Generalized Correlation Development for Viscosity Prediction in Pure Ionic Liquid Systems

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ABSTRACT

Ionic liquids are known as unique solvents with limitless potential. The study aimed to develop a generalized correlational model capable of predicting the viscosity of pure ionic liquid systems. Literature data was gathered using the ILThermo database and it was then trimmed and subjected to a modified pitzer correlation scheme for data analysis. From this computed viscosity of the data set, the viscosity of the other ionic liquids were predicted and compared with the values reported in the literature. The overall AAPD value for the model used is 157.07 %.
Keywords: ionic liquids; viscosity; generalized correlation; pitzer correlation; ilthermo database

INTRODUCTION

ILs are renowned as unique “designer” and “green” solvents, which display limitless potential from numerous combinations and eco-friendly traits, such as recyclability and non-volatility (Deetlefs & Seddon, 2014; Ratti, 2014). Despite the enticing benefits of using ILs, gathering experimental data for a specific IL is time-consuming, expensive, and unrealistic as there are more than 10^{18} ILs, obtainable by different sets of anions and cations (Yan et al., 2018). Therefore, having a preliminary understanding of a given property of an IL will aid its selection and design to its intended purpose. The study chose Viscosity as it provides significance in process equipment design used for heat transfer, process piping, and other units within important industries (Yuan et al., 2018; Gharagheizi et al., 2012).

The study had sought to build a generalized correlational model for viscosity prediction, having determined the most relevant data available from literature (IL Thermo Database) through the developed data trimming process while curve-fitting these through the use of MATLAB software. Since this centers on a purely computational experiment, gathering data based on the IL Thermo database. These data correspond with Pure IL System viscosities with varying temperatures, given pressure at or near one atm/100kpa. References considered from IL Thermo Database were limited from years 2015-2020 to improve the output relevance.

METHODOLOGY

Data Gathering. The data points of the viscosity of pure ILs were gathered from the ILThermo Database that have initially considered 6559 data points. The acentric factor, critical temperature, and pressure, which were required for the model, were considered from Valderrama et al.'s (2012) study on the critical properties of ILs. Inconsistent data or data that have missing parameters from literature were then trimmed. The acquired trimmed data were considered as the input data in evaluating the correlational model.

Prediction of η. A generalized Pitzer correlation for viscosity determination was utilized in the creation of the model, where viscosity (η) is fit as a function of temperature (T). The equation may be represented as:

$$\eta = T^{o} + \omega T^{l} \qquad (1)$$

Where ω is the acentric factor of the IL. For this study, the parameters T^{o} and T^{l} were defined as quadratic functions of the temperature:

$$T^{o} = A_1 + A_2\left(\frac{T}{Tc}\right) + A_3\left(\frac{T}{Tc}\right)^2 + A_4\left(\frac{P}{Pc}\right) + A_5\left(\frac{P}{Pc}\right)^2 \qquad (2)$$

$$T^{l} = A_6 + A_7\left(\frac{T}{Tc}\right) + A_8\left(\frac{T}{Tc}\right)^2 + A_9\left(\frac{P}{Pc}\right) + A_{10}\left(\frac{P}{Pc}\right)^2 \qquad (3)$$

Where A_n (n = 1 to 10) represents empirical constants, T_c is the critical temperature of the ionic liquid, and P_c is the critical pressure of the ionic liquid. The ratio T/T_c P/P_c is also the reduced temperature, T_r and reduced pressure, P_r.. The trimmed data was processed using the 2020 version MATLAB software (MATLAB R2020b), using the non-linear fit function as it produced the calculated viscosity, the residual values, and the absolute average percent deviation.

