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CFD MODELING OF NATURAL CONVECTION HEAT TRANSFER OF TIO_2-WATER NANOFLUID IN A CYLINDRICAL CONTAINER

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ABSTRACT

This work focuses on numerical validation of natural convection heat transfer of TiO_2-water nanofluids in a cylindrical container using COMSOL. The main aim of this study is to examine different available approaches to calculate effective thermal conductivity and compare them with experimental data available in the literature. Simulation results show that for considered mixture, average Nusselt number decreases by increasing Rayleigh number and particle volume fraction. It has been found that only one model was able to represent similar trends for given particle volume fractions, compared to experimental results.

Keywords: *Nanofluids, Natural convection, Heat transfer, Rayleigh-Bénard problem, Numerical simulation*

1. INTRODUCTION

Natural convection has been widely used in engineering applications such as cooling electronic devices and heat exchangers. In recent years, nanofluids, dispersions of nano-size particles in a base fluid, have been introduced as an innovative way to improve heat transfer rate. It has been observed that adding alumina and copper nanoparticles to water leads to an increase in heat transfer coefficient (Abu-Nada and Oztop, 2009; Gutierrez, 2008; Jang and Choi, 2004; Philip *et al.*, 2008). These observations have attracted the attention of many researchers to study about the effects of nanofluids and their applications in industrial scale.

However, some publications have reported paradoxical results in buoyancy-induced flows. For example, Putra et al. (2003) studied natural convection in a horizontal cylinder using water-based Al_2O_3 and CuO nanofluids. They found that Nusselt number of nanofluids was lower than that for base fluids. Wen and Ding (2005) reported a deterioration in heat transfer coefficient in a system combining of two horizontal discs separated by a gap using TiO_2-water nanofluids. Ho et al. (2010) investigated heat transfer rate in a square enclosure filled with Al_2O_3-water nanofluids experimentally. Comparing various volume fractions of nanoparticles in different test cells, they reported diminutions up to 30% in average Nusselt number. According to an observation by Li and Peterson (2010), the same trend was observed for Al_2O_3-water nanofluids in a cylindrical test cell considering volumetric fractions up to 6%.

Thermal conductivity, viscosity and density of nanofluids are the properties that affect fluid convection in an enclosure. According to separate experimental observations by Pak and Cho (1998), Ho *et al.* (2010) and Zhou and Ni (2008), thermal conductivity increases by an increase in temperature while viscosity and density decrease. In addition, an increase in volume fraction of nanoparticles leads to a reduction in heat capacity while increases density, thermal conductivity and viscosity.

Haddad *et al.* (2012) and Khanafer and Vafai (2011) published separately comprehensive reviews on the research progress on natural convection of nanofluids discussing different mathematical models as well as experimental correlations used to calculate thermo-physical properties of nanofluids. It seems that the problem of bottom-heated container is still an unsolved issue and computing thermo-physical properties of nanofluids is still challenging.

In the present work, the effects of adding TiO_2 nanoparticles to water in a vertical cylindrical cell, heated from below (Rayleigh-Bénard natural convection), is numerically investigated. First, various mathematical correlations are compared to show the effect of nanoparticle fraction on the evolution of thermo-physical properties. Then, heat transfer rate, in terms of Nusselt number, is investigated for different Rayleigh numbers and two nanoparticle concentrations. Contrary to common belief, some experimental observations have reported a decrease in Nusselt number by increasing nanoparticle concentration and the final aim of this work is to examine this statement for TiO_2 nanoparticles by comparing gathered numerical results with experimental data in the literature.

2. PHYSICAL PROPERTIES OF NANOFLUIDS

To calculate the heat transfer coefficient in this work, nanofluid is treated as a single phase mixture. Thermo-physical properties of the base fluid and TiO_2 nanoparticles are shown in Table 1.

Table 1 Thermo-physical properties of base fluid and nanoparticles (Bianco *et al.*, 2015)

Material	Dynamic viscosity (kg/(m.s))	Density (kg/m^3)	Heat capacity (J/kg.K)	Thermal conductivity (W/(m.K))
Water	9.93×10^{-4}	998.2	4182	0.597
TiO_2	-	4175	692	8.4

2.1 Thermal Conductivity

Four different theoretical models are used to calculate effective thermal conductivity of the nanofluid. These models are shown separately in Table 2.

