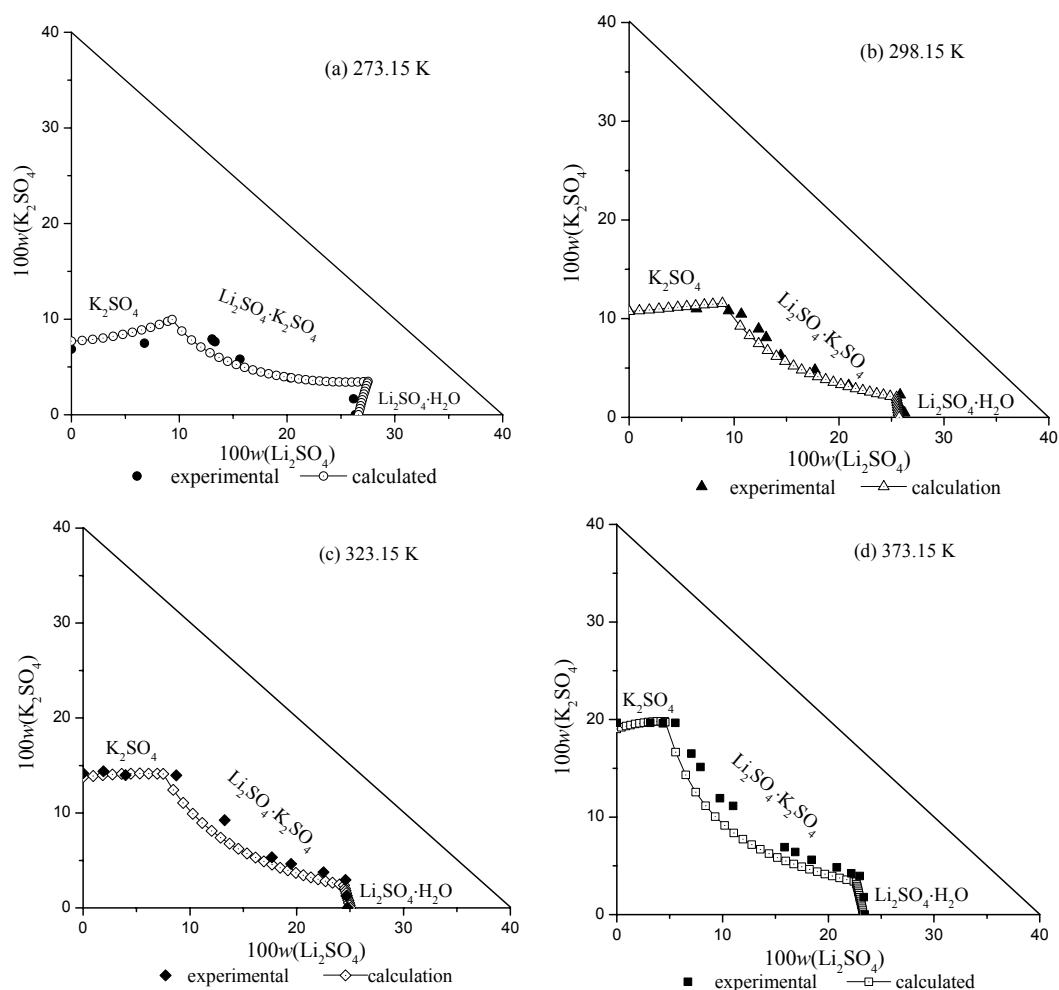


Fig. 2. The comparison between calculated and experimental phase diagrams of the system ($\text{Li}_2\text{SO}_4 + \text{K}_2\text{SO}_4 + \text{H}_2\text{O}$) at different temperatures

acknowledged.

References

- R.J. Spencer, N. Møller, and J.H. Weare, 1990. *Geochim. Cosmochim. Acta*, 3: 575–590.
 J.P. Greenberg, N. Møller, 1989. *Geochim. Cosmochim. Acta*, 53: 2503–2518.
 C. Christov, N. Møller, 2004. *Geochim. Cosmochim. Acta*, 68:

3717–3739.

- H.F. Gibbard, G. Scatchard, 1973. *J. Chem. Eng. Data*, 18: 293–298.
 H.F. Holmes, R.E. Mesmer, 1986. *J. Solution Chemistry*, 15: 495–518.
 A.D. Pelsha, 1975. *The manual on experimental data of solubilities of multi-component water-salt system Chemistry*, Press: Leningrad.