On the phononic and electronic contribution to the enhanced thermal conductivity of water-based silver nanofluids

V. Karthik, S. Sahoo, S.K. Pabi, S. Ghosh*

Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Kharagpur 721302, India

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ABSTRACT

Nanofluids often exhibit significantly higher thermal conductivity compared to the base fluid. Contributions of the phononic and electronic thermal transport between a heat source and frequently colliding nanoparticles to the enhanced thermal conductivity have been investigated for the first time, through multi-scale modeling. Classical molecular dynamics (MD) model has been used to estimate the phononic component of thermal transport from the heat source to colliding nanoparticles. A meso-continuum model has been used to estimate the same as well as the thermal transport from heat source to colliding nanoparticle due to the combined effect of phononic and electronic mechanisms. The data on thermal pickup by colliding nanoparticles from the heat source, obtained by rationally combining the predictions of MD and meso-continuum approach, have been fed to a higher length scale stochastic model to estimate the enhancement in the conductivity. The stochastic model keeps track of Brownian movement of nanoparticles within the base fluid and the convective heat dissipation of the absorbed thermal energy of the nanoparticles to the surrounding fluid. The present multi-scale model estimates 74% thermal conductivity enhancement in water-based silver nanofluid (0.1 vol%) having nanoparticles in the size range of 4–30 nm, and the results are in reasonable agreement with the experimental results reported in the literatures.

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1. Introduction

Significant enhancement in the thermal conductivity of the nanofluids due to the addition of small amount (<1 vol%) of nanoparticles has been reported by several researchers [1–6]. The thermal conductivity enhancement in nanofluids has been studied with nanoparticle dispersoids of ceramics [7,8], metals [9,10], intermetallics [11], carbon nanotubes [12], etc. The thermal conductivity enhancement of nanofluids depends on the different parameters like volume fraction, particle material, particle size, particle shape, temperature, base fluid, pH of nanofluid, and additives [13]. The rapid increase in the number of publications on nanofluids research is provoked by its potential heat transfer applications. Even though there are plenty of literatures available on nanofluids research, the lack of agreement in the experimental results published by different researchers still persists. The mismatch between the theoretical estimations and experimental values demands a better insight into the heat transfer mechanisms in nanofluids.

In the conventional continuum models such as Maxwell’s model, Hamilton–Crosser model, etc. do not include the effect of particle size and particle’s motion within the fluid [14]. These macroscopic models give a reasonably good prediction of thermal conductivity of slurries containing millimeter or micrometer-sized particles, but they underestimate the thermal conductivity of fluids containing nanoparticles. Several theoretical models based on different mechanisms have been analyzed in literatures to explain the thermal conductivity enhancement in the nanofluids [15–20]. The main mechanisms of heat transfer in nanofluids are Brownian motion of nanoparticles in the base liquid, ordered layering of liquid molecules at the liquid–particle interface, ballistic nature of heat transport in nanoparticle, and nanoparticle clustering [21]. Molecular level simulations have also been carried out to explain the mechanism for enhanced thermal transport in nanofluids [21]. Sarkar et al. [22] and Teng et al. [23] have used the MD simulations to estimate the nanofluids thermal conductivity enhancement, but they considered non-conventional Ar as base fluid for dispersing Cu nanoparticles. Only few MD studies have been reported for conventional nanofluids such as water–Pt [24], water–Ag [25] and ethylene glycol–Cu [26]. The heat transfer in MD is characterized only by atom vibrations (phonon heat transfer), hence the pure MD cannot account for electron movements, which plays a dominant role in the thermal conductivity enhancement.
role in heat transfer through metals. Therefore, pure MD simulations alone cannot explain the thermal transport mechanism in metallic nanofluids. Various theoretical and experimental works on nanofluids published over a past decade have been critically reviewed by different group of researchers [27–31]. All of them have concluded that the different mechanisms and models considered by them are not able to fully account for the experimental enhancement in thermal conductivity of nanofluids.

