Original Article

ASSESSMENT OF THE TiO₂/WATER NANOFLUID EFFECTS ON HEAT TRANSFER CHARACTERISTICS IN VVER-1000 NUCLEAR REACTOR USING CFD MODELING

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1. Introduction

Ordinary heat transfer fluids such as water and oil are widely used to prevent the overheating or to enhance the heat transfer rate of different systems used in microelectronics, industry, transportation, electronic, nuclear engineering, etc. However, the poor heat transfer properties of these coolants compared with those of most solids are the primary obstacle to high compactness and to the efficiency of the heat transfer systems. Therefore, many researchers have centralized their

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work on the improvement of high performance heat transfer fluids in recent times. In the early research, suspension and dispersion of millimeter or micrometer sized particles were employed. However, heat transfer fluids containing suspended particles of micrometer or millimeter sizes had major disadvantages like the erosion of the components by abrasive reactions, clogging in small passages, sedimentation of particles, and increasing the pressure drop. Nanofluid is a new class of fluid for improving both thermal conductivity and suspension stability in various industrial fields. It consists of uniformly dispersed and suspended nanometer-sized particles which were first pioneered by Choi and Eastman [1] in 1996. Compared with the suspensions of micrometer or millimeter sized particles, the heat transfer rate and stability of nanoparticles suspension are improved. Nanofluids have developed as a new class of heat transfer fluids and have grown tremendously in the past few years. Researchers are being challenged to figure out many unanticipated thermophysical features of these fluids, and to propose new models to explain their behavior. A plenary summary of the previous studies on the properties of nanofluids has recently been rendered by Duangthongsuk and Wongwises [2].

Sajadi and Kazemi [3] investigated the turbulent heat transfer characteristics of TiO$_2$/water nanofluid in a circular pipe for a maximum nanoparticles volume concentration of 0.25%. The results indicated that the addition of small amounts of nanoparticles to the base fluid considerably augments heat transfer, while Nusselt numbers are approximately the same for all nanoparticle volume concentrations. Recently, Abbasian Arani and Amani [4,5] presented an experimental study on heat transfer and pressure drop of TiO$_2$-water in a turbulent flow regime for 30 nm particles with a diameter of 30 nm. They carried out their experimental investigation for Reynolds numbers ranging between 8,000 and 51,000 and 0.002 and 0.02 volume concentrations. They concluded that by using a nanofluid at a high Reynolds number (>30,000) more power was needed to compensate for the pressure drop of the nanofluid, while increments in the Nusselt number for all Reynolds numbers are approximately equal.

In addition to the mentioned benefits of nanofluid, there are many phenomena which make nanofluid the best fluid for some specific applications. These phenomena include critical heat flux enhancement, accelerated quenching, wettability enhancement, etc. [6,7]. These characteristics make nanofluid a potential coolant for nuclear reactor systems such as core, Emergency Core Cooling System (ECCS) and In-Vessel Retention (IVR) coolant [8,9]. El-Wakil [10] shows that an annular with cosine heat flux (for a constant heat transfer coefficient) has a wall temperature profile as shown in Fig. 1. In this figure,

![Fig. 1](attachment:image1)

**Fig. 1** – Heat flux, clad temperature, and coolant bulk temperature of typical vertical annuli (constant heat transfer coefficient).

![Fig. 2](attachment:image2)

**Fig. 2** – Arrangement of various fuel assembly types in the core.
the axial temperature variation of the coolant, $t_f$, and cladding surface, $t_c$, are shown. The position of the cross sections at which maximum cladding surface temperature takes place is demonstrated. It is maximum center fuel and cladding temperatures that pose metallurgical limitations on reactor operation. The axial variation of neutron flux along the fuel element is given by:

$$f = f_c \cos \left( \frac{\pi z}{H} \right)$$

(1)

where $H$ is the height of the fuel element and $H_e$ is the extrapolated height [10]. Since each fuel element is usually uniform in cross-sectional dimensions and in fuel type and enrichment:

$$q^* = q_e \cos \left( \frac{\pi z}{H_e} \right)$$

(2)

where $q^*$ and $q_e$ are the volumetric thermal source strengths at any point, $z$, and the center of the fuel element, respectively.

