



Predictive Tait equation for non-polar and weakly polar fluids: Applications to liquids and liquid mixtures



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ABSTRACT

In this study, we describe a method based on the Tait equation which allows accurate estimation of density and isothermal compressibility of non-polar and weakly polar liquids and liquid mixtures over a wide range of pressures. We have applied the approach to various species in conditions ranging from 0.4 to 0.99 of the critical temperature and for pressures up to 150 MPa. If a reference experimental point of density is known and used as an input for this method, the approach yields average absolute deviations around 0.15% on density and around 2% on isothermal compressibility. In its fully predictive version, i.e. without experimental data point on density, this approach yields deviations on density around 0.3%, while deviations on isothermal compressibility are kept around 2%. Interestingly, when applied to compounds with a dipole moment larger than one Debye this approach is still able to provide reasonable results. In addition, this approach has been applied on binary liquid mixtures, using classical mixing rules. On different mixtures it has been found that the proposed approached yields results as good as on pure liquids emphasizing the consistency of the proposed methodology. All these results compare very favorably to those obtained from other approaches of the literature.

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1. Introduction

High-pressures densities and isothermal compressibilities of liquids are key quantities in the oil and gas industry [1,2]. To estimate these properties various methods, both correlative and theoretical ones, have been developed and reported in the literature [1–4]. Among them, the so-called Tait equation [5], a simple heuristic approach has shown its efficiency to deal with compressed liquids [5–16]. This approach has attracted a lot of attention as it only requires a value of density at a reference pressure and two numerical parameters, often noted B and C , to provide the density and the isothermal compressibility of a given liquid for pressures up to several MPa.

Rather surprisingly, the Tait equation has mostly been employed in a purely correlative manner and not as a predictive tool, i.e. B and C parameters are regressed for each fluid of interest using experimental data. This is probably due to the difficulties in physically interpreting these two numerical parameters [16–18], even if B is

viewed as a measure of the cohesive energy density of the liquid and C is closely linked to the repulsive force between molecules [7,16,17]. Thus, to the best of our knowledge, only two schemes based on a Tait equation are truly predictive for a large variety of species, those of Thomson et al. [8] and of Eslami and Azin [14]. However, these approaches usually yield non-negligible deviations compared to experimental data, their average absolute deviations (AAD) on density being of the order of 1% [8,14] which leads to AAD on isothermal compressibility of the order of 10% or even more.

In a recent work [15], we have recast the Tait equation in the framework of the extended corresponding states (CS) which allowed us to develop a “universal” function for the parameter B . This approach has shown to be accurate, with AAD compared to experimental data of the order of 0.1% and 1% on density and isothermal compressibility respectively [15]. However, this method requires an accurate value of the density and the isothermal compressibility at the reference point, the last being a quantity which is not always available even if it can be deduced, in some cases, from experimental compression at high pressures [19]. Thus, we propose in this article an extension of the developments of our previous work [15], which removes the need of experimental

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values of the density and the isothermal compressibility at the reference point. In addition, by combining this new model with mixing rules, we provide a methodology easily applicable to a large class of liquids and liquids mixtures in a predictive manner.

The structure of the article is as follow. In section 2, we describe the theoretical framework used to develop the proposed approach. Then, in section 3, we present and discuss the results obtained. Finally, the main conclusions are given in section 4.

2. Theoretical framework

2.1. Tait equation

Along a given isotherm, the so-called Tait equation describing the evolution of density with pressure is given by Ref. [5]:

$$\rho = \frac{\rho_{ref}}{\left[1 - C \ln\left(\frac{P+B}{P_{ref}+B}\right)\right]} \quad (1)$$

where ρ is the density, P is the pressure, ρ_{ref} and P_{ref} are the density and the pressure, respectively, at a reference point. B and C are numerical parameters that depend both on the chosen isotherm and on the studied materials. From Eq. (1), the isothermal compressibility, β_T , is straightforwardly deduced:

$$\beta_T = \frac{1}{\rho} \left(\frac{\partial \rho}{\partial P}\right)_T = \frac{1}{\left[1 - C \ln\left(\frac{P+B}{P_{ref}+B}\right)\right]} \frac{C}{P+B} \quad (2)$$

Interestingly, when using the Tait equation, the estimation of density of a liquid at a target pressure depends on the values of ρ_{ref} , B and C , whereas its isothermal compressibility only depends on B and C .

