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Research Article

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Numerical investigation of turbulent natural convection in a round bottom flask using a hybrid nanofluid

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Abstract

In this study, we conducted a numerical investigation of the turbulent natural convection of a hybrid nanofluid (HNF) in a flask equipped with an agitator, which is commonly used in organic chemistry synthesis. The bottom wall and the middle section of the flask were maintained at a constant high temperature $T_h$, while the upper, left, and right walls up to the middle of the flask were kept at a low temperature $T_c$. The HNF consisted of Graphene (Gr) and Carbon nanotube (CNT) nanoparticles (NP) dispersed in pure water. The governing equations were solved numerically using the finite size approach and formulated using the Boussinesq approximation. The effects of the NP volume fraction $\phi$ (ranging from 0% to 6%), the Rayleigh number $Ra$ (ranging from $10^4$ to $10^6$), and the Nusselt number were investigated in this simulation. The results indicated that the heat transfer is noticeably influenced by the $Ra$ number and the increase in the $\phi$ ratio. Additionally, the agitator rotation speed had a slight effect on the heat transfer.

Keywords: Turbulent natural convection; Hybrid nanofluids; Numerical simulation; Graphene; Carbon nanotube.

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1. Introduction

Numerous theoretical and experimental studies have focused on the investigation of natural convection in cavities containing nanofluids. (Choi et al. 1995) dispersed titanium oxide (TiO$_2$) nanoparticles in water and observed a 10.7% increase in thermal conductivity at a volume fraction of 4.35%. However, this improvement was significantly less compared to the 32% enhancement achieved for a nanofluid consisting of water and Al$_2$O$_3$ nanoparticles with the same concentration.

Several studies have been conducted on the natural convection of nanofluids. (Jou et al. 2006) conducted a numerical study of natural convection of nanofluids in a rectangular enclosure. They demonstrated that increasing the volume fraction improves heat transfer. (Oztop et al. 2008) carried out a numerical study of natural convection in partially heated rectangular enclosures, testing different types of nanoparticles. They found that the position of the heat source affects the thermal and dynamic fields, and heat transfer enhancement is
significant when the enclosure has a low aspect ratio. (Khanafer et al. 2003) numerically studied the natural convection of a nanofluid confined in a differentially heated enclosure. The results showed that heat transfer increases with an increase in nanoparticle volume fraction. Despite the abundance of work in the field of natural convection of nanofluids, most of these studies have been limited to cases of unpartitioned cavities, and very few studies have been conducted using nanofluids in partitioned cavities. Among these studies are (Mahmoudi et al. 2010; Hussein et al. 2014; Guiet et al. 2011; Hussein et al. 2013; Aminossadati et al. 2011; Wang et al. 2013).

In addition, work on the study of convective phenomena within ventilated cavities has mainly concerned simple and regular geometries (square, rectangular, etc.). On the other hand, few studies have dealt with the case of more complex geometries such as that of (Tmartnhad et al. 2008). The latter numerically analyzed the heat transfer, in a trapezoidal cavity ventilated and crossed by air.

The effectiveness of such processes is often limited by the thermophysical properties of the fluids used (Salhi et al. 2022). The development of research dealing with nanofluids aims to significantly improve heat transfer by introducing a low concentration of nanoparticles (size less than 100 nm) into a pure fluid (Choi et al. 1995; Shama et al. 2009; Salhi et al. 2015). Several studies have been carried out on the mixed convection of nanofluids (Sourtiji et al. 2014; Ehsan et al. 2017; Mojumder et al. 2015) whose numerical study focused on the heat transfer within a ventilated square cavity and crossed by a nanofluid (Al₂O₃-water). The latter varied the location of the discharge opening. It appears that the average Nusselt number increases with the increase in the Reynolds and Richardson numbers and the volume fraction. (Shahi et al. 2010; Farhad et al. 2010) carried out a numerical study concerning the mixed convection within a nanofluid (Cu-water) in a ventilated square cavity of which a portion of its base is subjected to a heat flow. Their results indicate the addition of nanoparticles leads to the increase of the average Nusselt number. Recently, there has been a growing interest in hybrid nanomaterials as a means to develop new nanofluids that can achieve the highest rates of heat transfer (Suresh et al. 2012; Nuim Labib et al. 2013; Sundar et al. 2014; Sheikholeslami et al. 2014; Suresh et al. 2011; Abbasi et al. 2013; Madhesh et al. 2014). In this context, (Kalidasan et al. 2017) considered in their numerical study the case of a ventilated square cavity with an adiabatic obstacle in its center. The authors were interested in the contribution of the use of a hybrid nanofluid (consisting of nanoparticles of diamond and cobalt oxide in water as a suspending fluid) on the thermal performance of the cavity.

