J Adv Chem Eng 2018, Volume 8
DOI: 10.4172/2090-4568-C3-012

PC-SAFT modeling and PpT measurements of benzyl alcohol at high temperature and pressure

Rokhsareh Mohammadkhani
Bu-Ali Sina University, Iran

The Perturbed Chain SAFT (PC SAFT) [1] model is an equation of state developed for modeling all types of substances: gases, solvents and polymers. This equation has been utilized to predict thermodynamic properties for the pure components and the mixtures [2-4]. PC-SAFT includes three pure compound parameters: the segment energy and size, the number of segments and in the cases with association extra parameters volume and energy. Determining these PC SAFT parameters for each component is the first challenge in using this equation. The aim of this work is to develop an approach for parameterizing the PCSAFT for benzyl alcohol up to high pressures and temperatures. For this purpose, new experimental density data were obtained from density measurements performed with a vibrating-tube density meter and carried out in the temperature range between (293.15 and 473.15) K and pressures ranging from (0.1–37.5) MPa. At the beginning, the parameters of the PC-SAFT for pure solvent are generally determined only by matching the liquid density experimental data. In this work, new correlations based on minimizing the total objective function of temperature, pressure and density simultaneously were developed to estimate the PC-SAFT parameters of benzyl alcohol which is an effective solvent in chemical synthesis and reactions. Benzyl alcohol is a useful solvent for inks, paints, lacquers, gelatin, cellulose acetate, and shellac [5]. Finally, we calculated the thermodynamic properties such as isothermal compressibility, T, thermal expansion coefficient, p, and speed of sound, u, from PC-SAFT equation. Using these calculated PC-SAFT parameters, PVT behavior and derived properties were reasonably well predicted.

r.mkhani@basu.ac.ir