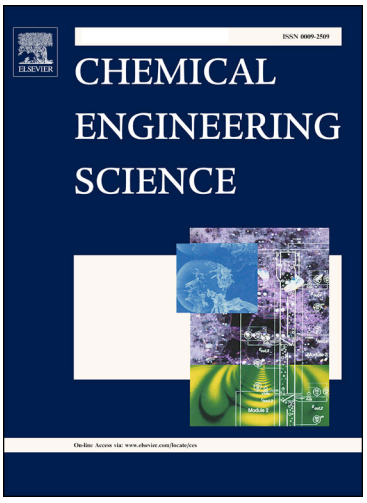

The Antoine equation of state: Rediscovering the potential of an almost forgotten expression for calculating volumetric properties of pure compounds

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The Antoine equation of state: Rediscovering the potential of an almost forgotten expression for calculating volumetric properties of pure compounds

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Abstract

Antoine is mainly known for the equation usually used for predicting vapor pressure of pure compounds that bears his name. In this article we show a little known equation of state (EoS), as well as its functionality to predict current PvT properties of more than forty compounds including industrial, noble, and organic gases. The Antoine EoS has been parameterized in three regions: $P_r < 1.2$, $1.2 \leq P_r \leq 10$ and $P_r > 10$ in order to improve its performance in the widest possible area. The proposed sets of optimized parameters were fitted by minimizing deviations after comparing predicted values with available experimental data in open literature.

The volumes predicted with the optimized Antoine EoS have been compared with those calculated with the widely-known Soave-Redlich-Kwong (SRK), Peng-Robinson-Stryjek-Vera (PRSV2) and Valderrama-Patel-Teja (VPT) equations of state. Results obtained by using the optimized Antoine EoS show better accuracy in the zone of high reduced pressures for all compounds and, in a more general way, for most of the compounds in the remaining zones than the other equations of state. The extension to noble gases and other compounds originally not taken into account by Antoine have been successfully achieved.

Keywords: Antoine; EoS; Volumetric properties; PvT

1. Introduction

The name of Antoine has been generally associated by the several generations of chemical engineers and chemists with the widely known empirical expression proposed for the direct calculation of vapor pressures of pure substances and, indirectly, of other related properties, such as the heat of vaporization. If it is true that one set (or, in some opportunities, several sets) of three constants, usually determined by the regression of experimental data are required for representing the vapor pressure-temperature relationship for pure liquids over a wide temperature range for each substance, its general utilization has been strongly recommended due to the associated relative simplicity of calculation, its relative highest precision compared with those of others of substantially greater mathematical complexity, and its ease for representing and extrapolating vapor pressure data.

This equation was not, however, the only contribution of this French pupil of the L'École des Mines to the calculations of properties of pure substances. In the period between 1875 and 1892, Louis Charles Antoine (1825 - 1898) proposed several equations for calculating volumetric and thermodynamic properties of pure compounds and some mixtures in gaseous state, which have been until now, as far as the authors

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