



# Model for predicting particle size evolution during nanoparticle aggregation in refrigerant–oil mixture

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## ABSTRACT

Nanorefrigerant–oil mixture is a promising energy-efficient refrigeration working fluid with superior thermophysical properties, and the prediction for its thermophysical properties requires the actual size of the particles in refrigerant–oil mixture. Due to the competitive adsorption of different liquid molecules on particle surface, the actual particle size of refrigerant–oil mixture cannot be predicted by the existing models developed for the nanofluids with single-component base fluid. This paper presents a model for predicting the particle size evolution during nanoparticle aggregation in refrigerant–oil mixture, considering the competitive adsorption behavior and its effects on particle movement and interaction. For model validation, the time-evolution of particle size distribution and the average size are calculated and compared with the existing experimental data. The model prediction agrees with 92% of the experimental data within deviation of  $\pm 10\%$  and the mean deviation is 3.7%. In addition, the model can reflect the influences of oil mass fraction, initial particle concentration, primary nanoparticle diameter and temperature on particle size evolution. It is found that the adsorption layer has a significant effect on the aggregation behavior and the particle size evolution.

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## 1. Introduction

Refrigeration system has been always a major sector in energy consumption in most of countries around the world. Driven by the growing emphasis on energy saving, many new techniques have been introduced to increase energy efficiency. Nanofluid is a technique that dispersing nanoparticles in conventional fluid, which has superior heat transfer performance [1]. In recent years, efforts have been made to utilize the nanofluid concept to increase the energy efficiency of refrigeration system. Researchers disperse nanoparticles in conventional refrigeration working fluids (i.e., refrigerant–oil mixture), forming the “nanorefrigerant–oil mixture”. It is reported that the use of nanorefrigerant–oil mixture could decrease the energy consumption of a domestic refrigerators by 26% [2]. As a type of nanofluids, nanorefrigerant–oil mixture is regarded as a promising energy-efficient refrigeration working fluid and attracts a great attention.

To design the refrigeration system using nanorefrigerant–oil mixture, a basic requirement is the knowledge on the thermophysical properties of nanorefrigerant–oil mixture. Previous studies have shown that most of the nanofluid thermophysical properties

(e.g., thermal conductivity, viscosity, and heat capacity) are functions of nanoparticle size [3–5]. However, nanoparticles are readily to aggregate due to the strong Brownian motion and high surface free energy, and the real particle size is changing during aggregation process [6,7]. For this reason, considerable error may occur if simply substitute the initial particle size (i.e., the particle size before nanofluid preparation) into the correlations or models for thermophysical properties calculation. To have more precise prediction for thermophysical properties, the particle size evolution during aggregation needs to be known. Since it is hard to measure the real-time particle size evolution in real situation, a prediction model is needed.

Prediction of particle size evolution requires modelling the nanoparticle aggregation as aggregation process is the cause of particle size evolution, and the core of aggregation modelling is to calculate the interactions between nanoparticles. In common, most of the existing aggregation models aim at the nanofluids with base liquid of single component, and calculate the interactions between nanoparticles on the basis of the classic Derjaguin–Landau–Verwey–Overbeek (DLVO) theory [8,9]. In nanofluids, either the base liquid is single-component or multi-component, liquid molecules form a neatly structured adsorption layer (also called “interfacial layer”) on the nanoparticle surface, as revealed by experimental observation [10] and molecular dynamic (MD) simulations