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2.2 Density

The density of the mixture is expressed as a linear average of density of base fluid and density of nanoparticles as given in Eq. 1.

$$\rho_{nf} = (1-\varphi)\,\rho_{bf} + \varphi\,\rho_p \quad (1)$$

Eq. 1 illustrates that the density of mixture increases with an increase in volume fraction of nanoparticles for nanoparticles with higher densities than the base fluid.

Table 2 Various thermal conductivity models for nanofluids

Thermal conductivity models	Expressions for $\frac{k_{eff}}{k_{bf}}$
(Maxwell, 1881)	$\frac{k_p + 2k_{bf} - 2\varphi(k_p - k_{bf})}{k_p + 2k_{bf} + \varphi(k_p - k_{bf})}$
Curve fitting of (Pak and Cho, 1998)	$1 + 2.92\varphi - 11.99\varphi^2$
(Bruggeman, 1935)	$\frac{(3\varphi-1)\frac{k_p}{k_{bf}} + \{3(1-\varphi)-1\} + \sqrt{\Delta}}{4}$ where $\Delta = \left[(3\varphi-1)\frac{k_p}{k_{bf}} + \{3(1-\varphi)-1\}\right]^2 + 8\frac{k_p}{k_{bf}}$
(Yu and Choi, 2003)	$\frac{k_p + 2k_{bf} + 2\varphi(k_p - k_{bf})(1+\beta)^3}{k_p + 2k_{bf} - \varphi(k_p - k_{bf})(1+\beta)^3}$

2.3 Heat Capacity

The same linear average approach can be used to calculate specific heat capacity of nanofluid (Eq. 2). However, a study by Zhou and Ni (2008) showed that Eq. 3 is more accurate compared to experimental data for Al_2O_3-water nanofluid. In this work, the second expression is assumed to be valid for TiO_2-water nanofluid as well.

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

$$C_{p,nf} = \frac{(1-\varphi)\,\rho_{bf}\,C_{p,bf} + \varphi\,\rho_p\,C_{p,p}}{\rho_{nf}} \quad (3)$$

2.4 Dynamic Viscosity

Although the viscosity of the nanofluid increases with the increase in the volume fraction of nanoparticles, there are few published results to validate available models for TiO_2-water mixture. Three different models are compared to predict the viscosity of the mixture. These models are shown in Table 3.

Table 3 Various dynamic viscosity models for nanofluids

Dynamic viscosity models	Expressions
(Einstein, 2005)	$\frac{\mu_{eff}}{\mu_{bf}} = 1 + 2.5\varphi$
(Brinkman, 1952)	$\frac{\mu_{eff}}{\mu_{bf}} = \frac{1}{(1-\varphi)^{2.5}}$
Curve fitting of (Pak and Cho, 1998)	$\frac{\mu_{eff}}{\mu_{bf}} = 1 + 5.45\varphi + 108.2\varphi^2$

2.5 Thermal Expansion Coefficient

In the present work, the thermal expansion coefficient is considered to be independent of concentration of nanoparticles. However its dependency on temperature of the base fluid is considered and is tabulated in Table 4.

3. COMPUTATIONAL MODEL

The geometry and grid were generated using COMSOL 4.4. 2D computational domain is shown in Fig 1. Upper boundary is considered as cold wall; right wall is assumed to be adiabatic and bottom wall to be at constant heat flux condition. Left wall in the domain is assumed axisymmetric. The single phase mixture is considered in thermal equilibrium. It means that the relative velocity between nanoparticles and base fluid is negligible.

Table 4 Thermal expansion coefficient of water for different average temperatures (Rashmi *et al.*, 2011)

Average temperature (K)	Thermal expansion coefficient, α_{nf} (K^{-1})
298.15	0.0002
307.55	0.0003
315.55	0.0004

Governing equations for this model are shown as below in Eq. 4-6.
Continuity equation:

$$\rho_{nf}\,\nabla.u = 0 \quad (4)$$

Momentum equation:

$$\rho_{nf}\,\frac{\partial u}{\partial t} + \rho_{nf}\,(u.\nabla)u = \nabla.\left[-pI + \mu_{nf}\,(\nabla u + (\nabla u)^T)\right] + \rho_{nf}\,\alpha_{nf}\,g\left[T - \tfrac{1}{2}(T_H + T_C)\right] \quad (5)$$