Ghosh et al. [32,33] have recently reported a new coupled atomistic-stochastic model to estimate the enhancement in the thermal transport of nanofluids based on collision induced phononic heat transfer mechanism. Their model suggests that the heat transfer during frequent collision of nanoparticles with the heat source due to Brownian motion of particles in nanofluids followed by dissipation of acquired heat by the nanoparticles during its Brownian motion to the surrounding fluid gives a significant contribution to the thermal conductivity enhancement. But their model ignores the heat transfer through electron movements during the collision. Further, the model considers mono-size particle dispersion in the base fluid. Shortfalls in that model have been overcome by the present multi-scale model, which incorporates the heat transfer due to movement of electrons with help of an additional meso-continuum model. The enhancement in the thermal conductivity of the nanofluids has been calculated for different particle sizes and their weighted average has been taken as the effective thermal conductivity enhancement of nanofluid. This approach has been used to estimate the thermal conductivity enhancement of water-based 0.1 vol% silver nanofluids.

2. Theoretical modeling

Heat pickup by a colliding nanoparticle within the nanofluid from the adjacent heat source has been estimated using both MD and meso-continuum approaches. MD simulation is required to capture the phonon transfer between the wall and nanoparticle as the transfer is characterized by fluctuations of kinetic energy with respect to space (nano-scale) and time. At the nano-scale the meso-continuum approach cannot reveal these features. The electronic component of the heat transfer between nanoparticle and wall has been estimated by carrying out two meso-continuum simulations, i.e., (i) assuming the nanoparticle conductivity to be phononic thermal conductivity and (ii) assuming the bulk thermal conductivity (i.e. conductivity due to both phonon and electron movement). Comparing the thermal pickup in the two cases gives an estimate of the contribution of the heat transfer due to movement of electrons. The ratio of the thermal pickup by assuming the actual conductivity to that assuming only the phononic conductivity \( R = \Delta T_{\text{total}} / \Delta T_{\text{ph}} \) has been multiplied to the heat pickup estimated by the MD simulation to get an accurate estimate of the thermal pickup. The estimated heat pickup by nanoparticle of different sizes, pre-collision temperatures and collision speed has been fed to the stochastic simulation to estimate the thermal conductivity of the nanofluids. Fig. 1 shows the pictorial representation of the different length and time scales used in the present multi-scale model. Water-based silver nanofluid in contact with silver heat source has been considered for the present study. Nanoparticles have been assumed to be spherical in shape and the heat source has been taken as a rectangular block.

2.1. Molecular dynamics model

MD simulations have been performed on LAMMPS platform [34] and post-processed for visualization using VMD software package [35]. Silver nanoparticles of different sizes have been made to collide with the heat source. Fig. 2 shows the heat source and nanoparticle configuration prior to the collision. Average collision velocities for particle of different sizes have been estimated from stochastic simulation. Before collision, the heat source has been equilibrated at 370 K, and nanoparticles have been equilibrated at four different temperatures viz. 298 K, 313 K, 333 K and 353 K. The Berendsen thermostat [36] has been used to rescale the velocities at every time step. The heat source and nanoparticles have been equilibrated for 10 ps. All equilibration simulations have been carried out using NVE ensemble with periodic boundary conditions, whereas collisions have been simulated with non-periodic boundary condition in the colliding direction. Particle temperature at every time step during the collision has been computed from the computed phase space.

2.1.1. Phase space evolution

Newton’s equations of motion have been integrated using velocity-verlet algorithm to calculate the position and velocity of any atom at a time increment of \( \Delta t \) from the known position and velocity at time \( t \), based on the following equations:

\[
\begin{align*}
\text{position: } & \quad \mathbf{r}_{n+1}(t) = \mathbf{r}_n(t) + \mathbf{v}_n(t) \Delta t + \frac{1}{2} \mathbf{a}_n(t) \Delta t^2 \\
\text{velocity: } & \quad \mathbf{v}_{n+1}(t) = \mathbf{v}_n(t) + \mathbf{a}_n(t) \Delta t
\end{align*}
\]
The contact area has been estimated from the impact dynamics configuration prior to collision. Table 2 shows the number of atoms and by averaging the temperature of all grid points lying within the temperature of the particle after the collision has been calculated used in meso-continuum approach are given in the Table 1. The material properties used in meso-continuum simulation [39,40]. Table 1

<table>
<thead>
<tr>
<th>Physical properties</th>
<th>Silver</th>
</tr>
</thead>
<tbody>
<tr>
<td>Phononic thermal conductivity</td>
<td>7.7</td>
</tr>
<tr>
<td>Bulk thermal conductivity</td>
<td>428</td>
</tr>
<tr>
<td>Density</td>
<td>10.5</td>
</tr>
<tr>
<td>Specific heat capacity</td>
<td>235</td>
</tr>
</tbody>
</table>

The stochastic model considers that the spherical nanoparticles suspended in a water-based nanofluid undergo Brownian motion, i.e., move randomly in the base fluid and repeatedly collide with a heat source (wall). The frequency of the collision depends on the
parameters like temperature and viscosity of the base fluid, size of the nanoparticle, etc. The nanoparticles will continuously exchange heat with the base fluid via convective mechanism depending on the temperature difference between the moving nanoparticle and the surrounding base fluid, and the velocity of the particle relative to the base fluid. During the collision of these particles with the heat source conductive heat transfer takes place from the heat source to the nanoparticles [33,41,42]. The Brownian stochastic model evaluates the trajectory and temperature history of the nanoparticles undergoing Brownian motion in water.

### 2.3.1. Average collision velocity and collision period

The Brownian stochastic model predicts the phase space evolution of a nanoparticle based on the following relationship [33,41,42]:

\[
p(x_0, t) = \frac{1}{\sqrt{2\pi \sigma^2(t)}} \exp \left\{ -\frac{(x - m(t))^2}{2\sigma^2(t)} \right\}
\]

where, \( p(x_0, t) \) is the probability density function for the \( x \)-component of velocity \( (u_x) \) of the nanoparticle, \( x_0 \) is the initial velocity component along \( x \)-direction, \( m(t) \) and \( \sigma^2(t) \) are the mean and variance of the distribution of \( x \)-component of the velocity, respectively. These are exponential functions of time \( t \), as follows:

\[
m_x(t) = e^{-\beta t} u_{0, x}
\]

and

\[
\sigma^2_x(t) = \frac{\sigma^2_0(t)}{2\beta} \left( 1 - e^{-2\beta t} \right)
\]

where, \( \sigma^2_0(t) \) is given by:

\[
\sigma^2_0(t) = \frac{2\beta k_B T}{M}
\]

where, \( M \) is the mass of the nanoparticle, \( T \) is the absolute temperature, \( \beta \) is a constant with dimensions of frequency, and \( k_B \) is the Boltzmann constant. \( \beta \) can be expressed as:

\[
\beta = \frac{6\pi \eta r_{np}}{M}
\]

where, \( \eta \) is the dynamic viscosity of the fluid medium (water), \( r_{np} \) is the nanoparticle radius.

The period of collision (\( \Delta t_c \)) for spherical nanoparticles has been calculated from the impact dynamics [38] as:

\[
\Delta t_c = \frac{2.94}{V_{coll}} r_{np}
\]

where,

\[
\zeta = \left[ \frac{5}{2} \pi^2 \rho \mu^2 \right]^{2/5}
\]

and

\[
\omega = \frac{1 - \mu^2}{4E}
\]

where, \( \mu \) is the Poisson’s ratio and \( E \) is the Young’s modulus. Apart from size and velocity, the collision period depends on the physical properties of nanoparticles, like Young’s modulus, density and Poisson ratio.

### 2.3.2. Tracking the temperature of nanoparticle during the Brownian motion

Based on the evolution of phase space, the variation of average particle temperature with time has been estimated by considering the following.

- In course of the Brownian motion when the nanoparticles collide with the heat source they extract thermal energy from the heat source.
- The collision induced heat transfer between the particles has not been considered, because the volume fraction of the nanoparticles in nanofluids is usually much smaller than 1%.
- Convective heat transfer takes place between the nanoparticles and the base fluid when the particles move in the fluid after the collision.

