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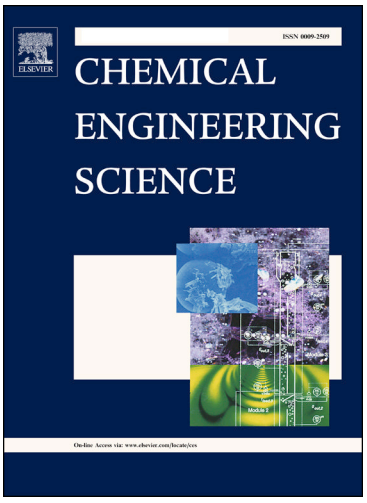

Simple correlation for critical isotherm of pure compounds

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Simple correlation for critical isotherm of pure compounds

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Abstract

A volumetric equation of state (PVT behavior of a fluid) is often based on a critical isotherm. Soave-Redlich-Kwong and Peng-Robinson are by far the most popular cubic equations of state. These equations use the first and second differential conditions at the critical point to obtain the parameters but fail to reproduce the P-V-T behavior near the critical point. A new simple equation is proposed for the critical isotherm which matches experimental data for a variety of molecules in the entire range from critical point to ideal gas condition as well as the liquid region. The new proposed critical isotherm equation matches experimental data of a wide variety of compounds much better than these cubic equations of state employed commonly.

Introduction

Equations of State aid in understanding the thermodynamics of various species including simple molecules, polar molecules and associating fluids. van der Waals' equation of state (van der Waals, 1873) was among the first one to successfully shed light on the thermodynamics of simple molecules. It took into consideration the repulsive and attractive intermolecular forces of attraction and consisted of the attractive parameter a and the co-volume parameter b. Although a very simple form, this equation explained the non-ideal behavior of gases to a great extent.

It was almost three quarters of a century later that new equations of similar type were proposed which improved on the shortcomings of the van der Waals' equation to the extent required. Redlich-Kwong equation (Redlich and Kwong, 1949) - a two parameter equation and its extension by Soave and others - converting it to three parameter form- and Peng-Robinson equation (Peng and

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