Energy Equation:

$$\rho_{nf}C_{p,nf}\frac{\partial T}{\partial t} + \rho_{nf}C_{p,nf}u.\nabla T = \nabla.(k_{eff}\nabla T) \quad (6)$$

Time-dependent (transient) solver was used to simulate natural convection in the cell. Simulation runs were performed until the volume-averaged Rayleigh number and surface-averaged Nusselt number reached their steady-state values (Each simulation was performed to model about 1200 seconds of heat transfer process in the enclosure.). Numerical iterations were performed until absolute tolerance reached 1×10^{-6}. Simulation results, then, were compared with published experimental data of (Wen and Ding, 2005).

Average Nusselt numbers were calculated using surface-averaged values of heat flux, bottom-wall temperature and thermal conductivity as given in Eq. 7. Volume-averaged Rayleigh numbers were then computed using Eq. 8.

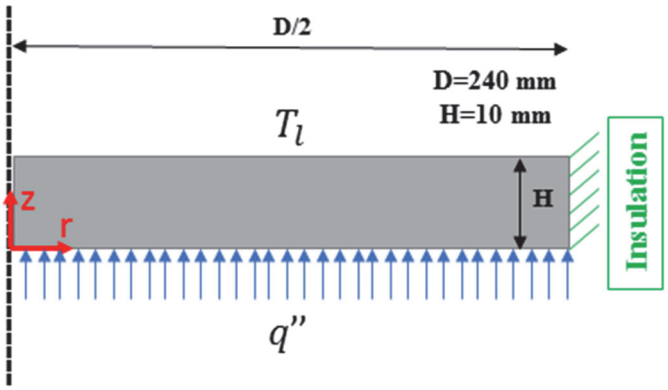

Fig. 1 2D axisymmetric scheme of computational domain

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$$Nu = \frac{q'' H}{(T_H - T_C)\, k_{eff}} \tag{7}$$

$$Ra = \frac{{\rho_{nf}}^2\, C_{p,nf}\, \alpha_{nf}\, g\, (T_H - T_C)\, H^3}{k_{eff}\, \mu_{nf}} \tag{8}$$

4. RESULTS AND DISCUSSION

The first step to create the model was to validate available models for thermal conductivity ratio with published data. A comparison between presented models in Table 2 is shown in Fig. 2. This figure clearly shows that the model of Yu and Choi with $\beta = 0.50$ is in well-agreement with previously reported data. It must be mentioned that β is a property of nanofluid which shows the impact of nanolayer on thermal conductivity of the nanofluid and decreases by increasing particle diameter.

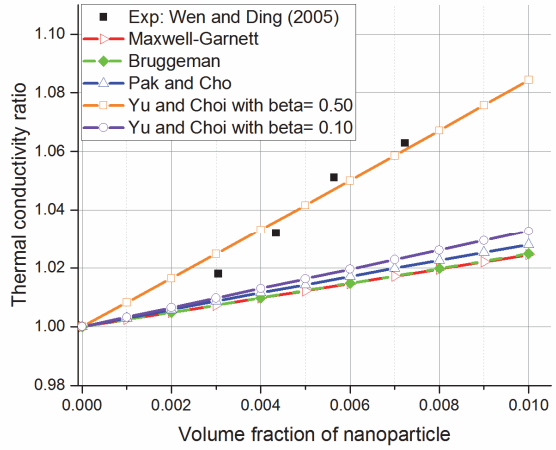

Fig. 2 Comparison between experimental data and different mathematical models for thermal conductivity enhancement ratio of TiO_2-water nanofluid

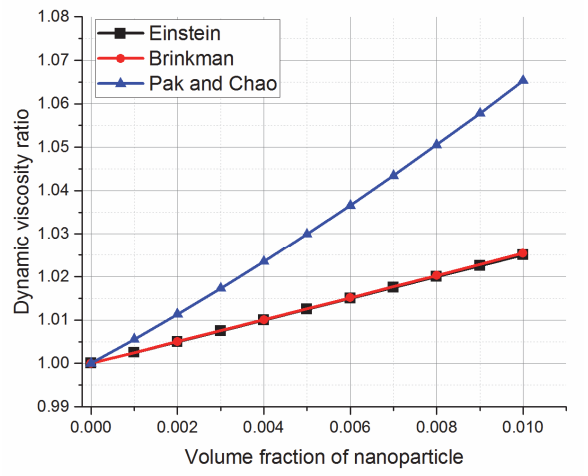

Fig. 3 Comparison between experimental data and different mathematical models for dynamic viscosity enhancement ratio of TiO_2-water nanofluid

In addition, different dynamic viscosity models were compared for the mixture (see Fig. 3). It was found that Einstein model and Brinkman model followed the same trend for given volume fractions. However, since the model of Pak and Cho for viscosity was developed by curve fitting of experimental data for Titania-water nanofluid, this model was taken into account for the rest of this work.