The convective heat transfer between the nanoparticle and the surrounding base fluid is described as follows. For the flow past a spherical nanoparticle in a fluid, the Nusselt number (\( Nu \)) can be approximated as [43,44]:

\[
Nu = Re^2 Pr^2
\]

where, \( Re \) is the Reynolds number and \( Pr \) is the Prandtl number. Using the Nusselt number the heat transfer coefficient can be calculated as:

\[
h = \frac{k_r}{d_{np}} Re^2 Pr^2
\]

where, \( k_r \) is the thermal conductivity of the base fluid, and \( d_{np} \) is the nanoparticle diameter. The Reynolds number can be expressed as:

\[
Re = \frac{V_{np} d_{np}}{\gamma}
\]

where, \( V_{np} \) is the velocity of the nanoparticle, \( \gamma \) is the kinematic viscosity of the medium. The nanoparticles velocity has been calculated as \( \sqrt{\nu_x^2 + \nu_y^2 + \nu_z^2} \), where the velocity components have been estimated from Brownian stochastic model. The heat transfer coefficient of any nanoparticle at any position in the liquid medium can be estimated from knowledge of flow past a sphere, which in turn yields the temperature variation of that nanoparticle with time in course of its Brownian movement as:

\[
\frac{dT_{np}}{dt} = \frac{1}{M C_{p, np}} \frac{dQ}{dt}
\]

where, \( T_{np} \) is the temperature of the nanoparticle, \( M \) is the mass of the nanoparticle, \( C_{p, np} \) is the specific heat of the constituent of nanoparticle, \( Q \) is the heat exchange between the nanoparticle and the fluid, \( t \) is the time. The rate of heat exchange between the nanoparticle and the fluid (water) is expressed as:
\[
\frac{dQ}{dt} = 4\pi r_{np}^2 h(T_{np} - T_w)
\]  
(17)

where, \(T_w\) is the temperature of the water medium, which depends on the location, i.e., the distance from the heat source. In order to incorporate the variation in \(T_w\) a thermal boundary layer in the base fluid having thickness (\(\delta_T\)) has been considered, which is given by

\[
\delta_T = \frac{6L}{(G_{RL})^{1/4}}
\]  
(18)

where, \(L\) is the length of heat source and \(G_{RL}\) is the Grashof number which is given as:

\[
G_{RL} = \frac{g\alpha\Delta T L^3}{\nu^2}
\]  
(19)

here, \(g\) is the acceleration due to gravity, \(\alpha\) is the volume expansion coefficient of water medium and \(\Delta T\) is the temperature difference between the heat source and the bulk fluid. The estimated thickness of the thermal boundary layer is found to be approx. 1 mm for the system.

When the particle strikes the heat source, it rebounds in accordance with the laws of impact dynamics. The thermal pickup by the nanoparticle during collisions has been estimated in stochastic simulation using linear expression, which has been generated from both MD and meso-continuum simulations. The ratio of the thermal pickup by assuming the actual conductivity (i.e. phononic plus electronic conductivity) to that assuming only the phononic conductivity obtained from meso-continuum simulation has been fed into the stochastic model to account the electronic part of heat transfer during the collision. The timestep chosen in this stochastic simulation is 10\(^{-5}\) s [33]. In the present model, collision occurring within a total time frame of 1 s has been taken into consideration for assessing the contribution of collisions to the enhanced thermal conductivity of the nanofluid. Further increase in this time frame up to 10 s is found to have negligible influence on the output.

### 2.3.3. Estimation of thermal conductivity enhancement of nanofluids

The thermal conductivity enhancement of nanofluids based on collision induced heat transfer mechanism can be estimated by the ratio of the heat transfer due to collision alone to the convective heat transfer through the fluid without particles. Heat transferred per unit time due to collision \((q_{coll})\) has been calculated as [33]:

\[
q_{coll} = fN H_{coll,avg}
\]  
(20)

where, \(f\) is the collision frequency of the nanoparticle, \(N\) is the number of nanoparticle in the volume element for the given volume fraction, and \(H_{coll,avg}\) is the average heat transfer per collision. Heat transfer per unit time has been calculated as:

\[
H_{coll} = M C_{p, np} \Delta T,
\]  
(21)

where, \(\Delta T\) is the change in the temperature of the nanoparticles before and after collision. Heat transfer per each collision has been evaluated in the stochastic model and averaged to obtain \(H_{coll,avg}\).

