Propose a Correlation to Approximate Nanofluids' Enthalpy of Vaporization - A Numerical Study

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Abstract—After studying available experimental data of nanofluids evaporation characteristics, a correlation was proposed by authors to approximate nanofluids' enthalpy of vaporization. Then the evaporation behavior of nanofuel droplets (fuel droplets containing nanoparticles) has been numerically investigated in order to evaluate this relation capability to predict nanofluids evaporation characteristics. Employing the relation in this numerical study led to results in good agreement with experimental data which means capability of this formula to predict nanofluids' heat of vaporization.

Index Terms—Enthalpy of vaporization, evaporation rate, fuel droplet, nanofluid, nanoparticles.

I. INTRODUCTION

Nanofluids, solutions containing a stable suspension of nanoparticles (e.g., metals, oxides, carbides, nitrides, or carbon nanotubes) with typical lengths of 10–100 nm, have attracted great interest recently [1]–[7]. Murshed *et al.* [8] provided a comprehensive review of nanofluids applications in transportation, micromechanics and instrumentation, heating, ventilating and air-conditioning (HVAC) and medical fields.

The present study is considered nanotechnology application in the field of combustion and fuels. In practical combustion systems such as gas turbines, diesel engine combustors and liquid rockets, liquid fuel is sprayed into the combustion chamber as a cloud of droplets [9]. Exposing into a hot environment causes quick evaporation of the droplets. In fact, droplet evaporation is an important process in liquid fuels combustion. However, studies on nanofluids evaporation characteristics are rare.

According to Madhusoodanan *et al.* [10], Aluminum oxide nanoparticles lead to a decrease in evaporation rate of water. Sefiane and Bennacer [11] found a reduction during the pinning phase in sessile droplet evaporation rate with presence of Aluminum nanoparticles compared to its base fluid, ethanol. Chen *et al.* [12] studied the effects of three different types of nanoparticles (Laponite, Ag and Fe₂O₃) on the evaporation process of deionized water (DW). They observed Clay and Sliver nanoparticles enhance DW evaporation rate, but Fe₂O₃ nanoparticles slow down it. Gan and Qiao [13] investigated evaporation characteristics of ethanol and n-decane fuel droplets with the addition of Al nanoparticles. Their results showed that Al nanoparticles tend to slow down the base fluid droplet evaporation rate.

Manuscript received July 4, 2013; revised September 1, 2013.

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Considering five different types of nanoparticles, Moghiman and Aslani [14] found that depending on type of nanoparticles, evaporation rate of free-surface water may be enhanced or slowed down.

As mentioned above, evaporation process is an important phenomenon in the combustion chambers. According to D²-law, evaporation rate of a single liquid droplet is inversely proportional to the enthalpy of vaporization [12]. If it is possible to estimate the effect of nanoparticles addition on heat of vaporization of base fluid, then influence of nanoparticles on evaporation characteristics of the base fluid can be predicted. Therefore having a correlation to estimate this property of nanofluids is significantly important. The aim of this paper is to first propose such relation for nanofluids' enthalpy of vaporization to predict evaporation behavior of nanofluid droplets and then evaluate the capability of this proposed correlation by comparing the obtained results with available experimental data.

II. DESCRIPTION OF PHYSICAL MODEL

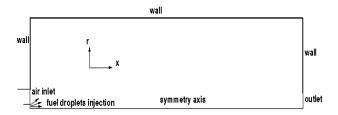


Fig. 1. Employed boundary conditions.

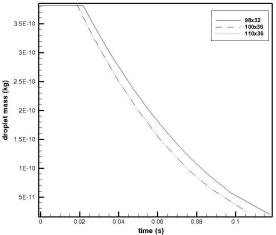


Fig. 2. Temporal evolution of droplet mass for three computational grid sizes.

The flow configuration investigated in this paper is based on a non-premixed swirl-burner. Fuel droplets are injected from the center of a combustion chamber while hot air stream

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flows around them. The flow has been considered to be two-dimensional and axi-symmetric. Air flow temperature is higher than boiling-point temperature of liquid fuel which causes quick evaporation of droplets. The Re number is around 100, the swirl number is set to 0.25 and air inlet axial velocity is 6 m/s. In Fig. 1, the employed boundary conditions are shown. In order to check grid independency of results, three grid meshes were tested. Fig. 2 presents the temporal evolution of droplet mass obtained by employing these grid meshes. From the figure, it is reasonable to select 100x36 grid nodes as a good compromise between accuracy and computational time.

III. MATHEMATICAL MODEL

The governing equations for the gas phase are Reynolds–Averaged Navier–Stokes, energy and species concentration. Turbulence stresses in gas phase equations are modeled by k- ϵ method, so two transport equations are also required for turbulent kinetic energy and eddy dissipation rate. The set of governing equations can be conveniently written in a general transport equation form as follows [15]:

$$\frac{\partial}{\partial t} (\rho \phi) + div (\rho u_i \phi) = div \left[\Gamma_{\phi} grad \phi \right] + S_{\phi}$$
 (1)

This generalized transport equation contains transient, convection, diffusion and source terms, respectively where the general variable ϕ may represent the mean value of any unknown variable in the aforementioned governing equations. The parameters Γ_{ϕ} and S_{ϕ} represent an effective diffusion coefficient of this general variable and the source term respectively. It has to be noted that in near-wall region, a wall-function approach is used. The gas phase governing equations are solved using SPRINT code [16] which has been validated before against experimental data.

