CERE
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CERE - SEMINAR

Thursday 2 November 2023
09:15 to 10:30 a.m.
Building 229, Room 003
(Light breakfast is served from 9:00, please bring your own coffee/tea)
Online from link in calendar invitation

"Effect of Free Volume in the Evaluation Diffusion and Thermodiffusion"

By

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Abstract
Diffusion and thermodiffusion are transport phenomena that play a fundamental role in numerous processes in different areas of science and industry [1], from industrial processes such as distillation, adsorption, liquid-liquid extraction [2], to thermal segregation in oil reservoirs [3]. Accurate modeling of diffusion and thermodiffusion is therefore essential not only for the efficient design and control of unit operations but also for the optimal exploitation of natural resources and many other applications.

Despite the relation between diffusion and thermodiffusion coefficients, the mathematical models to simulate these transport coefficients were built independently of each other, using different physical principles and empirical arguments [4]. Based on the statistical theory of fluctuations, a new unified thermodynamic modeling of diffusion and thermodiffusion was developed [5], where both coefficients are calculated in terms of the same sets of physical values, i.e. penetration distances and emission functions. Consequently, the simulation of diffusion coefficients allows the prediction of thermodiffusion coefficients.

In this work, which is a continuation of previous publications, we tested the impact of applying different equations of state (EoS) in describing experimental data on diffusion and thermodiffusion of binary systems. We also investigated the effect of introducing different approaches to free volume estimation into the mathematical model. The results indicate that the use of an effective co-volume, optimized together with the other parameters of the unified model, provides an accurate representation of both transport coefficients. Such accuracy has not been achieved by other models in the literature, including the previous publication. On the other hand, more research is needed because, even with the modification, the model is unable to adequately describe the diffusion data as a function of temperature.

References

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