The heat transfer per unit time through the liquid boundary layer, which contain no particles has been estimated as:

\[
q_{fluid} = \frac{k_l}{\delta_T} A (T_{hs} - T_{bf})
\]  
(22)

where, \(\delta_T\) is the thermal boundary layer thickness, \(A\) is the area of the heat source in contact with the volume element, \(T_{hs}\) is the temperature of the heat source, \(T_{bf}\) is the temperature of the bulk fluid (beyond the thermal boundary layer). The percentage enhancement in the thermal conductivity of nanofluids due to the presence of nanoparticles has been estimated by [33]:

\[
\text{Enhancement} = \frac{q_{coll}}{q_{fluid}} \times 100\%
\]  
(23)

### 3. Results and discussions

Stochastic simulation has been carried out to estimate the average collision velocity of silver nanoparticles of different sizes. Fig. 4 shows the variation of a collision velocity and collision period with particle size. Collision period (i.e. contact time) increases with increasing particle size, whereas the collision velocity decreases due to larger size and mass. The asymptotic behavior of collision velocity follows from the Brownian stochastic model. It can be seen from Eqs. (9) and (6) that the mean velocity exponentially decreases with increasing particle diameter. Eq. (10) explains the linear behavior of collision period with particle size.

MD simulations have been carried out for different sizes of nanoparticles, viz. 4, 5, 6, 7, 8, 9, 10, 11, 13, 14, and 15 nm with four pre-collision temperatures, viz. 298 K, 313 K, 333 K, and 353 K. As stated previously, during the MD simulation the pre-collision velocity imposed on the nanoparticle has been estimated from stochastic simulation.

Fig. 5 shows the temperature profile of 10 nm particle and heat source, during the collision, where the particle pre-collision temperature is 298 K. Temperature of the particles after collisions has been found from the MD simulation and linear expressions of thermal pickup in the nanoparticles due to collision have been generated. Fig. 6 shows the plot between post-collision and pre-collision temperature with linear fit equation of thermal pickup for 10 nm particle collision. Similarly, expressions for nanoparticle thermal pickup due to collision have been established for all particle sizes. Fig. 7 shows the thermal pickup by the particle during collision due to phononic heat transfer, as estimated from the MD simulation. These atomistic computations cost about 2–108 h in Windows XP machine (Intel\textsuperscript{®} Core\textsuperscript{TM} Quad CPU, 2.66 GHz, 2.99 GB RAM) depending on the size of the domain and collision period.

Meso-continuum simulations have been carried out for particle sizes ranging from 4 nm to 40 nm by assuming (i) the conductivity...
to be bulk thermal conductivity and (ii) the conductivity to be equal to the phonon conductivity. The grid interval size of 0.01 has been chosen after carrying out the grid independent test with grid sizes varying between 0.05, 0.025, 0.01 and 0.0075. Fig. 8 shows the temperature profile of the heat source and the nanoparticle (size: 25 nm, initial temperature: 298 K) after collision by assuming the conductivity to be phononic conductivity. The meso-continuum simulations took 1–65 h for completion, depending on the size and collision period. The temperature rise in the nanoparticles estimated from meso-continuum simulation by assuming phononic thermal conductivity and actual thermal conductivity has been shown in Fig. 9.

The time required for nanoparticles to approach the heat source temperature has been given in Table 3 and 4. When both electronic and phononic contributions are considered, the nanoparticle temperature approaches the heat source during the course of collision itself (Table 4). For the bigger size particles phonon transfer is insufficient to attain equilibrium with the heat source during the collision period.

