Postprint: Viscosity Calculation of Binary Mixtures Using the Modified McAllister Three-Body Model

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Abstract

The McAllister three-body model is widely regarded as the optimal correlation for liquid mixture viscosity. Based on a literature survey of viscosity data for three categories of binary mixtures (alcohol/alcohol, alkane/alkane, and alkane/alcohol), this study reveals that the interaction parameters (12 and 21) in the McAllister model exhibit systematic variations with the mixture' s equivalent molecular weight and temperature. Consequently, an improved McAllister three-body model was developed, and viscosities were calculated for ethanol with alcohols (including propanol, butanol, pentanol, hexanol, heptanol, octanol, nonanol, and decanol), n-butylcyclohexane with alkanes (including heptane, octane, nonane, decane, dodecane, and tetradecane), and isooctane with alcohols (including propanol, pentanol, hexanol, and heptanol). The results demonstrate an overall average absolute deviation of 1.00% between calculated and experimental values, with a maximum deviation of 9.75%.

Full Text

Improved McAllister Three-Body Model to Calculate Viscosities of Binary Mixtures

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Abstract

The McAllister three-body model is generally regarded as the best correlation for the viscosities of liquid mixtures. In this work, the viscosity data of three types of binary mixtures—alcohols/alcohols, alkanes/alkanes, and alkanes/alcohols—

were collected extensively from the literature. Investigation shows that the interaction parameters ($_{12}$ and $_{21}$) in the model exhibit regular trends along with equivalent molecular weights of binary mixtures and temperatures. Therefore, an improved McAllister three-body model was proposed. The new model was used to calculate the viscosities of different binary mixtures, including ethanol with alcohols (such as 1-propanol, 1-butanol, 1-pentanol, 1-hexanol, 1-heptanol, 1-octanol, 1-nonanol, and 1-decanol), n-butylcyclohexane with alkanes (such as 1-heptane, 1-octane, 1-nonane, 1-decane, 1-dodecane, and 1-tetradecane), and isooctane with alcohols (such as 1-propanol, 1-pentanol, 1-hexanol, and 1-heptanol). The results show that the overall average absolute deviation is 1.00% between calculated data and experimental values, and the maximum deviation is 9.75%.

Key words: McAllister three-body model; binary mixtures; viscosity calculation

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1. Introduction

Accurate prediction of liquid mixture viscosity is essential in chemical engineering design and process optimization. Among various predictive models, the McAllister three-body model has been widely recognized as one of the most accurate correlations for liquid mixture viscosity. Based on Eyring' s absolute rate theory, the McAllister model accounts for molecular interactions by introducing interaction parameters that account for three-body interactions between unlike molecules. However, the original model requires experimental data to determine these interaction parameters, limiting its predictive capability.

Previous studies by Asfour and coworkers have attempted to predict McAllister model parameters from pure component properties for specific systems such as n-alkane mixtures and regular binary liquid mixtures. While these approaches have shown promise, a generalized method for predicting interaction parameters across different classes of binary mixtures remains needed. This work investigates the systematic variation of McAllister interaction parameters with equivalent molecular weight and temperature, leading to the development of an improved predictive model.

2. Model Development

2.1 The McAllister Three-Body Model The McAllister three-body model for binary mixtures is expressed as:

$$\ln \nu_m = X_1^3 \ln \nu_1 + 3X_1^2 X_2 \ln \nu_{12} + 3X_1 X_2^2 \ln \nu_{21} + X_2^3 \ln \nu_2 - \ln\left(X_1 + X_2 \frac{M_1}{M_2}\right) + 3X_1^2 X_2 \ln\left(\frac{3 + M_2/M_1}{4}\right) + 3X_1 X$$

where is the kinematic viscosity of the mixture, $_1$ and $_2$ are the kinematic viscosities of pure components 1 and 2, $_{12}$ and $_{21}$ are the interaction parameters representing three-body interactions between unlike molecules, X_1 and X_2 are the mole fractions, and M_1 and M_2 are the molecular weights of the pure components.

The interaction parameters $_{12}$ and $_{21}$ are crucial for accurately representing the non-ideal behavior of the mixture. Traditionally, these parameters are regressed from experimental viscosity data, which is time-consuming and limits the model's predictive power.

2.2 Improved Predictive Model Analysis of extensive literature data reveals that the interaction parameters $_{12}$ and $_{21}$ exhibit systematic trends with respect to the equivalent molecular weight of the binary mixture and temperature. This observation allows for the development of a predictive correlation for these parameters.

The improved model establishes functional relationships between the interaction parameters and the equivalent molecular weight (M q) of the binary system. The temperature dependence is incorporated through an Arrhenius-type relationship, enabling parameter prediction across different temperatures without requiring experimental mixture data.

3. Results and Discussion

The variation of interaction parameters with equivalent molecular weight and temperature is illustrated for representative systems. For ethanol + alcohol mixtures, both $_{12}$ and $_{21}$ decrease monotonically with increasing equivalent molecular weight and show an inverse relationship with temperature.

[Figure 1: see original paper] Interactions among different molecules in binary systems

[Figure 2: see original paper] Variation of interaction parameter ($_{12}$ and $_{21}$) of ethanol + alcohols with equivalent molecular weight and temperature (solid lines represent the fitting results)

The predictive capability of the improved model was validated against three classes of binary mixtures:

1. **Alcohol/alcohol systems**: Ethanol with 1-propanol through 1-decanol
2. **Alkane/alkane systems**: n-Butylcyclohexane with C7–C14 n-alkanes
3. **Alkane/alcohol systems**: Isooctane with C3–C7 alcohols

For all systems studied, the model demonstrates excellent predictive accuracy. The overall average absolute deviation between calculated and experimental viscosity values is 1.00%, with a maximum deviation of 9.75%. This represents a significant improvement over conventional estimation methods and extends the applicability of the McAllister model to entirely predictive calculations.

4. Conclusion

An improved McAllister three-body model has been developed based on systematic analysis of interaction parameter trends in binary mixtures. By establishing correlations between the interaction parameters and equivalent molecular weight and temperature, the model eliminates the need for experimental mixture data. The model successfully predicts viscosities for diverse binary systems with an average absolute deviation of 1.00%, demonstrating its reliability and broad applicability for engineering calculations.

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Note: Figure translations are in progress. See original paper for figures.