The heat transferred between cladding and coolant, at any point, $z$, along the fuel element, per unit area of cladding surface (circumferential) is given by $h (t_c, t_f)$. Since $h$ has been assumed to be constant along the fuel element, the temperature difference $(t_c - t_f)$ is directly proportional to the volumetric thermal source strength $q^*$ at that point. Since the latter is a cosine function of $z$, the above temperature difference also has the form of:

$$t_c - t_f = (t_c - t_f_e) \cos \left( \frac{\pi z}{H_e} \right)$$

(3)

where $(t_c - t_f_e)$ is the temperature difference between the cladding surface and coolant at $z = 0$.

It is shown that the wall temperature profile has a maximum above the midpoint of the rod.

This study aimed to investigate the cooling effects of nanofluid in a VVER-1000 reactor. The VVER-1000 reactor is a Russian type pressurized water reactor that uses light water for the coolant and moderator. Its core consists of 163 fuel assemblies arranged in a hexagonal lattice with 311 fuel rods,
18 guiding channels for control rods and/or burnable absorber rods, and a central channel per assembly. The reactor core configuration is illustrated in Fig. 2.

Considering the advantages of nanofluids in improving the thermal properties of fluid, the key idea is to exploit the very high thermal conductivities of solid particles, which can be hundreds or even thousands of times greater than those of conventional heat transfer fluids such as water. The adjustable properties of nanofluids, including thermal conductivity and surface wettability, high specific surface area, and, therefore, more heat transfer surface between particles and fluids, motivated us to use a nanofluid in order to improve and enhance the heat transfer characteristics in VVER-1000 nuclear reactors. Due to easy access to TiO₂ and its good properties such as high thermal conductivity, the used nanofluid was TiO₂/water. These investigations were performed at normal coolant fluid flow and heat flux of a VVER-1000 reactor. The effects of size changes and of considered changes of the nanoparticles were also studied (Table 1).

### Table 2 – Fuel rod geometrical data for conventional VVER-1000.

<table>
<thead>
<tr>
<th>Clad inner diameter</th>
<th>7.73 (mm)</th>
<th>Pellet inner diameter</th>
<th>1.5 (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clad outer diameter</td>
<td>9.1 (mm)</td>
<td>Pellet outer diameter</td>
<td>7.57 (mm)</td>
</tr>
<tr>
<td>Pin pitch</td>
<td>12.75 (mm)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**Fig. 4** – Equivalent cells.

**Fig. 5** – Residual values with $5.6 \times 10^6$ meshes.

### 2. Thermohydraulic analysis of fuel rods in the hot channel

First, to simulate a fuel rod, Eq. (4) was used to obtain an equivalent cell that includes a fuel rod and its surrounding fluid in hexagonal assemblies of a VVER-1000 reactor as shown in Fig. 3.
The finite volume method, a grid network is created directly in the physical space. Consequently, the code using dynamic memory and a suitable structure of data enables control and flexibility of the calculations. In the grid network, the meshes were composed of three-dimensional (hexahedron) elements. The height of the elements is 1 mm.

2.1. Methodology

The differential equations governing the flow, turbulence, and heat transfer under the assumptions of steady, incompressible flow are given as follows [11]:

Conservation of mass:

\[ \nabla \cdot \rho \mathbf{u} = 0 \]  

Conservation of momentum:

\[ \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \mathbf{T} + \rho \mathbf{g} \]  

The stress tensor \( \mathbf{T} \) is given by:

\[ \mathbf{T} = \mu \left[ \nabla \mathbf{u} + \nabla \mathbf{u}^T \right] - \frac{2}{3} \rho \nabla \mathbf{u}^T \mathbf{u} \]  

where the second term on the right-hand side is the effect of volume dilation. For incompressible flow, \( \nabla \cdot \mathbf{u} \) becomes zero.

Conservation of energy:

\[ \nabla \cdot \left( \rho E + p \mathbf{u} \right) = \nabla \cdot \left( k \nabla T - \sum_j h_j f_j + \left( \mathbf{u} \cdot \nabla \right) T \right) \cdot \mathbf{u} \]  

Where \( k_s \) is the effective conductivity and \( k_s = k + k_t \), \( k_t \) is the turbulent thermal conductivity defined according to the turbulence model being used. The first three terms on the right-hand side of Eq. (8) represent energy transfer due to conduction, species diffusion, and viscous dissipation, respectively.