Numerical simulations were performed using different values of heat flux and two different volume fractions of TiO_2 for particles with average size of 170 nm. Numerical results are validated against experimental data for pure water (φ=0.0 % vol.) in Fig. 4.

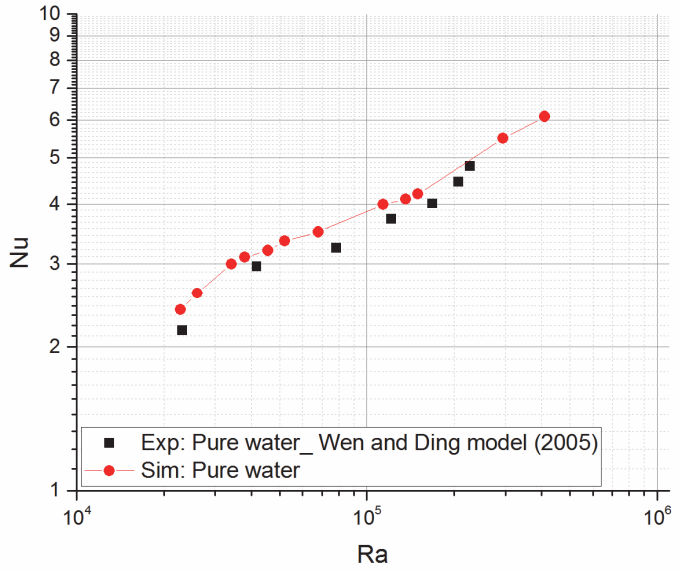

Fig. 4 Comparison between experimental data and simulation results for natural convection of pure water in the container heated from below

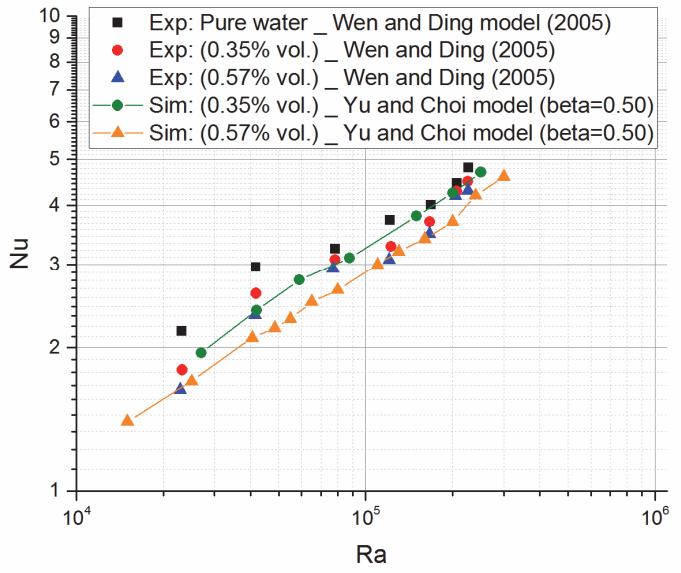

Fig. 5 Comparison between experimental data and simulation results (Implementation of the model of Yu and Choi with β=0.50) for natural convection of nanofluids with two different concentrations

Fig. 5 shows the effect of adding nanoparticles to pure water. This figure compares the numerical results of the model of Yu and Choi with $\beta = 0.50$ for volume fractions of 0.35% and 0.57% with experimental data. In contrast, Fig. 6 clearly illustrate that considering Yu and Choi model for thermal conductivity ratio with $\beta = 0.10$ (A typical value) led to an increase in heat transfer coefficient which was against experimental results.

