



# Application of perturbed hard-sphere equation of state to the study of volumetric properties of nano-fluids



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## ABSTRACT

This paper aimed to examine the application of a perturbed hard-sphere (PHS) scheme for modeling the volumetric properties of nanofluids. In this regard, PHS scheme has been employed to develop an analytical equation of state (EOS) to correlate and predict the volumetric properties of some nanofluids containing SnO<sub>2</sub>, ZnO, Co<sub>3</sub>O<sub>4</sub>, TiO<sub>2</sub>-anatase (-A), TiO<sub>2</sub>-rutile (-R), CuO and Al<sub>2</sub>O<sub>3</sub> as nanoparticles dispersed in ethylene glycol, poly ethylene glycol, water, poly ethylene glycol + water and ethylene glycol + water as base fluids. Two temperature-dependent parameters appeared in the EOS were expressed in terms of molecular scaling constants  $\sigma$ , the effective hard-sphere diameter, and  $\epsilon$ , the non-bonded interaction energy. The aforementioned scaling constants were correlated with melting temperatures and true densities which demonstrated the rationality of these constants. The performance of the proposed model was assessed by predicting 1348 density data, for which their measured values were available in the literature over the pressure range from 0.1 to 45 MPa and temperature range from 273 to 363 K. The overall average absolute deviation (AAD) of the correlated (at 0.1 MPa) and predicted (at elevated pressures) densities of 9 studied nanofluids from the experimental data was found to be 0.44%. Generally, this work showed that PHS is an appropriate scheme for the correlation and prediction of the properties of this class of fluids by the help of crossed interaction parameters between nanoparticles and base fluid molecules. The isothermal compressibility coefficients and excess volumes of studied nanofluids have also been investigated by the proposed model.

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## 1. Introduction

A nanofluid is defined as a dilute suspension of nanometer-size particles and fibers dispersed in a liquid. Some nanofluids are suspensions of metallic nanoparticles in conventional base fluids (denoted as nanoparticle/base fluid) [1]. As a result, when compared to the base fluid, changes in physical properties of such mixtures occur, e.g., viscosity and thermal conductivity. Recently, they came into focus as alternative heat transfer fluids flow [2–6]. Besides thermal conductivities which is crucial for use in the heat transferring phenomena, other thermophysical prosperities such as density is as critical as thermal conductivities in engineering systems [7]. In order to evaluate the fluid dynamic and heat transfer performances of nanofluids in thermal cycles, the density must be known accurately to compute matter and energy balances [8]. Since

the density data are scarce for nanofluids, specifically those reported at the elevated pressures, the development of empirical and semi-theoretical models such as  $P\rho T$  correlations and equations of state (EOSs) to supplement the available experimental data seems is useful.

Although the great efforts devoted to study the transport properties of nanofluids through empirical, semi-empirical, theoretical and molecular simulation methods [9–17], less emphasis has been placed on presenting analytical models for volumetric data of nanofluids. We briefly review the previous approaches within the calculation of volumetric data of nanofluids from the most widely used Tammann-Tait equation to those are related to computer-aided genetic algorithms as follows:

The densities of nanofluids and nanomaterial have been correlated based on the several EOSs and  $P\rho T$  correlations. The most widely used one is Tammann-Tait equation [18–20] and that was adopted for nanometer sized particles by Sharma-Kumar [21] and Pak-Cho [22]. Sharma and Kumar developed an EOS for nanomaterials as follows:

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$$P = a_1 \left(1 - \frac{V}{V_0}\right) + a_2 \left(1 - \frac{V}{V_0}\right)^2 \quad (1)$$

where,  $P$  is the pressure,  $V/V_0$  the relative change in volumes and 0 refers to their initial condition.  $a_1$  and  $a_2$  are the size-dependent parameters, which have been proposed to be determined from the definition of bulk modulus and its first order pressure derivative [21]. Very recently, Sugata and Piri [23] employed a perturbed-chain statistical associating fluid theory (PC-SAFT) coupled with Young–Laplace equation [24] to investigate and represent fluid-phase equilibria in nanosize pores. Pak and Cho [22] presented the general equation for representing the density of nanofluids as follows:

$$\rho_{nf} = \rho_{np}\varphi + \rho_{bf}(1 - \varphi) \quad (2)$$

where,  $\rho_{nf}$  is the density of the nanofluid,  $\rho_{np}$  is the density of the particle,  $\varphi$  is the particle volume concentration, and  $\rho_{bf}$  is the base fluid density. Vajjha et al. [25] employed Pak-Cho equation to calculate the nanofluid densities; the need for true values of base fluid and nanoparticle densities limits the applicability of the Pak-Cho equation.

The artificial neural network method has also been employed to correlate and predict  $P\rho T$  data of nanofluids. Karimi and Yousefi [26] correlated the experimental density of four nanofluids in the temperature range of 273–323 K and the nanoparticle volume fraction up to 10% with average absolute deviation (AAD) equal to 0.13% using neural network approach. It should be mentioned that these methods need large datasets for training.

