Energy Conversion and Management 111 (2016) 1–14

Contents lists available at ScienceDirect

Energy Conversion and Management

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

Stability of nanofluids: Molecular dynamic approach and experimental study

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ARTICLE INFO

Article history:
Received 25 September 2015
Accepted 16 December 2015
Available online 4 January 2016

Keywords:
Nanofluid
Dispersion stability
DLVO
Molecular approach
Experimental study

ABSTRACT

Nanofluids as volumetric absorbent in solar energy conversion devices or as working fluid in different heat exchangers have been proposed by various researchers. However, dispersion stability of nanofluids is an important issue that must be well addressed before any industrial applications. Conditions such as severe temperature gradient, high temperature of heat transfer fluid, nanoparticle mean diameters and types of nanoparticles and base fluid are among the most effective parameters on the stability of nanofluid. A molecular dynamic approach, considering kinetic energy of nanoparticles and DLVO potential energy between nanoparticles, is adopted to study the nanofluid stability for different nanofluids at different working conditions. Different forces such as Brownian, thermophoresis, drag and DLVO are considered to introduce the stability diagrams. The latter presents the conditions for which a nanofluid can be stable. In addition an experimental investigation is carried out to find a stable nanofluid and to show the validity of the theoretical approach. There is a good agreement between the experimental and theoretical results that confirms the validity of our theoretical approach.

1. Introduction

An overview on the rate of energy consumptions in different industrial installations indicates that improving thermal efficiency of the processes is very important. Various methods have been introduced to enhance heat transfer. Improving thermal characteristic of working fluid is one of the attractive methods for augmenting the performance of different thermal devices. Nanofluid as a volumetric absorption system in solar thermal energy or as a working fluid in different heat transfer equipments has been proposed by different researchers (for instance [1–4]) because of their interesting thermophysical properties such as thermal conductivity and absorption coefficient.

However, there are many serious problems that must be overcome prior to any application of nanofluids. Among them nanoparticles' aggregation and sedimentation or physicochemical stability of nanofluids, are the most important issues that must be well addressed. Sedimentation of nanoparticles causes severe problems on the hydrothermal behaviors of a process. However, various methods have been proposed for stabilization of nanofluid such as applying ultrasonic waves for breaking nanoparticle aggregates, coating nanoparticles with polymeric surfactants to prevent aggregation, external force field employment on nanofluid and changing of electrostatic properties of nanoparticles' surfaces by variation of PH. Although, some of these methods are effective on the stabilization of nanofluids to some extent but none of them can perfectly solve the problem of the nanofluid stability. It is well known that the interparticle forces in nanofluid play an important role on the nanofluid stability.

In 1917, Smoluchowski [5] made the first attempt to estimate the effect of direct motion of particles on coagulation. Fuchs [6] introduced a critical diameter for particles, above which aggregation dominates (about 1 μm). Xinfang et al. [7] studied the influence of hexadecyltrimethyl ammonium bromide (CATB) dispersant on the stability of copper nano-suspensions at different PH numbers. They introduced an optimum PH number in which maximum stability is achieved. Dongsheng et al. [8] investigates stability of alumina–water nanofluid at different PH numbers and various concentrations of sodium dodecylbenzenesulfonate (SDBS). They presented optimum values for PH number and SDBS concentration in which the stability of the nanofluid would be maximized. Xinfang et al. [9] also studied stability of copper water based nanofluid using CATB, TX-10 and SDBS surfactants. They

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http://dx.doi.org/10.1016/j.enconman.2015.12.044
0196-8904/

Nomenclature

a	diameter of base fluid molecule (m)	m_p	nanoparticle mass (kg)
A	Hamaker constant (J)	Re	Reynolds number
C_D	Drag coefficient	t	time (s)
C_C	Cunningham correction factor	T	temperature (K)
C_m	velocity slip coefficient	u_0	initial velocity of nanoparticle (m/s)
C_{tc}	thermal creep coefficient	V_1	bulk velocity (m/s)
C_t	temperature jump coefficient	V_p	nanoparticle velocity (m/s)
d_p	nanoparticle diameter (m)	V_{np}	nanoparticle volume (m^3)
E_{DLVO}	DLVO potential energy (J)	v	molecular volume of base fluid (m^3)
F_D	drag force (N)	x	nanoparticle location (m)
F_B	Brownian force (N)	ρ	base fluid density (kg/m^3)
F_T	thermophoresis force (N)	ρ_p	nanoparticle density (kg/m^3)
F_{DLVO}	DLVO force (N)	ν	kinetic viscosity of base fluid (m^2/s)
k_B	Boltzmann constant (J/K)	μ	dynamic viscosity of base fluid (Pa s)
k_f	nanofluid thermal conductivity (W/m K)	λ	molecular mean free path (m)
k_p	nanoparticle thermal conductivity (W/m K)	ε	relative permittivity of base fluid $\left(\frac{c^2}{J/m}\right)$
k_n	Knudsen number	ε_0	permittivity of free space $\left(\frac{c^2}{J/m}\right)$
K	kinetic energy of nanoparticle (J)	ϕ	volume fraction
k	inverse Debye length (1/m)	ψ_0	surface potential (V)
L	initial distance between nanoparticles (m)	ζ	Gaussian random number