Turbulent kinetic energy equation:

\[ \frac{\partial}{\partial t} (\rho k) + \frac{\partial}{\partial x_i} (\rho k u_i) = \frac{\partial}{\partial x_i} \left( \Gamma_k \frac{\partial k}{\partial x_i} \right) + G_k - Y_k + S_k \]  

Specific dissipation rate equation:

\[ \frac{\partial}{\partial t} (\rho \omega) + \frac{\partial}{\partial x_i} (\rho \omega u_i) = \frac{\partial}{\partial x_i} \left( \Gamma_\omega \frac{\partial \omega}{\partial x_i} \right) + G_\omega - Y_\omega + D_\omega + S_\omega \]  

where \( \Gamma_k = \mu + \frac{\mu_t}{\sigma_k} \)
\( \Gamma_\omega = \mu + \frac{\mu_t}{\sigma_\omega} \)
\( \sigma_k = 1.176, \sigma_\omega = 1.0, \sigma_{k,1} = 1.0, \sigma_{k,2} = 1.0, \sigma_{\omega,1} = 1.168 \) [12].

In order to obtain heat transfer parameters, nanofluid properties such as density, specific heat, viscosity and thermal conductivity should be measured or calculated by theoretical models.

2.1.1. Density and specific heat

The effective density of the nanofluid is given by Wang and Mujumdar [13]:

\[ \rho_{nf} = (1 - \phi) \rho_f + (\phi) \rho_{np} \]  

The heat capacitance is defined as [11]:

\[ \left( c_p \right)_{nf} = \frac{(1 - \phi)\left( \rho_f c_{pf} \right) + (\phi)\left( \rho_{np} c_{pnp} \right)}{(1 - \phi)\rho_f + (\phi)\rho_{np}} \]  

2.1.2. Dynamic viscosity of nanofluid

In this study, the model by Brinkman et al was used for obtaining viscosity [14].

\[
\mu_{nf} = \frac{1}{(1 - \phi)^{\frac{1}{2}}}\mu_{bf}
\]  

(13)

2.1.3. Thermal conductivity

Many theories have been presented for calculating the conductivity coefficient of nanofluids. In the model by Chon et al [15], the effect of Brown’s motion, shape, and size of the nanoparticles and base fluid were considered.

\[
\frac{k_{nf}}{k_{bf}} = 1 + 64.7\phi^{0.748} \left(\frac{d_{np}}{d_{bf}}\right)^{0.369} \left(\frac{k_{np}}{k_{bf}}\right)^{0.7576} Pr^{0.9955} Re_{np}^{1.2321},
\]  

(14)

\[
Pr = \frac{\mu_{bf}}{\rho_{bf} \alpha_{bf}}
\]  

(15)

\[
Re_{np} = \frac{\rho_{np} \kappa T}{3 \pi \mu_{bf} d_{np}}
\]  

(16)

Where \( \kappa \) is Boltzmann’s constant \((1.38066 \times 10^{-23} \text{ J/K})\). This correlation is applicable for nanoparticles with a diameter between 10 nm and 150 nm, and a volume concentration between 0.2% and 9%, where \(d_{nf}\) is the equivalent diameter of base fluid molecule, given by:

\[
d_{nf} = 0.1 \left(\frac{6M}{N\pi\rho_{bf}}\right)^{\frac{1}{3}}
\]  

(17)

which \(M\) is the molecular weight of the base fluid, \(N\) is the Avogadro number, and \(\rho_{bf}\) is the mass density of the base fluid calculated at temperature \(T = 293\) K.

All of these equations are solved using FLUENT 6.3.26 code. User defined functions (UDFs) are also written in C programming language to ensure the accuracy and stability of solutions. The implicit first-order upwind scheme is used for solving the above equations.

The convergence criterion is fixed such that the residual values are lower than \(10^{-8}\) and the number of grids which satisfies the convergence criterion was obtained equal to \(5.6 \times 10^5\). For this purpose, several numbers of meshes have been investigated and at \(5.6 \times 10^5\), the convergence criterion was satisfied very well, as shown in Fig. 5. Also, the grid independency for the chosen meshes was done, which is shown in Fig. 5, for the maximum temperature of the clad and output coolant temperature. As shown in Fig. 6, by increasing 

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**Fig. 8** – Vertical annulus modelled in the Computational Fluid Dynamics code.