Conveniently, an increase in volume fraction of nanoparticles leads to a slight increase in thermal conductivity and increases heat transfer rate. This process has been reported by many researchers, as mentioned before. However, a sharp increase in thermal conductivity like the observations of (Wen and Ding, 2005) or (Karthikeyan *et al.*, 2008) may cause a considerable degradation in heat transfer in the cell by reducing average Nusselt number and fluid motion in the enclosure. In other words, it is necessary to predict the correct correlation between thermal conductivity ratio and nanoparticles fraction.

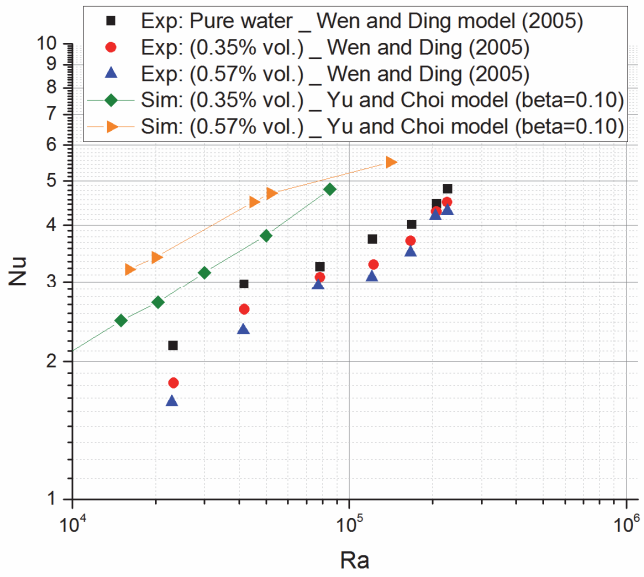

Fig. 6 Comparison between experimental data and simulation results (Implementation of the model of Yu and Choi with β=0.10) for natural convection of nanofluids with two different concentrations

In the present work, the model of Yu and Choi with $\beta = 0.10$, which might be suitable for higher volume fractions and other nano materials, overestimated heat transfer coefficients while altering β to 0.50 led to better heat transfer prediction. For other models of Table 2 like M-G model or Bruggeman model, higher deviations from experimental results are expected since they failed in predicting conductivity ratio.

Figs 7-10 show velocity and temperature profiles for two different heat fluxes ($200\ \frac{W}{m^2}$ and $1000\ \frac{W}{m^2}$) and two different volume fractions (0.35% vol. and 0.57% vol.). Rayleigh-Bénard cells were formed in the enclosure heated from below. Hot layers of fluid rise in the domain reaching the cold upper boundary while cold layers descend due to the density difference between hot and cold layers.

It can be seen that by an increase in heat flux, velocity of nanofluid layers increases. Moreover, velocity at the center of each cell is around zero which means that the fluid in the middle of each Bénard's cell remains stable and hot and cold layers of water circulate around it continuously (Rayleigh-Bénard effect). In addition, comparing Figs 7 and 8 shows that under constant heat flux condition of $200\ W/m^2$, increasing solid volume fraction leads to a decrease in maximum velocity from 0.85 mm/s to 0.79 mm/s. The same trend can be seen by comparing Figs 9 and 10 (from 2.08 mm/s to 1.97 mm/s) for heat flux of $1000\ W/m^2$. This means that increasing Titania nanoparticle fraction decreases natural convection within the enclosure. Maximum velocity was observed where two next raised hot layers or two next descended cold layers encountered each other leading to hot and cold spots in temperature profiles. In other words, there are some spots with constant hot or constant cold temperatures that have the maximum velocity within the enclosure while the center of each cell has the average temperature.

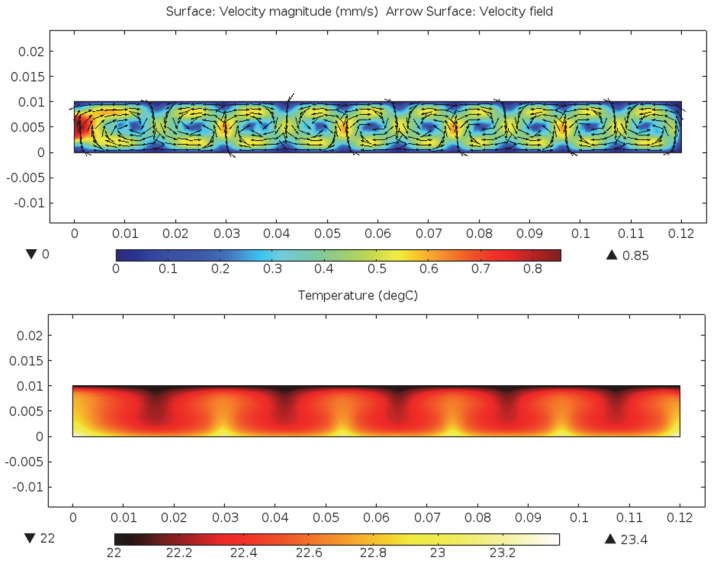

Fig. 7 Steady-state velocity and temperature profiles for 0.35% vol. Titania-water nanofluid ($q'' = 200\ W/m^2$)

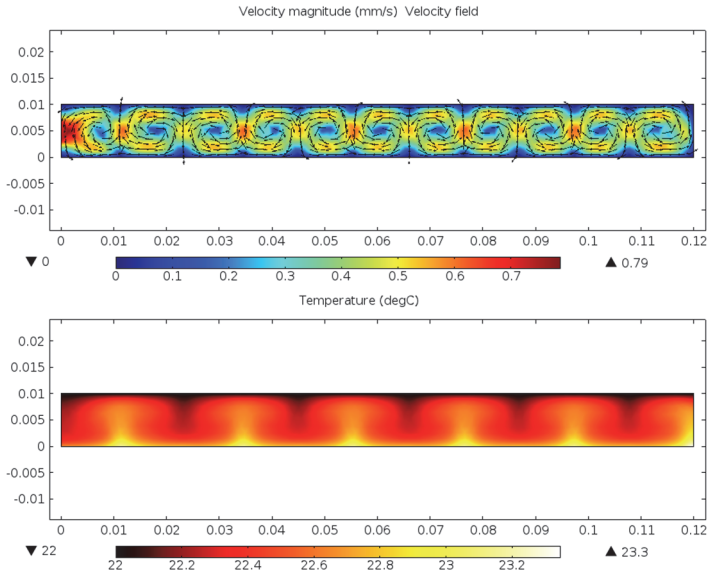

Fig. 8 Steady-state velocity and temperature profiles for 0.57% vol. Titania-water nanofluid ($q'' = 200\ W/m^2$)

5. CONCLUSION

The effect of adding TiO_2 nanoparticles (less than 1% vol.) to pure water was investigated numerically in a vertical cylinder in COMSOL. Different mathematical correlations were compared for dynamic viscosity and thermal conductivity in order to find the most suitable expressions for nanofluids compared to literature findings. It was found that the model presented by Pak and Chao for dynamic viscosity ratio and the modified model of Yu and Choi for thermal conductivity ratio were able to represent experimentally measured thermo physical properties.

Experimental results were compared with simulation results for pure water and water-based nanofluids for two different volume fractions in terms of Nusselt number. By comparing different thermal conductivity ratio correlations, it was found that considering Yu and Choi model with $\beta = 0.50$ led to better predictions of Nusselt number. Nusselt number reduced by increasing Rayleigh number and increasing

nanoparticle volume fraction which was in agreement with experimental findings. Using $\beta = 0.10$ in considered thermal conductivity model overestimated Nusselt number and led to an increase of about 60% in convective heat transfer rate within the enclosure.

Moreover, it was seen that increasing heat flux increased flow circulation in the enclosure for pure water as well as nanofluids while increasing nanoparticle fraction led to a decrease in natural convection within the nanofluid as well as high temperature under constant flux condition. So in accordance with experimental observations, Titania-water nanofluid decreases Rayleigh-Bénard convection in the enclosure.

