A Modification for the Peng-Robinson Equation of State for Prediction of Phase Equilibrium of Pure Substances and Their Mixtures

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Since the van der Waals equation of state was proposed in 1873, hundreds of different cubic equations of state have been developed to introduce more accurate and efficient predictions of thermodynamic properties. Although many of them can provide reasonable values for the vapor region of hydrocarbons, the great majority fail to predict saturated liquid molar volumes of hydrocarbons and some other polar compounds like water and alcohols. Also, it is well known that the actual cubic equations of state fails near the critical region. For this reason, a new thermodynamically consistent alpha cohesion function for the Peng-Robinson cubic equation of state was developed. This new alpha function must be of class C^2; this implies that the first and second derivatives of the alpha function must be continuous. This new modification is in order to improve the prediction in vapor pressure of a considerable number of pure substances and their mixtures belonging to different chemistry families such as: hydrocarbons, aromatic compounds, gases, alcohols, sulfur compounds, and refrigerants. For non-polar and polar substances, the results obtained for the prediction of vapor pressure are in good agreement with experimental data published in the international literature (maximum deviation of 3 %). Besides, the proposed modification allowed other thermodynamic properties to be calculated such as: heat capacity at constant pressure, inversion Joule-Thomson coefficient, and Boyle temperature.