determined the optimum values of PH number and concentration of surfactants in order to achieve maximum nanofluid stability. Hwang et al. [10] used various methods for stabilization of different nanofluids. They studied different physical treatment techniques based on two-step production method, including stirrer, ultrasonic bath, ultrasonic disruptor, and high-pressure homogenizer, to verify the versatility of methods for preparing stable nanofluids. They concluded that high-pressure homogenizer is the most effective method to break down the agglomerated nanoparticles suspended in the base fluids. They produced Ag nanoparticles with the diameter of about 3 nm by modified magnetron sputtering method that is also an effective one-step method to prepare stable nanofluids. Huang et al. [11] studied the stability of two different, alumina and copper, water based nanofluids at different PH numbers. By studying of the influence of PH on zeta potential layer, they introduced an optimum PH number in which zeta potential layer has its maximum thickness on particle's surface whereupon maximum stability for nanofluid is achieved. These works have tried to prepare stable nanofluids but none of them investigated the conditions for which the nanofluids remain stable. Weiting et al. [12] modeled the process of aggregation and sedimentation of nanoparticles in nanofluids based on an analytic solution of nanoparticle's motion in the base fluid. They calculated the speed and location of nanoparticle and presented the variations of nanoparticle concentration with time. However the nanoparticles' aggregation in nanofluids was not discussed.

As mentioned, researches focused on stabilization of nanofluid at a certain condition during the preparation process. Their attempts on nanofluid stabilization were limited to amplifying zeta potential layer around the nanoparticles. Furthermore, in some cases experimental works have been carried out on breaking aggregated particles down to smaller ones. At the author knowledge there is not any attempt to show and to present the conditions for which the nanofluid would be stable and the nanoparticle aggregation does not occur during the working process. Thus it is very important to have a new and deep look on the nanofluid dispersion stability. The objective of this study is to propose stability diagrams for nanofluid at different thermophysical conditions. This is done based on a molecular dynamic approach by considering different forces, to represent conditions that nanofluid be stable. Hence, the energy approach for different cases (2, 3 and 7 particle methods) is implemented to study the dispersion stability of nanofluid at different thermophysical conditions. Then the stability diagram for various nanofluids at different conditions are generated based on the nanofluid characteristics including nanoparticle diameter, types of nanoparticles, types of base fluids, fluid temperature and flow field temperature gradient. An experimental investigation is carried out to see and to verify the results obtained theoretically.

2. Forces on the nanoparticles

There are different effective forces on dispersed nanoparticles in a base fluid. However, each of these forces has a particular range of effectiveness and some limitations to be effective. Forces between nanoparticles can be attractive or repulsive. They may also be short-range or long-range forces [13]. Some of the forces have more important role on particles aggregation at nano-scale. These forces are drag, thermophoresis, Brownian, Van der Waals and electrical double layer force. Van der Waals and electrical double layer forces are interparticle forces that combination of them was introduced as DLVO theory [14]. Other forces are hydrodynamic forces acting on each particle individually. These forces mathematically can be defined as follows:

2.1. Drag force

Recommended correlation for drag force, given by [15]

$$F_D = \frac{18\mu}{\rho_p d_p^2} \times \frac{C_D Re}{24} \times (v_1 - v_p) \times m_p \tag{1}$$

Here v_p is the particle velocity, v_1 is the fluid velocity, m_p is nanoparticle mass, C_D is drag coefficient, ρ_p is density of nanoparticle, μ is dynamic viscosity of base fluid, and d_p is the particle diameter. Re is the relative Reynolds number, given by

$$Re = \frac{\rho d_p |V_p - V_1|}{\mu} \tag{2}$$

There are various models of the drag coefficient C_D for nanoparticles. Stoke's law seems to be appropriate [16]. By substituting of C_D from Stoke's law Eq. (1) becomes: