Modelling of Excess Molar Volume of Binary Mixtures of Water-Alkanol: a New Application of the Eras Model

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Following our study of modeling of excess properties [1-6], in this work a new expression has been developed to describe excess molar volume of binary liquid mixtures of water-alkanol at different temperatures and atmospheric pressure. The model combines the ERAS Model [7] with a term which takes into account hydrophobic effects. The effects contain two contributions: (1) a hydrophobic hydration term to account for the formation of clathrate hydrate, and (2) a hydrophobic interaction term to account for the formation of a solvation complex of two clathrates hydrate. These two terms suppose chemical equilibrium between species in solution. Application of the proposed expression to represent excess molar volume shows a good agreement with experimental data for the systems water-methanol, or -ethanol, or -1-propanol, or -2-propanol, or -t-butanol over the whole composition range in temperature 288.15-303.15 K range.

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