World Academy of Science, Engineering and Technology
International Journal of Chemical and Materials Engineering
Vol:10, No:01, 2016

Densities and Volumetric Properties of {Difurylmethane + [(C5 – C8) N-Alkane or an Amide]} Binary Systems at 293.15, 298.15 and 303.15 K: Modelling Excess Molar Volumes by Prigogine-Flory-Patterson Theory

Authors : Belcher Fulele, W. A. A. Ddamba

Abstract : Study of solvent systems contributes to the understanding of intermolecular interactions that occur in binary mixtures. These interactions involves among others strong dipole-dipole interactions and weak van de Waals interactions which are of significant application in pharmaceuticals, solvent extractions, design of reactors and solvent handling and storage processes. Binary mixtures of solvents can thus be used as a model to interpret thermodynamic behavior that occur in a real solution mixture. Densities of pure DFM, n-alkanes (n-pentane, n-hexane, n-heptane and n-octane) and amides (N-methylformamide, N-ethylformamide, N,N-dimethylformamide and N,N-dimethylacetamide) as well as their [DFM + ((C5-C8) n-alkane or amide)] binary mixtures over the entire composition range, have been reported at temperature 293.15, 298.15 and 303.15 K and atmospheric pressure. These data has been used to derive the thermodynamic properties: the excess molar volume of solution, apparent molar volumes, excess partial molar volumes, limiting excess partial molar volumes, limiting partial molar volumes of each component of a binary mixture. The results are discussed in terms of possible intermolecular interactions and structural effects that occur in the binary mixtures. The variation of excess molar volume with DFM composition for the [DFM + (C5-C7) n-alkane] binary mixture exhibit a sigmoidal behavior while for the [DFM + n-octane] binary system, positive deviation of excess molar volume function was observed over the entire composition range. For each of the [DFM + (C5-C8) n-alkane] binary mixture, the excess molar volume exhibited a fall with increase in temperature. The excess molar volume for each of [DFM + (NMF or NEF or DMF or DMA)] binary system was negative over the entire DFM composition at each of the three temperatures investigated. The negative deviations in excess molar volume values follow the order: DMA > DMF > NEF > NMF. Increase in temperature has a greater effect on component self-association than it has on complex formation between molecules of components in [DFM + (NMF or NEF or DMF or DMA)] binary mixture which shifts complex formation equilibrium towards complex to give a drop in excess molar volume with increase in temperature. The Prigogine-Flory-Patterson model has been applied at 298.15 K and reveals that the free volume is the most important contributing term to the excess experimental molar volume data for [DFM + (n-pentane or n-octane)] binary system. For [DFM + (NMF or DMF or DMA)] binary mixture, the interactional term and characteristic pressure term contributions are the most important contributing terms in describing the sign of experimental excess molar volume. The mixture systems contributed to the understanding of interactions of polar solvents with proteins (amides) with non-polar solvents (alkanes) in biological systems.

Keywords : alkanes, amides, excess thermodynamic parameters, Prigogine-Flory-Patterson model
Conference Title : ICLMMP 2016 : International Conference on Liquid Matter Modern Problems
Conference Location : Singapore, Singapore
Conference Dates : January 07-08, 2016