International Journal of Heat and Mass Transfer 99 (2016) 630-637

Contents lists available at ScienceDirect



International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Dependency of the thermophysical properties of nanofluids on the excess adsorption



HEAT and M

Marzieh Tamizi, Mohammad Kamalvand*, Mansoor Namazian

Department of Chemistry, Faculty of Science, Yazd University, Yazd 89195-741, Iran

ARTICLE INFO

Article history: Received 27 October 2015 Received in revised form 27 March 2016 Accepted 11 April 2016 Available online 22 April 2016

Keywords: Nanolayer Adsorption Density functional theory Density profile Nanofluid

ABSTRACT

The difference between the experimental thermophysical properties of nanofluids and the values obtained by ideal mixture theory was investigated. It is shown that by ignoring fluid adsorption around nanoparticles in a nanofluid, ideal mixture theory underestimates the density, thermal conductivity, and viscosity and overestimates the heat capacity and thermal expansion coefficient of the nanofluids. Dependency of these deviations upon the adsorption of nanofluid molecules on the surface of nanoparticles was investigated and a linear correlation was observed at different temperatures, concentrations, and nanoparticle diameters. The excess adsorption of the nanofluid molecules is obtained by using an accurate version of the density functional theory.

© 2016 Elsevier Ltd. All rights reserved.

1. Introduction

Nanofluid is a stable and uniform suspension consisting of nanoparticles in fluids such as water or ethylene glycol [1]. Following the presentation of nanofluid by Choi in 1995 [1], a large number of researchers have focused on studying the thermophysical properties of nanofluids such as thermal conductivity, viscosity, heat capacity, and density. Experimental results show that the nanofluids have improved thermophysical properties compared to the bulk fluid or colloidal fluids containing micrometer sized particles [2]. For example, by adding 1.5 wt% of carbon coated Cu, Al, and Fe nanoparticles, the thermal conductivity of polyethylene glycol can be enhanced up to 49%, 40%, and 30%, respectively [3]; for a nanofluid containing ethylene glycol and 0.3 vol% of Cu nanoparticles, the effective thermal conductivity increases by up to 40% [2] or with increase in nanoparticle volume fraction by up to 5%, the viscosity of Al₂O₃/water nanofluid can increase by up to 60% [4] and the specific heat of nanofluid containing 4 vol% of CuO nanoparticles in water is 20% lower than that of the pure water [5].

One of the oldest models to predict thermal conductivity of a solid–liquid mixture is the Maxwell model. This model has been proposed for an ideal liquid–solid mixture and by ignoring interactions between these two parts [6],

$$k_{th} = \frac{k_{sp} + 2k_{bf} + 2(k_{sp} - k_{bf})}{k_{sp} + 2k_{bf} - (k_{sp} - k_{bf})\varphi}$$
(1)

where, k is thermal conductivity, sp and bf denote solid particle (like spherical nanoparticles) and base fluid, respectively, and k_{th} refers to the theoretical value of nanofluid's thermal conductivity. However, many experimental results show that the Maxwell model underestimates thermal conductivity of the nanofluids.

Although the reason for the improvement in thermophysical properties of nanofluids is not clear, some mechanisms, for example for thermal conductivity enhancement of nanofluid, have been proposed: Brownian motion of the nanoparticles, the nature of heat transport in the nanoparticles, and the effects of nanoparticle clustering and interfacial molecular layering of the fluid. Among these mechanisms, Evans et al. [7] and Babaei et al. [8] showed that the effect of Brownian motion of the nanoparticles on the enhancement of thermal conductivity of nanofluids is not considerable. In contrast, layering of liquid molecules on the nanoparticle surface has an important role in the anomalous enhanced thermal conductivity of nanofluids [9–17]. It has been shown that the thermal conductivity of nanofluids depends on the nanolayer structure, and there is a linear regularity between thermal conductivity enhancement and total excess adsorption of fluid molecules on the nanoparticle surface [18].

