

Modeling the VLE Behavior and Liquid Viscosity of Non-Ideal Mixtures: a Consistent Approach

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A previously developed Eyring-theory-based model [Macías-Salinas et al., *Fluid Phase Equilibria*, **210**, 319 (2003)] proved to give an accurate description of viscosity behavior of highly non-ideal liquid solutions within wide ranges of temperature and pressure. The model makes use of a cubic equation of state (CEoS) along with modern mixing rules of the Wong-Sandler type to reasonably compute volumetric properties and the excess activation energy of flow for the liquid mixture of interest. However, the excellent performance of the viscosity model was achieved at the expense of adversely affecting VLE calculations since the excess Gibbs energy of the mixture obtained from the CEoS was manipulated to match the experimental excess activation energy of flow. To fix this inconsistency, in this work we propose a new modeling approach by the introduction of a residual term for the excess activation energy aimed to keep the same accuracy in viscosity calculations without altering the VLE behavior computed from the CEoS. Various binary non-aqueous and aqueous mixtures exhibiting a maximum and/or minimum in the viscosity-composition function were considered to confirm the versatility of the present modeling approach.