The study of heat transfer by natural convection in the prepared round bottom flask for the composition of organic chemistry, such as the ease of isolation after the reaction, the low cost and the simplicity of operation (Chafai et al. 2022), it is of great importance in the study of the mechanisms of chemical reactions. Thus, the objective of the present work consists of a characterization of the turbulent force convective heat transfer of hybrid nanofluid in round bottom flask contains an agitator. Accordingly, we numerically study the turbulent natural convection of a hybrid nanofluid (HNF) in a round bottom flask containing an agitator, it is one of the laboratory flasks used in organic chemistry synthesis. The bottom wall and to the middle of the flask are maintained at a constant high temperature $T_h$ with the agitator rotation speed fixed at 250 rpm. While the upper, left and right walls to the middle of the flask are maintained at low $T_c$. The HNF comprises Gr and CNT nanoparticles suspended in pure water. The governing equations are solved numerically using the finite size approach and formulated using the Boussinesq approximation. In this simulation, we investigated the effects of
NP volume fraction $\phi$ from 0% to 6%, Rayleigh number ($Ra$) from $10^4$ to $10^6$, the rotation speed of the agitator and the Nusselt number.

2. Problem description and mathematical formulation

Fig. 1 illustrates the round bottom flask cavity considered in the present study. As shown, the left and right walls have straight and circular surfaces, while the top wall is straight. In addition, the cavity has a height $H$ = 115 mm, diameters $D_0 = 64$ mm, $d_1 = 32$ mm, and flask neck $d_2 = 32$ mm, for the agitator $d_3 = 3$ mm and $L = 10$ mm.

The simplifying assumptions used in our study are as follows:

- The basic fluid used is a Newtonian fluid, incompressible and which satisfies the hypothesis of Boussinesq.
- The nanofluid is assumed to be incompressible and the flow is turbulent, stationary and two-dimensional.
- The thermophysical properties of the hybrid nanofluid are constant, except for the variation of the density, which is estimated by the assumption of Boussinesq.

![Fig. 1 Geometry of the studied configuration.](image)

The mathematical formulations and the numerical solution procedure are described as follows:

**Continuity equation:**

$$\frac{\partial (\rho u)}{\partial x} + \frac{\partial (\rho v)}{\partial y} = 0$$

(1)

**Momentum equation in the (x,y)-direction:**
\[
\rho_\text{nf} \frac{\partial u}{\partial x} + \rho_\text{nf} v \frac{\partial u}{\partial y} = -\frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( 2 \frac{\partial u}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right]
\] (2)

\[
\rho_\text{nf} \frac{\partial v}{\partial x} + \rho_\text{nf} v \frac{\partial v}{\partial y} = -\frac{\partial P}{\partial y} + \frac{\partial}{\partial x} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( 2 \frac{\partial v}{\partial y} \right) \right] + \frac{\partial}{\partial y} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) \right] + g \rho_\text{nf} \beta_\text{nf} (T - T_{\text{ref}})
\] (3)

Energy equation:

\[
\rho_\text{nf} \frac{\partial T}{\partial x} + \rho_\text{nf} v \frac{\partial T}{\partial y} = \frac{\partial}{\partial x} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( \frac{\partial T}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( \frac{\partial T}{\partial y} \right) \right]
\] (4)

Turbulent kinetic energy:

\[
\rho_\text{nf} \frac{\partial k}{\partial x} + \rho_\text{nf} v \frac{\partial k}{\partial y} = \frac{\partial}{\partial x} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( \frac{\partial k}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( \frac{\partial k}{\partial y} \right) \right] + (P_k)_\text{nf} + (G_k)_\text{nf} - \rho_\text{nf} \epsilon
\] (5)