Thermal performance of a nanofluid depends not only on its thermal conductivity, but also on its other thermophysical properties which include heat capacity, viscosity, and density [19]. Density measurement of nanofluids demonstrated an increase in

^{*} Corresponding author. Tel.: +98 353 112 2641; fax: +98 353 821 0644. *E-mail address:* kamalvand@yazd.ac.ir (M. Kamalvand).

density by increasing volume fraction of nanoparticles [20]. In addition, the heat capacity of nanofluid plays an important role in the heat transfer process [21]. Specific heat capacity of nanofluids depends on many factors, such as specific heat capacity of fluid and nanoparticles, concentration, shape and size of nanoparticles, and temperature of suspension [17]. According to the experimental results, the specific heat capacity of nanofluids decreases with an increase in volume fraction of the nanoparticles [22,23]. The specific heat capacity of nanofluids also increases with increasing temperature. The solid-fluid interaction energy, absence of thermal equilibrium between nanoparticles and fluid molecules, and layering of liquid molecules on the surface of nanoparticles are several proposed mechanisms for how nanoparticles affect heat capacity of the nanofluid [24]. The reduced specific heat capacity of nanofluids is due to the lower specific heat capacity of nanoparticles. Although, in the literature, there is no satisfactory mechanism for the reduced specific heat capacity of nanofluids, theoretical studies have been performed to obtain models to predict it. By ignoring the interaction between the nanoparticles and the fluid molecules, the specific heat capacity of nanofluids is usually predicted by:

$$C_{p,nf} = \varphi C_{p,sp} + (1 - \varphi) C_{p,bf} \tag{2}$$

where, φ is the volume fraction of solid particles (like nanoparticles); *nf, sp*, and *bf* refer to the nanofluid, solid particle, and base fluid, respectively; and C_p is the specific heat capacity. In this model, the nanofluid is assumed to be an ideal mixture. Experimental results demonstrate that using this model leads to an overestimation in the calculated specific heat capacity values [22]. Also, two similar equations for density (ρ) and thermal expansion coefficient (α) of the nanofluids are reported:

$$\rho_{nf} = \varphi \rho_{sp} + (1 - \varphi) \rho_{bf} \tag{3}$$

$$\alpha_{nf} = \varphi \alpha_{sp} + (1 - \varphi) \alpha_{bf} \tag{4}$$

It should be noted that Eq. (3) underestimates density and Eq. (4) overestimates the thermal expansion coefficient of nanofluids. In addition to the above properties, viscosity of the nanofluid is more than that of the base fluid and it is dependent on temperature, volume fraction, and nanoparticles diameter. At first, Einstein proposed a simple correlation, $\eta = \eta_f (1 + 2.5\varphi)$, for viscosity of a solid–liquid mixture, where η is viscosity. After Einstein, Brinkman generalized the Einstein model for non-interacting hard-sphere particles suspension [25]:

$$\eta_{nf} = \frac{\eta_{bf}}{\left(1 - \varphi\right)^{2.5}} \tag{5}$$

The Brinkman model underestimates viscosity of the nanofluids, too. Deviation of Eqs. (1)-(5) from experimental values clearly shows that the interaction between nanoparticles and the base fluid molecules should be considered. Therefore, based on the assumption of thermal equilibrium between the nanoparticles and the base fluid, Eq. (2) was improved by Xuan and Roetzelas [26]:

$$C_{p,nf} = \frac{\varphi \rho_{sp} C_{p,sp} + (1 - \varphi) \rho_{bf} C_{p,bf}}{\varphi \rho_{sp} + (1 - \varphi) \rho_{bf}}$$
(6)

In this model, the effects of density of nanoparticle and fluid (ρ_{sp} and ρ_{f} , respectively) are also considered; and the deviation of heat capacity estimated by this model from experimental data is lower than that by Eq. (2). Generally, there is a large deviation between the specific heat capacity values obtained from Eqs. (2) and (6) [27]. Also, a similar modified equation is reported for accurate calculation of the thermal expansion coefficient [28]:

$$\alpha_{nf} = \frac{\varphi \rho_{sp} \alpha_{sp} + (1 - \varphi) \rho_{bf} \alpha_{bf}}{\varphi \rho_{sp} + (1 - \varphi) \rho_{bf}}$$
(7)

