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ISS 実験との比較による過剰エンタルピーモデルでのソーレ係数予測精度の評価

Evaluation of the Prediction Accuracy for the Soret Coefficients in the Excess Enthalpy Model by Comparison with the ISS Experiment

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1. Introduction

The Soret effect is a mass transport phenomenon in which a concentration difference is formed by a temperature difference as a driving force. The direction and the amount of mass transport due to the Soret effect are defined as the Soret coefficient S_T. Several theoretical models have been proposed to predict the Soret coefficient. Kempers model[1)] is one of the accurate models for predicting the Soret coefficient. Recent years, Shimizu *et al.* developed a Kempers model by modified liquid standard[2)] from gas standard. However, there is no study that evaluates the accuracy of the value obtained from the modified Kempers model by comparing with the Soret coefficient obtained from the ISS experiment, and discusses the error factors in modified Kempers model. Therefore, the objective of this study is to clarify the prediction accuracy of the modified Kempers model with the excess enthalpy and to introduce a thermodynamic correction.

2. Experimental Apparatus and Method

Figure.1 (a) and **(b)** shows the schematic diagram of the Calvet calorimetry (C80) and the excess enthalpy measurement. The lower section of the sample cylinder was filled with Salol and the upper section with *tert*- butanol (TBA) partitioned

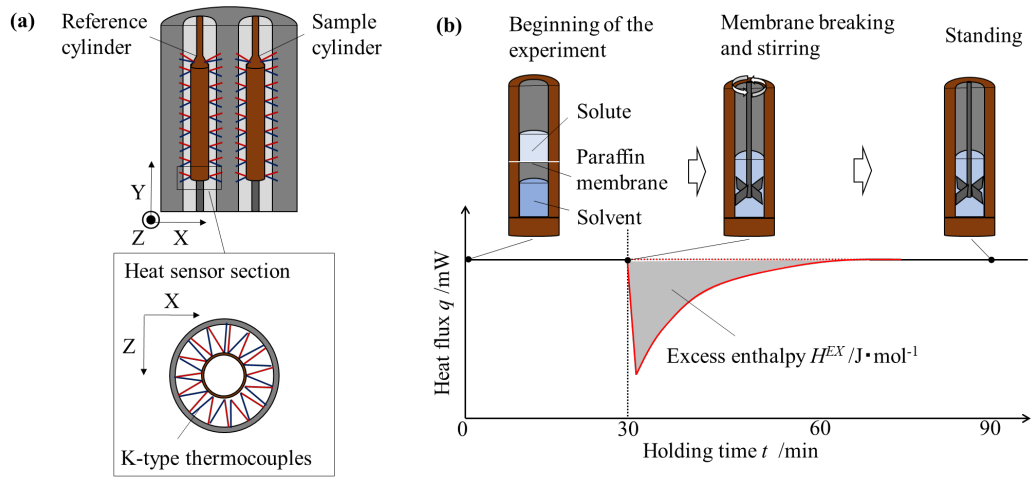

Fig.1 Schematic diagram of **(a)** the Calvet calorimetry (C80) and **(b)** the excess enthalpy measurement

with a paraffin membrane (TBA molar fractions X_{TBA} = 0.01, 0.03 and 0.1). First, the temperature of the entire cylinder was raised to 323 K, and then it was isothermally stabilized for 30 min. After the membrane was broken and the solution was stirred by stirring rod, the heat flux of the solution was calculated from the temperature change measured by thermocouples until 90 min. The excess enthalpy generated during the mixing process was calculated by integrating the observed total heat flux.

3.Results

As the molar fraction X_{TBA} increased, the amount of excess enthalpy increased. In addition, since the excess enthalpy was positive, the mixing of Salol/TBA was found to be an endothermic mixture. The Soret coefficients calculated by using modified Kempers model (KEM model) are negative and in the order of 10^{-2} K^{-1}.

4.Discussion

We compared the KEM model value and the Eslamian Model[3] value with the Soret coefficients of the measured value of ISS measurement[4]. The Eslamian model (ESL model)[3], which is considered to have a good estimation accuracy of the Soret coefficients, was introduced as a comparison model. In addition, the Soret coefficients of Water/Ethanol[5] were also compared in the same way. The results suggest that the KEM model can predict the Soret coefficient to the same extent as the ESL model. In addition, the KEM model values are closer to the measured values in both systems in the high temperature region. This is because it does not include a term expressing the Soret effect of physical action. Therefore, using the heat of transport due to thermal oscillations in solids[6,7], we introduced a physical term into the KEM model. As a result, the value S_T = -1.39×10^{-2} K^{-1} obtained by this model is closer to the measured value S_T = -1.46×10^{-2} K^{-1} than the ESL model value S_T = -2.02×10^{-2} K^{-1}. This trend was observed in both systems. These results suggest that the KEM model added with physical term is a highly effective model for predicting the Soret coefficient of a liquid.

5.Conclusion

Introducing the heat of transport term due to thermal oscillations in the solid state has the effect of improving the prediction accuracy of the Soret coefficients in the liquid state as the physical term. The KEM model added with physical term can predict the sign of the Soret coefficients accurately, $|S_T|$ with an error of about 10% and grad S_T with an error of about 70%. Therefore, this model is effective in predicting the Soret coefficient.

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