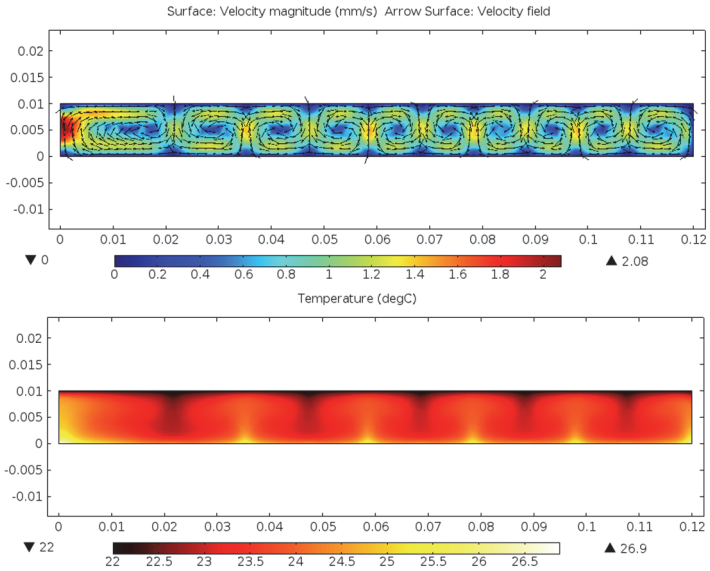

Fig. 9 Steady-state velocity and temperature profiles for 0.35% vol. Titania-water nanofluid ($q'' = 1000\ W/m^2$)

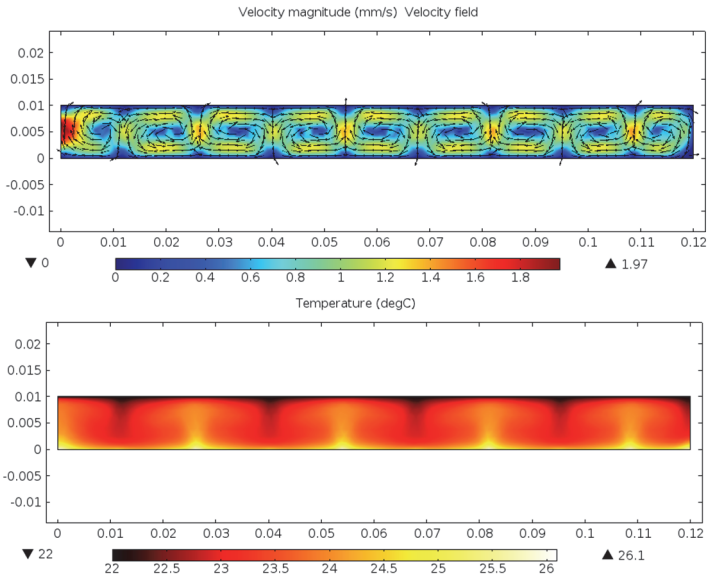

Fig. 10 Steady-state velocity and temperature profiles for 0.57% vol. Titania-water nanofluid ($q'' = 1000\ W/m^2$)

It seems that predicting the correct correlation between thermal conductivity ratio and solid volume fraction has a major contribution in predicting the correct evolutions. More effort must be made in order to introduce better correlations for thermal properties particularly thermal conductivity ratio and dynamic viscosity ratio.

NOMENCLATURE

$C_{p,bf}$	Specific heat of the base fluid (Water) $(\frac{J}{kg.K})$
$C_{p,p}$	Specific heat nanoparticles $(\frac{J}{kg.K})$
$C_{p,nf}$	Specific heat of the nanofluid $(\frac{J}{kg.K})$
D	Diameter of the cylindrical fluid container (m)
g	Acceleration due to gravity $(\frac{m}{s^2})$
H	Height of the cylindrical fluid container (m)
k_{eff}	Effective thermal conductivity $(\frac{W}{m.K})$
k_{bf}	Thermal conductivity of base fluid (Water) $(\frac{W}{m.K})$
k_p	Thermal conductivity of nanoparticles $(\frac{W}{m.K})$
Nu	Average Nusselt number
p	Pressure (Pa)
q'',	Input flux $(\frac{W}{m^2})$
Ra	Average Rayleigh number
T	Nanofluid temperature (K)
T_H	Temperature of hot wall (Lower wall) (K)
T_C	Temperature of cold wall (Upper wall) (K)
u	Velocity $(\frac{m}{s})$
μ_{bf}	Dynamic viscosity of the base fluid (Water) $(\frac{kg}{m.s})$
μ_{nf}	Dynamic viscosity of nanofluid $(\frac{kg}{m.s})$
ρ_{bf}	Density of the base fluid (Water) $(\frac{kg}{m^3})$
ρ_p	Density of nano particles $(\frac{kg}{m^3})$
ρ_{nf}	Density of nanofluid $(\frac{kg}{m^3})$
φ	Volume fraction of nanoparticle
α_{nf}	Thermal expansion coefficient $(\frac{1}{K})$

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