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Modeling ionic liquids mixture viscosity using Eyring theory combined with a SAFT-based EOS

Khalid Mujasam Batoo [a], Youssef Ali Naeem [b], Shaima Haithem Zaki [c], Subhash Chandra [d], Hussam Abdali Abdulridui [e], Ahmed Ahmed Ibrahim [f], Bouchaib Zazoum [g], Waleed Mohammed Khazaal [h], Khaldoon T. Falih [i], Eftikhaar Hasan Kadhum [j], Batool Ali Ahmed [k], Laith H. Alzubaidi [l,m,n], Reza Shariyati [o,*]

[a] King Abdullah institute For Nanotechnology, king Saud University, Riyadh 11451, Saudi Arabia
[b] Al-Manara College for Medical Sciences, Maysan, Iraq
[c] Department of Anesthesia Techniques, Al-Noor University College, Nineveh, Iraq
[d] Department of Electrical Engineering, GLA University, Mathura 281406, India
[e] Al-Hadi University College, Baghdad 10011, Iraq
[f] Department of Physics and Astronomy, College of Science, King Saud University, P.O. Box 2455, 11451 Riyadh, Saudi Arabia
[g] Department of Engineering & Physics, Southern Arkansas University, Magnolia, AR 71753, USA
[h] Mazaya university college, Iraq
[i] New Era and Development in Civil Engineering Research Group, Scientific Research Center, Al-Ayen University, Thi-Qar, Iraq
[j] National University of Science and Technology, Dhi Qar, Iraq
[k] Department of medical engineering, Al-Nisour University College, Baghdad, Iraq
[l] College of technical engineering, the Islamic University, Najaf, Iraq
[m] College of technical engineering, the Islamic University of Al Diwaniyah, Iraq
[n] College of technical engineering, the Islamic University of Babylon, Iraq
[o] Universiti Malaysia Pahang Al-Sultan Abdullah (UMPSA), Kuantan Pahang, Malaysia

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ABSTRACT

This work aims to calculate the viscosities of ionic liquid mixtures using the Eyring theory combined with the SAFT-VR Morse EOS. The free volume theory was used to correlate the pure viscosity of ionic liquids (ILs) and solvents. Three model parameters have been adjusted using experimental viscosity data of ILs between 282 K and 413 K and 1 bar to 350 bar. The average ARD%, Bias%, and rmsd between model estimation and viscosity experimental data for pure ILs have been obtained 4.9 %, 1.015 %, and 0.67, respectively. The average error of the proposed model tends to increase at a pressure higher than 200 bar. The average ARD% for $[C_2mim][Tf_2N]$ and $[C_6mim][Tf_2N]$ is about 3.8 % and 3.4 % at pressures lower than 200 bar, while the average ARD% values increase sharply at higher pressures. This is due to the weak performance of the SAFT-VR Morse EOS for the calculation of IL density at high pressures. The SAFT-VR Morse EOS has been coupled with the Eyring theory, and the Redlich-Kister mixing rule to estimate the mixture viscosity of ILs-ILs and ILs-solvent systems. The thermal contribution of excess activation free energy has been calculated using the Redlich-Kister mixing rule with four adjustable parameters. The average ARD%, rmsd, and Bias% for fifteen binary mixtures have been obtained 3.9 %, 2.51, and 0.57 %, respectively. The average error values for mixture viscosity of ILs-polar solvent are higher than non-polar solvents. In the case of binary IL-IL systems, the model results are in good agreement with experimental data. The model performance has been evaluated using the viscosity deviation property. The SAFT-VR Morse EOS predicts the negative viscosity deviation. The strong attractive interaction in the mixture than a pure component is the major contribution to negative viscosity deviation. The results show that the new model can calculate the mixture viscosity and viscosity deviation of binary systems satisfactory. The obtained error values of mixture viscosity show that the Eyring theory can be coupled with a SAFT-based EOS to calculate the viscosity of ILs over a wide range of pressures and temperatures satisfactory.

* Corresponding author.
E-mail address: rshariyati.iau@gmail.com (R. Shariyati).

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