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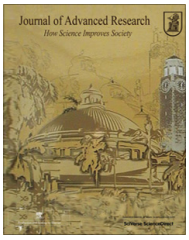

ORIGINAL ARTICLE

An efficient reliable method to estimate the vaporization enthalpy of pure substances according to the normal boiling temperature and critical properties

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ABSTRACT

The heat of vaporization of a pure substance at its normal boiling temperature is a very important property in many chemical processes. In this work, a new empirical method was developed to predict vaporization enthalpy of pure substances. This equation is a function of normal boiling temperature, critical temperature, and critical pressure. The presented model is simple to use and provides an improvement over the existing equations for 452 pure substances in wide boiling range. The results showed that the proposed correlation is more accurate than the literature methods for pure substances in a wide boiling range (20.3–722 K).

Introduction

Vaporization enthalpies are used frequently in adjusting enthalpies of formation of liquids to the standard state and in evaluating environmental transport properties. Accurate thermodynamic correlations are required to enhance the reliability of such simulations. Of the thermodynamic properties, heat of vaporization is one of the most important parameters for a multi-component multistage vapor–liquid equilibrium process as it is the one which controls the temperature as well as liquid and vapor profiles in a column [1]. Moreover, this property is sometimes used in the prediction or correlation of other thermodynamic properties. There is thus engineering and theoretical interest in the measurement and correlation of values of this property [2–12].

The normal boiling enthalpy can be calculated using either equations of state applied to the liquid and vapor phases or more simply by means of empirical correlations that allow calculating the enthalpy of vaporization of pure fluids [6–22]. Some of them are general analytical expressions that only require as input parameters certain properties of the fluid, such

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as the critical temperature, critical pressure, normal boiling point temperature, and molecular weight [6,23].

In this study, an accurate empirical correlation was presented by incorporating the normal boiling temperature and critical points of the pure substances. This equation can predict the heat of vaporizations for pure substances over the entire range of normal boiling point temperatures of practical interest.

Methodology

In this research, we considered some of well known analytical models that do not require specific adjustable coefficients for each substance, but rather are based on a knowledge of some properties of the liquid–vapor equilibrium (critical properties mainly) or on molecular properties. In particular, we selected seven specific expressions that are valid only for the calculation of the vaporization enthalpy. These are including the correlation of Riedel [13], Chen [15], and Zhao et al. (ZNY) [17], the simplest method defined as Trouton rule [19], two models presented by Vetere [20,21] and a more recent proposal of Liu [22].

Riedel model [13]

$$\Delta H_{vb} = 1.093\ RT_b \frac{\ln P_c - 1.013}{0.93 - T_b/T_c} \tag{1}$$

where ΔH_{vb} is vaporization enthalpy (J mol^{-1}), R is universal gas constant (8.3145 J mol^{-1} K^{-1}), T_b is normal boiling point (K), T_c is critical temperature (K), and P_c is critical pressure (bar).

Chen model [15]

$$\Delta H_{vb} = RT_b \frac{3.978(T_b/T_c) - 3.958 + 1.555\ln P_c}{1.07 - T_b/T_c} \tag{2}$$

Trouton rule [19]

$$\Delta H_{vb} = 88\,T_b \text{ J mol}^{-1} \tag{3}$$

Zhao et al. model (ZNY) [17]

$$\Delta H_{vb} = T_b(36.6 + 8.314\ln T_b) \tag{4}$$

Vetere model (V-79) [21]

$$\Delta H_{vb} = RT_b \times \frac{(1 - T_b/T_c)^{0.38}[\ln(P_c - 0.513 + 0.5066T_c^2/(P_cT_b^2)]}{1 - T_b/T_c + [1 - (1 - T_b/T_c)^{0.38}]\ln(T_b/T_c)} \tag{5}$$

Vetere model (V-95) [20]

– For hydrocarbons:

$$\Delta H_{vb} = 4.1868T_b\left(9.08 + 4.36\log_{10}T_b + \frac{0.0068T_b}{M} + \frac{0.0009T_b^2}{M}\right) \tag{6}$$

– For alcohols:

$$\Delta H_{vb} = 4.1868T_b\left(18.82 + 3.34\log_{10}T_b - \frac{6.37T_b}{M} + \frac{0.036T_b^2}{M} - \frac{5.2\times10^{-5}T_b^3}{M}\right) \tag{7}$$

where M is molecular weight (kg/kmol).

Liu [22]

Table 1 Tuned coefficients of new proposed model.

Coefficients	Values
A	0.01290
b_1	0.00086
b_2	−0.00206
b_3	0.01150
c_1	−0.01983
c_2	0.00632
c_3	−0.04279
d_1	0.02086
d_2	−0.00459
d_3	0.03544

$$\Delta H_{vb} = RT_b\left(\frac{T_b}{220}\right)^{0.0627} \times \frac{(1 - T_b/T_c)^{0.38}\ln(P_c/P_a)}{1 - T_b/T_c + 0.38(T_b/T_c)\ln(T_b/T_c)} \tag{8}$$

where P_a is atmospheric pressure in bar.

New proposed vaporization enthalpy correlation

In this study, we tried to find a more accurate and rapid model to calculate vaporization enthalpies of pure substances based on experimental data [14,24–26]. Thermophysical properties of compounds are obtained from the literatures [6,23]. By investigation of more than 452 data points vaporization enthalpy of pure substances and using 352 points of them in multiple regression analysis, a new empirical correlation is suggested to accurately prediction of vaporization enthalpy with the wide ranges of normal boiling temperatures (20.3–722 K).

The new presented model has three dependent variables (P_c, T_c, and T_b) and 10 independent variables as follows:

$$\Delta H_{vb} = RT_b(A + BT_{br} + CT_{br}^2 + DT_{br}^3) \tag{9}$$

$$B = b_1 + b_2P_c + b_3\ln(P_c) \tag{10}$$

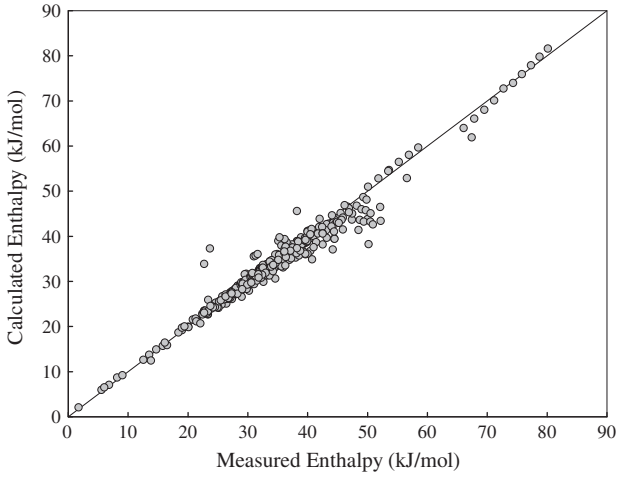

Fig. 1 Accuracy of presented model versus experimental data points from the literatures.