The time-dependent Lagrangian momentum equations for liquid phase are solved numerically to determine velocity and position of droplets [17], [18]. The mass conservation equation for liquid phase is obtained using correction factor introduced by Nikos and Dean [19]. Also by using the correlation reported by Faeth [20] the heat transfer equation is obtained. Clausius—Clapeyron equation of state [21] is employed to predict phase behaviors of system.

The effect of nanopaticles on liquid phase equations is modeled by revising the thermo-physical properties according to following equations [22], [23] for density (ρ), molar mass (M) and heat capacity (C_p). In below equations, subscript "NF" represents nanofluid.

$$\rho_{nf} = (1 - \varphi)\rho + \varphi \rho_s \tag{2}$$

$$M_{nf} = (1 - \varphi)M + \varphi M_s \tag{3}$$

$$\left(\rho C_{p}\right)_{nf} = \left(1 - \varphi\right)\rho C_{p} + \varphi \rho_{s} C_{p} \tag{4}$$

where properties with subscript "s" are for nanoparticles

whereas without subscripts are for basefluid. The variable φ in above equations represents nanoparticles volume fraction.

Nanofluids' enthalpy of vaporization has been rarely studied and there is no proposed relation for it yet. After studying published experimental data of Gan and Qiao [13] and Chen et al. [12], following model (equation (5)) was proposed by authors to approximate this property. This model is based on this assumption that the nanofluid behaves more like a fluid rather than a conventional solid-fluid mixture [23]. Nanofluid heat of vaporization (h_{fg}) should be a function of enthalpy of vaporization of base fluid and nanopartilees and also nanopartilees volume fraction. Further investigation reveals that density is also a significant parameter in evaporation behavior of droplets. According to [13], boiling temperature has an important influence on droplets lifetime and therefore on evaporation rate of droplets. Therefore effect of base fluid boiling temperature and nanopartilees' has been considered in this formula of enthalpy of vaporization.

$$\left(\rho h_{fg}\right)_{nf} = \left(1 - \varphi\right)\rho h_{fg} + IMF * \varphi \rho_s h_{fg,s} \tag{5}$$

where properties with subscript "s" are for nanoparticles whereas without subscripts are for basefluid and the parameter IMF (impact factor) has been defined as:

$$IMF = T_{b,bf} / T_{b,np} \tag{6}$$

where T_b (K) is the boiling point temperature and subscripts "bf" and "np" are for base fluid and nanoparticles, respectively. During numerical code execution, nanofluid properties are continuously calculated at every time step using (2)-(6). Hence variation in particle concentration because of evaporation will be included in calculations.

IV. RESULTS AND DISCUSSION

A. Evaluation of the Proposed Relation by Comparing Obtained Results with Findings of [13] for Decane Fuel Droplets

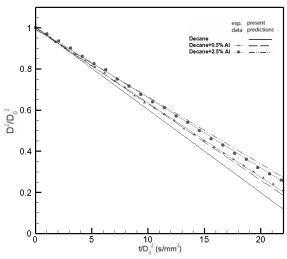


Fig. 3. Comparing this numerical study results with results of [13] for decane-based fuel droplets.

Fig. 3 compares temporal evolution of non-dimensionalised droplet square diameter of decane-based fuel obtained from this numerical study and experimental results of [13]. Note that as suggested by droplet evaporation classical theory [9], the droplet diameter (D) was scaled by the initial droplet diameter (D_0) . All nanoparticles concentrations are in weight percent. It has also to be noted that there was no available data for pure decane in reported data of [13]. The figure reveals that present findings are in good agreement with the experimental data which approve the proposed relation capability to approximate enthalpy of vaporization of nanofluids.

B. Evaluation of the Proposed Formula by Comparing Obtained Results with Findings of [13] for Ethanol Fuel Droplets

The temporal evolution of non-dimensionalised droplet square diameter for ethanol-based fuel obtained from this study is compared with experimental results of [13] in Fig. 4. From the figure, it can be observed that present predictions are consistent with the experimental data confirming the capability of proposed relation to approximate nanofluids' enthalpy of vaporization.

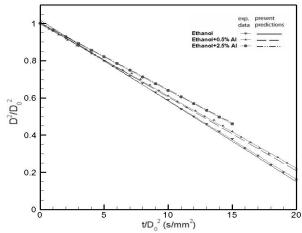


Fig. 4. Comparing this numerical study results with results of [13] for ethanol-based fuel droplets.

V. CONCLUSION

The present study is the first work on proposing a formula to approximate nanofluids' heat of vaporization. The evaporation characteristics of nanofluid droplets by employing this proposed correlation for nanofluids' enthalpy of vaporization were numerically investigated. The results obtained by using this relation were found to agree well with available experimental data which reveals this relation capability to predict heat of vaporization of nanofluids. However this formula produces good prediction for evaporation behavior of nanofluids studied in this paper, further investigation are still needed to improve this relation, since this property may also be dependent upon other thermo-physical properties such as surface tension and viscosity.

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natural gas temperature effects on the flame luminosity and NO emission," *International Journal of Spray and Combustion Dynamics*, vol. 4, pp. 175-184, 2012. 3) M. Vaezi, M. Passandideh Fard, M. Moghiman, and M. Charmchi, "Gasification of heavy fuel oils: A thermochemical equilibrium approach", *Fuel*, vol. 90, pp. 878-885, 2011. His previous research interests were in the fields of numerical modeling of Industrial processes, turbulent combustion flame simulation, pollutants emission modeling, and air conditioning. Currently he also focuses on nanotechnology applications in engineering-related systems. He has registered an invention under title of "Carbon Black Gas Furnace" in National Iranian Gas Company (NIGC).

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