Several researchers tried to correlate high-pressure volumetric data of nanofluids based on Tammann-Tait equation [16,17]. Although the Tammann-Tait equation leads to the quit accurate results for the density correlation of nanofluids, however, in the case of nanofluids the applicability of that equation is limited to the fitting of numerous coefficients to each nanoparticle concentration. This issue limits the use of Tammann-Tait equation for the practical purposes. It should be added that Tammann-Tait equation does not make significant contributions to understand the molecular interactions operating between nanoparticle surface and base fluid molecules.

By employing molecular-based EOS, one can both predict accurately the  $P\rho T$  data of nanofluids and investigate the effect of molecular interactions on their volumetric behavior using the crossed interaction terms. Using a perturbed hard sphere (PHS) equation of state is a proper route to achieve this goal. The PHS EOS is based on the molecular theories of statistical mechanics [27], in which the reference physical model serves as the hard-sphere repulsion and a perturbation part denotes the dispersion forces. Likewise, PHS EOS belongs to a long history and comprehensive theoretical backgrounds among the literature [28–30]. Numerous researchers [29,31–34] brought PHS EOS in focus over the past 2 decades and consequently, the performance of such model has been well-established for various classes of liquids [28,35–42].

In the present work, for the first time, we examine the applicability of a perturbed hard-sphere scheme to correlate and predict the volumetric properties of nanofluids. As mentioned above, it was found that, regardless of the fact that the PHS scheme had to be extended by orders of magnitude, it was still an appropriate scheme to model the properties of highly non-simple fluids by the help of crossed interaction parameters between nanoparticles and base fluid molecules; this fact is attributed to its theoretical basis. Also, we show that our PHS model yields nanoparticle parameters that correlate regularly with the melting temperatures and true densities of compacted nanopowder.

## 2. Theory

### 2.1. Equation of state for pure base fluid

In the framework of the perturbation theory of liquids [27], the compression factor of a dense fluid comprises hard-sphere contributions and dispersion forces. According to the perturbation theory, the general frame of the PHS EOS of interest is that of Carnahan-Starling-van der Waals equation which was proposed by Song et al. [28,43], viz;

$$Z = \frac{P}{\rho k_B T} = 1 + b(T)\rho g(\sigma^+) - \frac{a(T)\rho}{k_B T}, \quad (3)$$

Where  $Z$  is the compression factor,  $P$  is the pressure,  $\rho$  is the number (molar) density and  $k_B T$  is the thermal energy per molecule.  $a(T)$  and  $b(T)$  parameters represent respectively, attractive forces between the pairs of hard-sphere and the van der Waals co-volume.  $g(\sigma^+)$  denotes the radial distribution function (RDF) of hard-spheres at contact developed by Carnahan-Starling [44], which reads as:

$$g(\sigma^+) = \frac{1 - \eta/2}{(1 - \eta)^3}, \quad (4)$$

Here  $\eta$  is packing fraction of hard-sphere fluid defined as:

$$\eta = \frac{b(T)\rho}{4}, \quad (5)$$

Eq. (3) has two parts; 1) the Carnahan–Starling expression [44] taken as physical reference hard-sphere model and 2) van der Waals (vdW) attraction term to represent dispersion forces. Two temperature-dependent parameters of Eq. (3) i. e. the strength of attractive forces between two spheres  $a(T)$  and the molecular size,  $b(T)$  are theoretically related to the pair-potential function and temperature. Until now several approaches have been proposed to evaluate these parameters. Generally, one may perform the integral equations derived by Song and Mason [32,43,45] which require the pair potential energy function of physical systems of interest. However, the pair-potential function is seldom accurately known for most physical systems especially for inhomogeneous mixtures such as nanofluids, in which the interaction between the nanoparticles and the base fluid are due to a combination of factors such as ionic double repulsive layer in the nanoparticle surface and also nanoparticle size [46]. In this respect, the determination of these parameters through the integral equations is not straightforward. The temperature-dependent parameters,  $a(T)$  and  $b(T)$ , can be expressed in terms of suitable reducing constants. They are universal function of the reduced temperature. In the following, we show how to express two temperature-dependent parameters appeared in the PHS EOS, using the universal functions of reduced temperature,  $T_r$ , in terms of molecular scaling constants  $\sigma$ , the effective hard-sphere diameter, and  $\varepsilon$ , the non-bonded interaction energy and in corresponding states form as:

$$a(T) = \frac{2\pi}{3} \sigma^3 \varepsilon F_a(k_B T/\varepsilon) \quad (6)$$

$$b(T) = \frac{2\pi}{3} \sigma^3 F_b(k_B T/\varepsilon) \quad (7)$$

Where,  $\varepsilon$  is the dispersive energy parameter and  $\sigma$  denotes the hard-core diameter. Further,  $F_a$  and  $F_b$  are the universal functions of the reduced temperature,  $k_B T/\varepsilon$  which can be written as the following empirical formula [47,48]:

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