2.2. Corresponding states formulation

In a recent study [15], we have reformulated the Tait equation in the extended corresponding states framework, i.e. using critical pressure, critical temperature and acentric factor as scaling parameters. This allowed us to build a generic function describing the B parameter. This function is applicable to a large variety of not-highly-polar compounds over a wide range of temperature and pressure and writes for a given liquid:

$$B(T) = P_c \left\{ -2 + \left(1 + \kappa \left[1 - \sqrt{T_r}\right]\right)^2 \right\} \quad (3)$$

where, P_c is the critical pressure, $T_r = \frac{T}{T_c}$ where T_c is the critical temperature, and κ is a parameter function of the acentric factor given by:

$$\kappa(\omega) = -0.883\omega^2 + 14.34\omega + 10.17 \quad (4)$$

It should be pointed out that, to develop Eqs. (3) and (4), we have used a reference pressure in the Tait equation, Eq. (1), taken at $1.5P_c$ [15]. In the following, P_{ref} and ρ_{ref} taken at $1.5P_c$ will be noted $P_{1.5P_c}$ and $\rho_{1.5P_c}$, respectively.

3. Results

3.1. Development of the P-Tait scheme

Once the parameter B is obtained thanks to Eqs. (3) and (4), the application of the Tait equation to determine density and

isothermal compressibility only requires the knowledge of parameter C and $\rho_{1.5P_c}$. To determine these quantities, a general framework is described below. The so-developed scheme, applicable to liquids and liquid mixtures, is noted as P-Tait in the following and its corresponding flowchart is provided in Fig. 1 for sake of clarity.

3.1.1. C parameter function

To define a generic function describing the C parameter we have used an extended CS framework [20,21]. More precisely, we have first studied the variations of the parameter C with the reduced temperature, T_r , when Eqs. (3) and (4) are used to compute the B parameter. To do so, using the accurate NIST database [22], we have adjusted the values of C with T_r for sixteen non-polar and weakly-polar pure compounds over a wide range of temperature and pressure, in which the adjustments are carried out based on the isothermal compressibility data [15], i.e. using Eq. (2), see Table 1 for the studied systems and the range of thermodynamic conditions. We recall here that the reference point has been taken at $P_{ref} = 1.5P_c$ consistently with our previous work [15]. However, as it will be shown later on, the scheme proposed in this work can be straightforwardly extended to any reference point (e.g. the saturation pressure).

Results shown in Fig. 2 indicate that the so-fitted parameter C depends both on the studied compounds and on the reduced temperature. This means that the usual assumption of a parameter C independent on the temperature could lead to non-negligible deviations when dealing with a wide range of temperatures. This would be particularly noticeable on the isothermal compressibility as this property is strongly dependent on C , see Eq. (2). In addition, Fig. 2 shows that compounds possessing a similar acentric factor do not yield superimposing C versus T_r curves, e.g. butane and sulfur hexafluoride or heptane and octafluorocyclobutane. This indicates that the parameter C does not depend only on T_r and ω as in the classical extended corresponding states framework. However, as shown in Fig. 2, the deviations between the curves associated to compounds possessing similar acentric factors occur when the ratios between the triple point temperature, T_t , and the critical temperature, T_c , differs noticeably. Hence, to take into account this effect and so to go beyond the classical extended corresponding states framework, we have used the T_t/T_c ratio as an extra variable to correlate the parameter C .

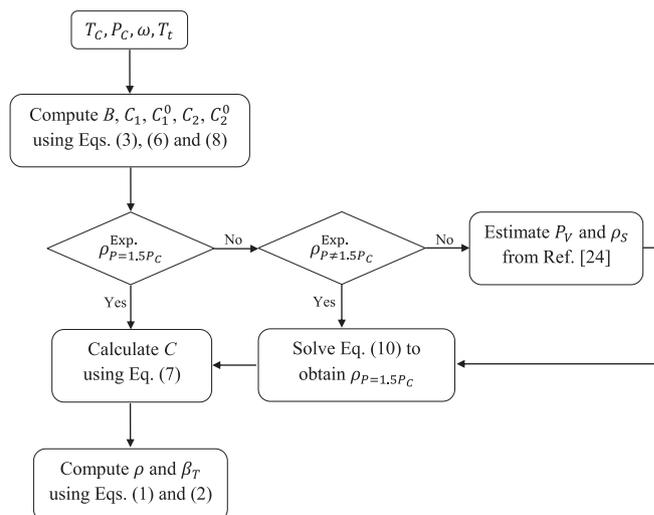


Fig. 1. Flowchart of the P-Tait scheme proposed in this work. T_t is the triple point temperature, P_v is the vapor pressure and ρ_s is the saturation liquid density.

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