RESULTS

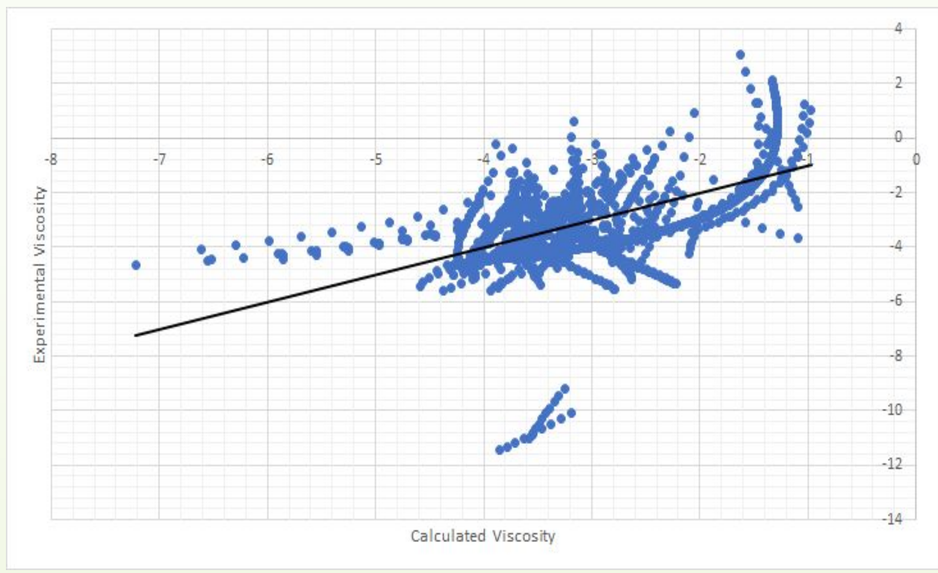

Fig. 1. Experimental Values vs. Calculated Values for Viscosity

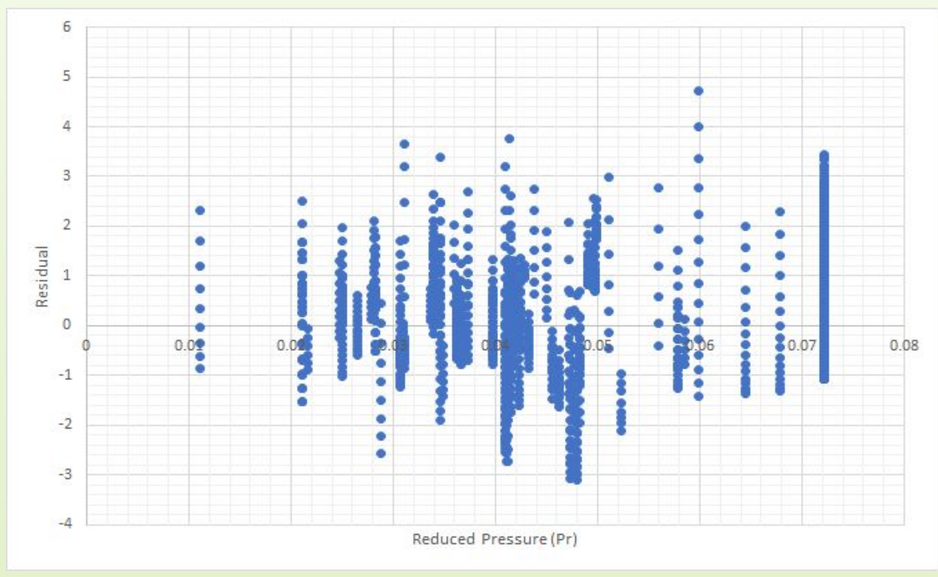

Fig. 2. Residual plot of Reduced pressure

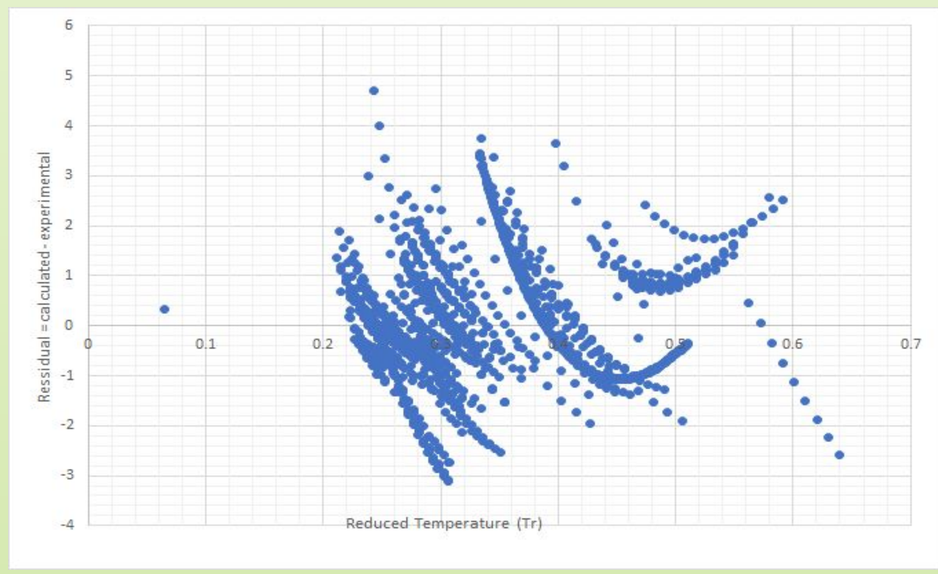

Fig. 3. Residual plot of Reduced Temperature

CONCLUSIONS

The study considered the use of a generalized pitzer correlation to predict the viscosities of ILs. The resulting viscosity model resulted in an absolute average percent deviation of 157.07 %. The resulting average percent deviation is considered to be high giving poor predictions and therefore not acceptable for use. The possible reasons for this case may be due to inconsistencies found in the literature, as well as the model not being a good fit for use when viscosity data is inputted. Changing the model or making further refinements to the parameters of the model is needed to improve the accuracy of its estimation.