Rate of energy dissipation:

\[
\rho_\text{nf} \frac{\partial \epsilon}{\partial x} + \rho_\text{nf} v \frac{\partial \epsilon}{\partial y} = \frac{\partial}{\partial x} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( \frac{\partial \epsilon}{\partial x} \right) \right] + \frac{\partial}{\partial y} \left[ (\mu_\text{nf} + (\mu_t)_\text{nf}) \left( \frac{\partial \epsilon}{\partial y} \right) \right] + (C_{\epsilon 1} f_1 (P_k)_\text{nf} + C_{\epsilon 3} (G_k)_\text{nf}) - \rho_\text{nf} \epsilon
\] (6)

With

\[ C_{\epsilon 1} = 1.44, C_{\epsilon 2} = 1.92, \sigma_k = 1, \sigma_\epsilon = 1.33 \]

Stress production:

\[
(P_k)_\text{nf} = (\mu_t)_\text{nf} \left[ 2 \left( \frac{\partial u}{\partial x} \right)^2 + 2 \left( \frac{\partial v}{\partial y} \right)^2 + \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 \right]
\] (7)

Buoyancy term:

\[
(G_k)_\text{nf} = \frac{(\mu_t)_\text{nf}}{\sigma_t} g \rho_\text{nf} \beta_\text{nf} \frac{\partial T}{\partial y}
\] (8)

Prandtl number:
\[ Pr_{nf} = \frac{C_{p_{nf}} \cdot \mu_{nf} \cdot k_{eff}}{C_{p_f} \cdot \mu_f \cdot k_{nf}} \cdot Pr \quad (8) \]

The eddy viscosity:

\[ (\mu_e)_{nf} = \rho_{nf} \cdot C_{\mu} \cdot f_{nf} \cdot \frac{k^2}{\epsilon} \quad (9) \]

The thermo-physical properties of the hybrid were predicted nanofluid using the following models (Xu et al. 2019; Tiwari et al. 2007; Devi et al. 2016; Jasim et al. 2021):

**Density of the hybrid nanofluid:**

\[ \rho_{hbf} = (1 - \varphi_1 - \varphi_2) \rho_f + \varphi_1 \rho_{np1} + \varphi_2 \rho_{np2} \quad (10) \]

**Heat capacitance of the hybrid nanofluid:**

\[ (\rho C_p)_{hbf} = (1 - \varphi_1 - \varphi_2) (\rho C_p)_f + \varphi_1 (\rho C_p)_{np1} + \varphi_2 (\rho C_p)_{np2} \quad (11) \]

**Thermal conductivity of the hybrid nanofluid:**

\[ k_{hbf} = \frac{k_{np2} + (M - 1)k_{mf} - (M - 1)\varphi_2(k_{mf} - k_{np2})}{k_{np2} + (M - 1)k_{mf} + \varphi_2(k_{mf} - k_{np2})} k_{mf} \quad (12) \]

With: \( M = 3 \) and

\[ k_{mf} = \frac{k_{np1} + (M - 1)k_f - (M - 1)\varphi_1(k_f - k_{np1})}{k_{np1} + (M - 1)k_f + \varphi_1(k_f - k_{np1})} k_f \]

**Viscosity of the hybrid nanofluid:**

\[ \mu_{hbf} = \frac{\mu_f}{(1 - \varphi_1 - \varphi_2)^{2.25}} \quad (13) \]

Where the dimensionless numbers are:

\[ Ra = \frac{g \beta H}{H} (T_h - T_c) \quad (14) \]

\[ Pr = \nu / \alpha \quad (15) \]

The Nusselt number can be expressed as:

\[ Nu = \frac{hH}{k_f} \quad (16) \]

The heat transfer coefficient is expressed as:

\[ h = \frac{q_w}{T_h - T_c} \quad (17) \]

Thermal conductivity:
\[ k_{nf} = -\frac{q_w}{\partial T/\partial x} \]

Average Nusselt number:
\[ Nu_{avg} = \int_0^y Nu(y)dy \]  \hspace{1cm} (19)

3. Code validation and Grid testing

The obtained results related to the Gr-CNT-Water mixture \((\phi=0.02), Ra=10^5\) and are presented in Table 1. From this table, it appears that the nodes number of 17139 is sufficiently fine to carry out the numerical simulations.

