Implementation of Isochoric Slopes for Mixture Properties Calculations

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The physical properties of fluid mixtures have been a research focus for more than a century. Some important reasons were and continue to be the need for efficient and economical industrial processes, engineering design calculations and purely scientific curiosity. Accurate prediction of physical and calorimetric properties of fluid mixtures by an equation of state requires an accurate description of the effects of intermolecular forces between both like and unlike molecules. The effects of the unlike interactions are especially challenging, because they exist only in mixtures, and they may have strong composition dependence. Experimental measurements for mixtures are necessary, and the number of measurements required should be minimized. Experimental measurements of derivatives such as $\partial P/\partial T$ have been used previously to evaluate the thermodynamic consistency of equations of state and the impact of using numerical and analytical derivatives during equation development. In this work, we have explored, using different sets of data covering wide pressure and temperature ranges, the use of isochoric slopes ($\partial P/\partial T$) obtained from PρT measurements to develop correlations that improve the predictions of excess properties. Isochoric slopes are attractive for this application, because they are directly related to energy and entropy calculations, and they depend strongly upon composition but weakly upon temperature in the single-phase region. The excess properties are calculated using properties for pure substances calculated using reference equations of state and mixture properties that have been measured experimentally. The predicted mixture properties then are compared to experimental data.