Evaluation of the PC-SAFT, SAFT and CPA equations of state in predicting derivative properties of selected non-polar and hydrogen-bonding compounds

In order to provide a comprehensive understanding of the potential and limitations of the PC-SAFT, SAFT and CPA equations-of-state, this study offers insight into their application for the prediction of derivative properties over extensive ranges of pressure and temperature. The ability of these models to predict selected properties (heat capacities, pressure-volume derivative, pressure-temperature derivative and speed of sound) are evaluated for n-alkanes and 1-acohols. For n-alkanes, it is shown that the cubic term of CPA is unable to describe the pressure-volume derivative at high pressures, which is a major shortcoming in predicting derivative properties compared to SAFT-based models. Although PC-SAFT and SAFT provide a substantially better prediction of the pressure-volume derivative than CPA, they are still not accurate enough to obtain good speed of sound predictions. All three models are unable to accurately correlate the isochoric heat capacity, indicating an incorrect temperature dependency in these models. PC-SAFT shows peculiar behaviour in the description of the isobaric heat capacity of alkanes that can be traced back to the incorrect description of the pressure-temperature derivative. For 1-alcohols, both CPA and PC-SAFT accurately predict the isobaric heat capacity when modelled with the 3B association scheme, while SAFT is unable to capture the singularities present in the property irrespective of the association scheme used. None of the models are able to predict the speed of sound accurately, because the terms describing physical interactions result in poor estimates of the pressure-volume derivative that governs the property. © 2012 Elsevier B.V.