The ratio of temperature rise predicted by MD simulation to that of predicted by meso-continuum approach \( R = \Delta T_{\text{ph}} (\text{MD}) / \Delta T_{\text{ph}} (\text{Meso-continuum}) \) has been listed in Table 5. The ratio suggests that for lower particle size the thermal pickups predicted from MD simulation are significantly larger than those predicted by the meso-continuum approach. However, with increase in the particle size the prediction of the meso-continuum simulation approaches that of the more rigorous MD simulation (i.e. \( R \approx 1.0 \)). At higher pre-collision temperatures, the MD temperature rise predictions are higher than the meso-continuum predictions (Table 5). MD simulations have been carried out for larger particle size (20 nm) at high pre-collision temperatures (333 K and 353 K) and it has been found that the \( R \) values are 1.04 and 1.33 (approaching to 1.0). Since the ratio \( R \) is approaching 1.0, the computationally intensive MD simulations are not necessary for particle sizes significantly higher than 20 nm.
The ratio of the temperature rise in the nanoparticle due to total thermal conductivity to the temperature rise due to phononic thermal conductivity \( R = \frac{\Delta T_{\text{total}}}{\Delta T_{\text{ph}}} \), estimated by meso-continuum simulation has been used to estimate the actual thermal pickup by the colliding nanoparticles. Fig. 10 shows the variation in the ratio with the diameter of nanoparticle. For lower particle sizes the phonon heat transfer was sufficient to raise the temperature of the particle to that of heat source.

The percentage enhancement in the heat transfer rate (i.e. thermal conductivity enhancement) of base fluid due to the presence of nanoparticles has been estimated from the stochastic simulation, as explained previously. Fig. 11 shows the percentage enhancement in the thermal conductivity of base fluid due to the presence of nanoparticles of different sizes. Fig. 12 shows the contributions of phononic and electronic thermal transport to the thermal conductivity enhancement for bigger size particles. The phononic enhancement has been obtained from stochastic model by coupling MD simulation results alone. The electronic contribution further improves the enhancement for bigger particles (Fig. 12). Even though the bigger size particles have good amount of contribution from electronic thermal transport, they show low percentage of enhancement than the smaller particles because of lesser number of particles per unit volume, leading to lesser number of collisions.

Synthesis of the nanoparticles with unique size is not possible in experiments; always it will be a mixture of different sized nanoparticles. By considering this fact an arbitrary size distribution has been generated for nano fluids having 1 vol.% of nanoparticles, which is shown in Fig. 13.

Table 3
Collision period and time to reach equilibrium temperature vs. particle size for combined electronic and phononic contribution.

<table>
<thead>
<tr>
<th>Size (nm)</th>
<th>Time required for equilibrium (ps)</th>
<th>Collision period (ps)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>23</td>
<td>23</td>
</tr>
<tr>
<td>10</td>
<td>86</td>
<td>86</td>
</tr>
<tr>
<td>15</td>
<td>94</td>
<td>94</td>
</tr>
<tr>
<td>20</td>
<td>135</td>
<td>135</td>
</tr>
<tr>
<td>25</td>
<td>183</td>
<td>183</td>
</tr>
<tr>
<td>30</td>
<td>226</td>
<td>226</td>
</tr>
</tbody>
</table>

Table 4
Collision period and time to reach equilibrium temperature vs. particle size for only phononic heat transfer.

<table>
<thead>
<tr>
<th>Size (nm)</th>
<th>Time required for equilibrium (ps)</th>
<th>Collision period (ps)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2.5</td>
<td>17</td>
</tr>
<tr>
<td>5</td>
<td>4.5</td>
<td>23</td>
</tr>
<tr>
<td>6</td>
<td>10</td>
<td>29</td>
</tr>
<tr>
<td>7</td>
<td>11</td>
<td>36</td>
</tr>
<tr>
<td>8</td>
<td>23</td>
<td>42</td>
</tr>
</tbody>
</table>

Table 5
The ratio of temperature rise \( R_1 \) predicted by MD to that of predicted by meso-continuum approach.

