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An Enhanced Algorithm for Calculation of Supercritical PVT Properties by Saeki's EOS and the Adomian Decomposition Method

Hooman FATOOREHCHI, Omid TAVAKOLI
School of Chemical Engineering, College of Engineering, University of Tehran, Tehran, IRAN, ISLAMIC REPUBLIC OF

✉otavakoli@ut.ac.ir

Saeki developed a semi-empirical equation of state for supercritical fluids in form of $P=P^*-a_kXe^{-x}-b_k\,(X+c_k)^4X$ where P^*, a_k, b_k and c_k are temperature-dependent parameters, X is defined by $X=(V-V_c)/V$ and suffix k indicates the liquid-like region or the gas-like region of the supercritical state ($T>T_c$). Obviously, according to the Saeki EOS, the P-V relation at a specified temperature is highly nonlinear. Therefore, the calculation of density for supercritical fluids via Saeki's EOS would be a computationally difficult task. In this paper, we propose a fast and robust algorithm, based on a semi-analytical mathematical ansatz known as the Adomian decomposition method, which excels common univarate root-finders such as the Newton-Raphson algorithm in terms of accuracy and economy of computation. For the sake of illustration, the densities of carbon dioxide, water, methyl chloride, methanol, ethanol, and n-pentane are calculated by the proposed algorithm at supercritical conditions. The obtained results are of high accuracy, compared to the Benedict-Webb-Rubin (BWR) and the Beattie-Bridgeman equations of state, and are in good agreement with experimental data.