The main reason for deviation of Eqs. (1)–(5) from experimental data is the entropic effects and energetic interactions between nanoparticles and the base fluid molecules that are ignored in these equations. These interactions lead to aggregation of the base fluid molecules around nanoparticles [29]. In fact, in a dense fluid, the molecules accumulate on the surface of a central molecule and form a solid-like layered structure [30]. Although there are no long-range Van-der Waals forces between nanoparticles and fluid molecules, there is an entropic attraction between them due to which the nanolayer is formed [29]. In the nanofluid, distribution of molecules around the nanoparticle is named nanolayer. Density and hence other thermophysical properties of the nanolayer are different from those of the base fluid. Therefore, a part of the base fluid molecules in the nanofluid has different properties from those of the base fluid; and this difference is ignored in Eqs. (1)–(5). The local structure of a nanolaver can be shown by one-body density distribution function (density profile), $\rho(r)$ [31]. Density profile is affected by factors such as diameter of central molecule, temperature, and intermolecular interactions. Increasing size of the nanoparticle leads to increase in tendency of the molecules to be adsorbed on the surface of the central molecule [31]. Due to the large diameter (in comparison with fluid molecules diameter) of the nanoparticles, the number of adsorbed molecules in a volume element about the nanoparticle surface is usually greater than that in the pure fluid. These additional adsorbed molecules are shown with a property called excess adsorption. Excess adsorption may be calculated by the following equation [30]:

$$\Gamma = \int \left[\rho(\mathbf{r}) - \rho_b\right] d\mathbf{r} = 4\pi \int \left[\rho(r) - \rho_b\right] r^2 dr \tag{8}$$

where, Γ is excess adsorption of fluid molecules on the surface of each nanoparticle, ρ_b is average bulk density, and r is the distance between the surface of nanoparticle and the center of fluid molecules. $\Gamma_N = \Gamma \times N$ is the total excess adsorption around all nanoparticles in which N is the number of all nanoparticles dispersed in the nanofluid. In this paper, dependency of the anomalous behavior of the thermophysical properties of nanofluids on excess adsorptions will be investigated. To calculate the excess adsorption of fluid molecules on the surface of nanoparticle, the density profile can be obtained by using experimental or theoretical methods. One of the powerful and accurate theoretical methods is density functional theory (DFT) by which the density profile of the base fluid around nanoparticles can be obtained.

The remainder of this paper is organized as follows. In Section 2, DFT method is explained briefly; in Section 3, the effects of excess adsorption on the density, thermal expansion coefficient, specific heat capacity, thermal conductivity, and viscosity of nanofluids are investigated; and in Section 4, some concluding remarks are exposed.

2. Density functional theory

In the density functional theory of an inhomogeneous fluid, the grand potential, Ω , of the system related to its Helmholtz free energy, *F*, is obtained via a Legendre transformation [32],

$$\Omega[\rho(\mathbf{r})] = F_{int}[\rho(\mathbf{r})] + \int d\mathbf{r} \rho(\mathbf{r})[V^{ext}(\mathbf{r}) - \mu]$$
(9)

where, $\rho(\mathbf{r})$ is the one-body density distribution, $V^{\text{ext}}(\mathbf{r})$ is the external field due to the nanoparticles, μ is the chemical potential, and $F_{int}[\rho(\mathbf{r})]$ is the intrinsic Helmholtz free energy of the fluid. The intrinsic Helmholtz free energy functional can be expressed as an ideal-gas contribution $F^{id}[\rho(\mathbf{r})]$ plus an excess term $F^{ex}[\rho(\mathbf{r})]$ that accounts for the non-ideal interactions [32],

$$F_{int}[\rho(\mathbf{r})] = F^{id}[\rho(\mathbf{r})] + F^{ex}[\rho(\mathbf{r})]$$
(10)

Download English Version:

https://daneshyari.com/en/article/656483

Download Persian Version:

https://daneshyari.com/article/656483

Daneshyari.com