<table>
<thead>
<tr>
<th>Particle size (nm)</th>
<th>298 K</th>
<th>313 K</th>
<th>333 K</th>
<th>353 K</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>2.43</td>
<td>2.63</td>
<td>4.43</td>
<td>9.45</td>
</tr>
<tr>
<td>5</td>
<td>2.43</td>
<td>3.01</td>
<td>3.81</td>
<td>7.62</td>
</tr>
<tr>
<td>7</td>
<td>1.89</td>
<td>2.07</td>
<td>3.14</td>
<td>6.11</td>
</tr>
<tr>
<td>8</td>
<td>1.96</td>
<td>1.98</td>
<td>2.79</td>
<td>6.65</td>
</tr>
<tr>
<td>10</td>
<td>1.44</td>
<td>1.64</td>
<td>1.97</td>
<td>3.42</td>
</tr>
<tr>
<td>15</td>
<td>1.09</td>
<td>1.28</td>
<td>1.48</td>
<td>1.70</td>
</tr>
</tbody>
</table>

Fig. 9. Temperature rise vs. particle size at different pre-collision temperature estimated from meso-continuum simulations: (a) phononic thermal conductivity and (b) total thermal conductivity.

Fig. 10. Variation of ratio \( R_1 \) with particle size at 298 K estimated from meso-continuum approach.

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The percentage enhancement in the thermal conductivity of the present fluid due to the presence of 0.1 vol.% silver nanoparticles of above chosen particle size distribution has been estimated as:

\[
\text{Total enhancement} = \sum_i \phi_i E_i
\]

where, \(i\) is the particle size, \(\phi_i\) is the volume fraction of the particle size \(i\) and \(E_i\) is the percentage enhancement in the base fluid due to the presence of 0.1 vol% of \(i\) sized particles. From this equation, the total enhancement in the thermal conductivity of water-based 0.1 vol% silver nanofluids has been estimated as 73.9%. The order of magnitude matched well with the experimentally reported ones [6,11]. The particle size distribution has significant effect on total thermal conductivity enhancement, a narrow size distribution at lower particle size will result in higher enhancement. The enhancement value estimated by the present model is much higher than the value predicted by Maxwell’s model and proves that the frequent collision of nanoparticles with heat source plays the key role in the enhancement of thermal conductivity.

4. Conclusions

1. A multi-scale model for estimating the enhancement in the thermal conductivity of fluids due to the addition of nanoparticles has been developed. The nano-scale heat exchange between a nanoparticle and heat source has been modeled using both MD simulations as well as meso-continuum approach. At a higher length scale, where large numbers of nanoparticles are moving in a fluid and frequently colliding with the heat source, a stochastic model described the movement and the thermal state of the nanoparticles.
2. For particles sizes less than or equal to 15 nm, phononic contribution to the thermal pickup has been estimated using MD simulation as well as meso-continuum approach.
3. For particle sizes greater than 15 nm, thermal pickup by the particle has been estimated by meso-continuum approach only.
4. For lower particle sizes (<10 nm) the prediction of thermal pickup due to phonon transfer made by MD simulation was significantly higher than that predicted by the meso-continuum approach. However, with increase in the particle size the prediction of the meso-continuum simulation approaches that of the atomistic simulation.
5. For nanoparticles having sizes greater than 30 nm, the thermal pickup is not appreciable if the electronic movement is not taken into account.
6. Meso-continuum approach has been used to estimate the ratio of thermal pickup by combined phononic and electronic mechanisms to that by phononic mechanism only. By multiplying this ratio with the thermal pickup due to phonon transfer as computed by the MD approach, the thermal pickup by the nanoparticle during collision has been estimated and fed to the stochastic model for prediction of enhancement in thermal conductivity.
7. The present model predicts that the 0.1 vol% addition of silver nanoparticles in the size range of 4–30 nm to the water enhances the thermal conductivity of water by 74%.
8. Eventhough, the bigger particles have longer collision time and good extent of contribution from electronic part of heat transfer, their contribution in enhancement has been limited by the lesser number of particles per unit volume.
References


