



Comparison of bulk modulus as Benzene dense fluid using the LIR equation of state with the extended coefficients and comparison with Peng-Robinson equation of state

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ABSTRACT

New parameters of the linear isotherm regularity, the so-called LIR equation of state, are used to calculate the bulk modulus of dense fluids. In this work, we derive an expression for the bulk modulus of dense fluids (CO, C₆H₆, C₆H₅CH₃) using the linear isotherm regularity (LIR). In later stages, bulk modulus calculated by Peng-Robinson (PR) equation of state as a test of the other equation of state. Comparison of the calculated values of bulk modulus with the extended coefficients of the linear isotherm regularity with the values obtained experimentally shows the accuracy of this method to be general, quite good.

1. Introduction

The bulk modulus is a scalar quantity relating an isotropic pressure to an average change in volume. It is the average of the three inverse linear compressibilities (change of length induced by pressure). The bulk modulus is defined as:

$$B = -\frac{1}{\rho} \left(\frac{\partial p}{\partial V} \right)_T = \rho \left(\frac{\partial p}{\partial \rho} \right)_T \quad (1)$$

Huang and O'Connell [1] discovered a regularity in which all isotherms of the reduced bulk modulus of a compressed liquid as a function of density intersect at a common point called 'common bulk modulus point'. The reduced bulk modulus is defined as:

$$B_r = \left(\frac{\partial p}{\partial \rho} \right)_T / RT \quad (2)$$

where B_r is the reduced bulk modulus and R is the gas constant. Huang and O'Connell checked the regularity for more than 250 fluids and used it as the basis of a correlation scheme for the volumetric properties of compressed liquids and liquid mixtures. Boushehri et al. [2] presented a theoretical basis for this regularity in terms of a statistical-mechanical equation of state [3].

The linearity of bulk modulus as a function of pressure: More than 100 years ago, a regularity has been discovered by Tait [4] in which isotherms of bulk modulus (reciprocal isothermal compressibility), $1/\beta = \rho(\partial p / \partial \rho)_T$, of a liquid as a function of pressure vary linearly [5-8].

A new scale for measuring the overall elastic stiffness of these compounds is introduced and its correlation with the calculated bulk modulus and lattice constants is analyzed. The overall elastic stiffness is calculated and found to be directly proportional to bulk modulus and inversely proportional to lattice constants. Bulk modulus has been found to correlate well with strength and hardness in many materials and those with largest the bulk moduli are usually expected to be the hardest materials [9]. Therefore, one of the important parameters that characterize the physical property of a material system is the material stiffness and its corresponding bulk modulus which measures the degree of stiffness or the energy required to produce a given volume deformation. The bulk modulus reflects important bonding characters in the material and, for many applications, is used as an indicator for material strength and hardness. Early

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