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## Nomenclature

$A$	Hamaker constant [J]
$c$	particle concentration [ $\text{kg m}^{-3}$ ]
$D_f$	fractal dimension
$d_m$	molecular diameter [m]
$d_p$	particle diameter [m]
$\bar{d}_p$	average particle diameter [m]
$d_{p0}$	primary nanoparticle diameter
$d_{p,DLS}$	average diameter measured by DLS right after preparation
$e$	electron charge ( $1.60 \times 10^{-19}$ C)
$\bar{F}_B$	Brownian force [N]
$\bar{F}_g$	gravity [N]
$\bar{F}_d$	drag force [N]
$\bar{F}_{buo}$	buoyancy [N]
$\bar{G}$	Gaussian vector
$\bar{g}$	gravitational acceleration [ $\text{N kg}^{-1}$ ]
$H$	unretarded geometrical function
$h_a$	adsorption layer thickness [m]
$h_{a0}$	thickness of a single molecular layer
$h_p$	Planck constant ( $6.626 \times 10^{-34}$ J s)
$I$	ionic strength [M]
$i, j$	particle index
$k_B$	Boltzmann constant ( $1.38 \times 10^{-23}$ $\text{m}^2 \text{kg s}^{-2} \text{K}^{-1}$ )
$L$	side length of simulation domain [m]
$M$	molecular weight [kg]
$N_A$	Avogadro's number ( $6.022 \times 10^{23}$ $\text{mol}^{-1}$ )
$N_{a0}$	number of molecular layers
$n$	number of primary nanoparticles contained in a particle
$n_m$	number of molecules adsorbed on the surface of a particle
$P$	deposition probability
$r_p$	particle radius [m]
$S$	height of simulation domain [m]
$S'$	height of actual suspension [m]
$s$	separation distance between two particles [m]
$T$	temperature [K]
$\Delta t$	time step [s]
$U_{elec}$	electrostatic repulsion potential [J]
$U_{vdw}$	van der Waals attraction potential [J]
$\Delta u$	cohesive energy density difference between nanoparticle and liquid [MPa]
$\vec{v}$	particle velocity vector [ $\text{m s}^{-1}$ ]
$\vec{x}$	particle location vector [m]
$x$	x coordinates of particle location [m]
$Y$	dimensionless effective surface potential
$y$	y coordinates of particle location [m]
$z$	z coordinates of particle location [m]

## Greek symbol

$\delta_D$	dispersive solubility parameter [ $\text{MPa}^{-1/2}$ ]
$\delta_P$	polar solubility parameter [ $\text{MPa}^{-1/2}$ ]
$\delta_H$	hydrogen bonding solubility parameter [ $\text{MPa}^{-1/2}$ ]
$\varepsilon$	dielectric permittivity [ $\text{F m}^{-1}$ ]
$\varepsilon_0$	absolute dielectric constants ( $8.85 \times 10^{-12}$ $\text{F m}^{-1}$ )
$\zeta$	zeta potential [V]
$\eta$	refractive index
$\kappa$	inverse Debye length [ $\text{m}^{-1}$ ]
$\lambda$	randomly-generated number
$\mu$	viscosity [ $\text{kg m}^{-1} \text{s}^{-1}$ ]
$\nu_e$	main electronic absorption frequency in the ultraviolet region ( $3 \times 10^{15}$ $\text{s}^{-1}$ )
$\rho$	density [ $\text{kg m}^{-3}$ ]
$\sigma$	standard deviation of the associated normal distribution
$\sigma'$	standard deviation of log normal distribution
$\tau$	mean of the associated normal distribution
$\tau'$	mean of log normal distribution
$\psi$	particle surface potential [V]
$\omega$	oil mass fraction [%]

## Subscripts

0	initial
a	adsorption layer
a0	single molecular layer
ad	after deposition
b	bulk liquid
bd	before deposition
$k$	bulk liquid (b), adsorption layer (a), or particle (p)
$k'$	bulk liquid (b) or adsorption layer (a)
l	liquid
new	new particle
o	oil
p	particle
p-o	particle–oil
p-r	particle–refrigerant
r	refrigerant

## Abbreviation

CLL	cell-linked list
DLS	dynamic light scattering
DSMC	direct simulation Monte Carlo
HSP	Hansen solubility parameters
MC	Monte Carlo
MD	molecular dynamics
PBE	particle population equation
PSD	particle size distribution

[11–15]. For single-component liquid (i.e., pure liquid), the composition of the adsorption layer is the same with the bulk liquid, thus the adsorption layer can be neglected while calculating the interactions using DLVO theory. For multi-component fluid (i.e., liquid mixture), the particle affinities of different liquid molecules are different, causing that the molecules of different liquids adsorb on nanoparticle surface competitively [16,17], and the composition of adsorption layer is different with that of bulk liquid. At this point, the interacted particle system becomes “particle–adsorption layer–liquid–adsorption layer–particle” from “particle–liquid–particle”, and the classic DLVO theory cannot be directly used to calculate the interactions in liquid mixtures. Thus, a new model incorporating the adsorption layer needs to be established to calculate the

interactions between nanoparticles in refrigerant–oil mixture, and describe the aggregation behavior of nanoparticles.

In order to incorporate the adsorption layer in aggregation model, the thickness and composition of adsorption layer should be known. Most of the existing studies estimate the adsorption layer thickness by empirical hypothesis [18–20] or molecular dynamic simulation [12–15], and few studies develop analytical calculation [21,22]. In these studies, the base fluids of nanofluids are single-component, and the composition effect on thickness calculation is not considered. However, the adsorption layer thickness for nanorefrigerant–oil mixtures could be a function of the composition of adsorption layer, thus the existing approaches cannot be utilized directly. As for the composition of adsorption layer, there is still

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