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A NEW APPROXIMATION METHOD FOR THE ESTIMATION OF VISCOSITIES OF LIQUID MIXTURES USING UNIFAC-VISCO MODEL

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ABSTRACT

Viscosity is considered as one of the most significant transport properties in the scientific point of view and for various chemical applications. With an increased popularity of process and reservoir simulators, there is always an acute need for consistent, reliable as well as accurate predictive methods for viscosity calculations. The present study reports the viscosities of 14 binary liquid systems involving various types of alcohols, aromatics, and ketones predicted in the entire range of composition and at different temperatures. Computations were performed by employing the UNIFAC-VISCO model. To investigate its predictive capability, the UNIFAC-VISCO model has also been tested critically by considering group interaction parameters belonging to two different categories: α_{nm} from original UNIFAC-VISCO and β_{nm} from the UNIFAC-VLE. Consideration of β_{nm} parameters in line with α_{nm} has further led to easier predictions of both the dynamic and the kinematic viscosities of various organic liquids in a wider range.

Keywords: UNIFAC-VISCO, liquid mixtures, viscosity, predictive model, group interaction parameter.

INTRODUCTION

From theoretical points of view, transport properties have long been used to understand molecular interactions in liquids. A prior knowledge of thermodynamics and transport properties of multi-component mixtures is extremely important at early stages of designing chemical processes (Sohrevardi et al., 2017). With the increased popularity of chemical process and reservoir simulators, there is always an acute need for some consistent, reliable as well as accurate predictive methods for viscosity which is considered as one of the most significant transport properties for scientific studies and their subsequent chemical applications (Hossain et al., 2016; Wu, 1986; Zhao and Jacquemin, 2017). Models used for estimating viscosity of liquid mixtures may be classified as correlative or predictive in type. In correlative methods, the experimental data for mixtures are used for evaluation of model parameters (Kijevčanin et al., 2008). Whereas, properties of pure components are utilized in the predictive models (Billah et al., 2018; Kijevčanin et al., 2008; Zhang et al., 2018). In predictive approach-based group contribution method mixture viscosities are calculated using data of only pure components and the relevant functional group parameters. Moreover, group contribution models are appropriate for obtaining a faster evaluation of thermo-physical properties under different thermodynamic conditions.

In this work, estimation of viscosities is made for various binary liquid systems employing predictive model known as UNIFAC-VISCO (Chevalier et al., 1988; Gaston-Bonhomme et al., 1994). To improve the prediction results, a new approximate technique has been developed to overcome the