<table>
<thead>
<tr>
<th>Nodes</th>
<th>9111</th>
<th>12351</th>
<th>17139</th>
<th>26323</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\psi_{max})</td>
<td>1.3547</td>
<td>1.7249</td>
<td>1.8667</td>
<td>1.8669</td>
</tr>
</tbody>
</table>

Table 1

Values of the stream function for different nodes number.

Fig. 2 presents a comparison between the results of the present study and those of \((\text{Quiet et al.}, 2011)\). The comparison concerns the mean Nusselt number. It is clear that the results of our code are in good agreement with those proposed by Quiet et al.

4. Results and discussion

The main purpose of this study was to determine the effect of different parameters such as the volume ratio of mixed nanoparticles \((0 \leq \phi \leq 0.06)\), the rotational speed of the agitator \((250, 275, 300 \text{ and } 350 \text{ rpm})\) and Rayleigh number \((10^4 \leq Ra \leq 10^6)\) on the flow behavior and convective heat transfer in a round bottom
flask of the resulting CNT-Gr-water hybrid nanofluid. The thermophysical properties of water and the tested nanoparticles are regrouped in Table 2.

<table>
<thead>
<tr>
<th>Property</th>
<th>Water</th>
<th>Gr</th>
<th>CNT</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_p$ (J.kg$^{-1}$.K$^{-1}$)</td>
<td>4179</td>
<td>717</td>
<td>425</td>
</tr>
<tr>
<td>$\rho$ (kg. m$^{-3}$)</td>
<td>997.1</td>
<td>1800</td>
<td>2600</td>
</tr>
<tr>
<td>$K$ (W.m$^{-1}$.K$^{-1}$)</td>
<td>0.613</td>
<td>5000</td>
<td>6600</td>
</tr>
<tr>
<td>$\beta \times 10^{-5}$ (K$^{-1}$)</td>
<td>21</td>
<td>2.84</td>
<td>0.85</td>
</tr>
</tbody>
</table>

Fig. 3 shows us isothermal contours, and as expected, in the absence of nanoparticles, the heat distribution is much lower than in their presence. Also, Fig. 3 shows that the isotherms conform to the shape of the round bottom flask. This outcome is unsurprising since weak circulation structures are formed under low Rayleigh number conditions, resulting in minimal heat transfer. However, at high Rayleigh number conditions ($Ra = 10^6$), the circulation structure's strength within the cavity intensifies, and heat transfer within the cavity is predominantly controlled by it. Moreover, the isothermal lines are predominantly clustered near the round bottom portion of the hot wall and the left and right portions of the cold circular walls, as expected in the Rayleigh-Bénard experiment. Thus, substantial temperature gradients arise in the bottom portion of the hot wall. In addition, we can clearly see from Fig. 3 that the intensity of the buoyancy effect rises when the volume fraction of the hybrid nanofluid increases, and this may be confirmed by the increasing of the circulation shape inside the cavity.
Fig. 3 Isotherms for different $Ra$ and volume fraction.

The streamlines contours are depicted in Fig. 4. We clearly observe from Fig. 4 that the streamlines differ from one case to another according to the proportion of nanoparticles and according to the high value of the Rayleigh number. Generally, we notice an evident difference in the angle and shape of the vortex rotation system.

Fig. 4 reveals that the streamlines exhibit mostly symmetrical behavior. It is noteworthy that increasing the Rayleigh number generally results in higher values of the stream function. At low Rayleigh numbers ($Ra = 10^4$), the stream function exhibits its lowest value and secondary vortexes are formed. In contrast, at high Rayleigh numbers ($Ra = 10^5$), the vortexes expand both horizontally and vertically, and their strength intensifies. Additionally, we observed that the thickness of the thermal boundary layer adjacent to the heated wall is influenced by the presence of nanoparticles and their volume fraction. The emergence of these vortexes can be attributed to the strong vorticity of the hybrid nanofluid particles in these regions.

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Fig. 4 Velocity streamline for different $Ra$ and volume fraction.

