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Mutual diffusion in concentrated liquid solutions: A new model based on cluster theory

Amin Kamgar¹, Ali Bakhtyari¹, Sajjad Mohsenpour¹, Carmine D'Agostino², Geoff Moggridge², Mohammad Reza Rahimpour^{1*}

¹*Chemical Engineering Department, Shiraz University, Shiraz 71345, Iran*

²*Department of Chemical Engineering and Biotechnology, University of Cambridge, Pembroke Street, Cambridge CB2 3RA, UK*

Abstract

In dilute solutions, diffusion is dominated by motion of single molecules. Conversely, in non-ideal concentrated solutions, mass transfer by diffusion can be heavily influenced by molecular clustering. Cluster theory in concentrated solutions can be approached using the Cussler model, which has been used to explain experimental mutual diffusion data in highly concentrated solutions. In this work, using the Cussler model and the critical point theory as a starting point, a new model for predictions of mutual diffusion coefficients in binary mixtures over the whole composition range was developed. The model is based on modifications of the concentration correlation function and explains well the experimental mutual diffusion data and their dependence on composition and activity coefficients. The model does not require any knowledge of intra-diffusion coefficients and can be used to predict mutual diffusion coefficients over the whole composition range.

Keywords: Diffusion; Cussler equation; Cluster theory; Concentrated solution; Thermodynamics

* Corresponding author. E-mail addresses: rahimpour@shirazu.ac.ir (M.R. Rahimpour).

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