Fig. 5 shows us the isotherms in the case of changing the rotational speed of the mixer in the absence and in the presence of nanoparticles. Accordingly, we notice a difference in the distribution of heat depending on the speed of rotation. Also, the difference in temperature distribution significantly increases upon adding nanoparticles.

V1=250 rpm  V2=275 rpm  V3=300 rpm  V4=350 rpm
The effect of the rotational speed of the agitator on the velocity streamlines in the absence and in the presence of nanoparticles is presented in Fig. 6. In the absence of nanoparticles, pure water flows tangentially along the agitator to the wall of the round bottom flask. Due to the effects of reflection and gravity on the wall, the liquid moves tangentially along the normal direction of the agitator, resulting in a circulating water flow from the bottom-up. Increasing the agitator speed leads to the formation of three non-symmetrical vortexes, and the speed of rotation significantly influences the maximum value of the streamline. The maximum value of the streamline ($\psi_{\text{max}} = 1.9765$) is achieved at a speed of 350 rpm.

Furthermore, the presence of nanoparticles results in the formation of four symmetrical vortexes. Additionally, it is evident that the maximum values of the streamline slightly increase with the introduction of nanoparticles ($\varphi = 0.04$). Hence, for this reason, the rotational speed of 250 rpm was chosen.

Fig. 7 illustrates how the Nu number varies with the NP volume fraction $\varphi$ for different Rayleigh numbers. Previous research on this subject has demonstrated that the addition of nanoparticles to the base fluid
results in two counteracting effects on intracavity convective heat transfer. The first effect is an increase in \( Nu \) due to the enhanced thermal conductivity of the mixture resulting from the presence of nanoparticles. The second effect, arising from the viscosity increase due to the addition of nanoparticles, suppresses convective motion and thereby reduces \( Nu \). The dominant mechanism among these two antagonistic effects depends on the type of particles used, the convective strength (\( Ra \)), and the model utilized to estimate the viscosity and thermal conductivity of the mixture.

The findings presented in Fig. 6 in this study reveal that, for a given \( Ra \) value, a monotonic rise in \( Nu \) can be achieved by introducing nanoparticles. Moreover, it is demonstrated that \( Nu \) increases monotonically with increasing \( Ra \) for a given \( \phi \) value. This is because elevating the Rayleigh number augments convection.

![Fig. 7 Variation of average Nusselt number \( Nu \) with HNP volume fraction \( \phi \) at different Rayleigh numbers \( Ra \).](image)

The mean Nusselt number versus Rayleigh number for different types of NFs (Gr, CNT, and Gr-CNT) is illustrated in Fig. 8. The graph demonstrates that an increase in the Rayleigh number leads to an increase in the Nusselt number and total heat transfer within the cavity, under these conditions. Moreover, the NF type affects the average Nusselt number and heat transfer within the cavity. The highest mean Nusselt number is observed for Gr-CNT-water HNF at a Rayleigh number of \( 10^6 \).
5. Conclusion

In this study, the impact of the Rayleigh number, the volume fraction ($\phi$) of nanoparticles, the rotational speed and the type of nanofluid on the flow streamlines, isotherm distribution, and mean Nusselt number was investigated. The main findings are summarized as follows:

✓ The stream functions and Nusselt number increase with increasing Rayleigh number. Furthermore, it was observed that increasing the Rayleigh number results in enhanced heat transfer for a given volume fraction.

✓ The flow circulation cell and the best heat transfer performance were observed at rotation speed of 275 rpm.

✓ The performance of Gr and CNT nanofluids and Gr-CNT hybrid nanofluid was compared to pure water, and they demonstrated better heating implementation.

✓ The presence of Gr and CNT nanoparticles led to an increase in the Nusselt number.

✓ For high Rayleigh numbers, the difference in heat transfer increased with increasing volume fraction of nanoparticles.

✓ The Gr-CNT hybrid nanofluid exhibited the highest heat transfer performance.

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Data availability These research data are not shared, all data generated or analyzed during this study are included in this published article.

Statements and Declarations
Conflict of interest
On behalf of all authors, the corresponding author states that there is no conflict of interest.

Ethical approval
Ethical approval is not required for this review. Not Applicable.

Consent to participate
Not required for this article.

Consent for publication
Not required for this article.

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