**Fig. 9** – Wall temperature. Comparison of numerical and experimental method \((\text{Re} = 3,500)\).

**Fig. 10** – Wall temperature. Comparison of numerical and experimental method \((\phi = 1\%)\).
the number of grids to $5.6 \times 10^6$, maximum temperature of the clad and output coolant converge to the fixed values and are independent from the number of grids. Therefore, the validation of the numerical method is clearly assessed in the considered range of parameters such as grid and convergence. The pressure correction approach using the SIMPLE algorithm was used. Mass flow rate was specified at the inlet whereas static pressures given at the outlet. Static temperature of the fluid (ambient value) is specified at the inlet and is $T_{in} = 563$ K. These input conditions are estimated indirectly from the chosen Reynolds number value. An adiabatic and no slip wall boundary are assumed for the outer wall of the annulus. The turbulence model was chosen after applying various two-equation turbulence models available in the software. It was found by experimenting with different turbulence models that the best model for good convergence is $k-\varepsilon$ SST as it has predicted the flow in the wake of the cylinder very well [12].

![Fig. 11 – Heat transfer coefficients. Comparison of numerical and experimental method (Re = 4,200).](image)

**Table 3 – Relative errors between the experimental and numerical values.**

<table>
<thead>
<tr>
<th>Height (m)</th>
<th>Fig. 8</th>
<th>Fig. 9</th>
<th>Fig. 10</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$Re = 3,500$</td>
<td>$Re = 3,500$</td>
<td>$Re = 4,200$</td>
</tr>
<tr>
<td></td>
<td>$\phi = 1%$</td>
<td>$\phi = 1%$</td>
<td>$\phi = 1%$</td>
</tr>
<tr>
<td>0.5</td>
<td>0</td>
<td>0.038462</td>
<td>0</td>
</tr>
<tr>
<td>0.4</td>
<td>0.01923</td>
<td>0.017037</td>
<td>0.018519</td>
</tr>
<tr>
<td>0.3</td>
<td>0.01667</td>
<td>0.030303</td>
<td>0.030303</td>
</tr>
<tr>
<td>0.2</td>
<td>0.014706</td>
<td>0.029412</td>
<td>0.01389</td>
</tr>
<tr>
<td>0.1</td>
<td>0.013158</td>
<td>0.027778</td>
<td>0.012658</td>
</tr>
<tr>
<td>-0.1</td>
<td>0.012195</td>
<td>0.025</td>
<td>0.012195</td>
</tr>
<tr>
<td>-0.2</td>
<td>0.012195</td>
<td>0.025641</td>
<td>0.011765</td>
</tr>
<tr>
<td>-0.3</td>
<td>0.011905</td>
<td>0.026316</td>
<td>0</td>
</tr>
<tr>
<td>-0.4</td>
<td>0.013514</td>
<td>0.027778</td>
<td>0.012195</td>
</tr>
<tr>
<td>-0.5</td>
<td>0.013889</td>
<td>0.029412</td>
<td>0.013514</td>
</tr>
</tbody>
</table>

![Fig. 12 – Temperature of the fuel center in terms of height of fuel rod at different concentrations and nanoparticle size of 10 nm.](image)
2.2. Validation of the presented CFD code

In order to validate the CFD simulation code with written UDF which has been used in this paper, the written CFD simulation code is performed on a vertical annulus with nonuniform heat flux in a nonradiation environment which has been used by Abbassi and Talebi [16] to investigate the TiO$_2$/water nanofluid effects on heat transfer characteristics experimentally. A comparison was made between the written CFD simulation code and the experimental data [16]. Comparison results show the superiority and accuracy of the CFD simulation code with written UDF.

The experimental apparatus is a vertical annulus which is designed to simulate flow over nuclear fuel rods in a nonradiation environment as shown in Fig. 7. Electrically produced heat flux has a cosine shape. Inner and outer diameters of annuli are 33 mm and 55 mm, respectively, and the length is 1.44 m. Both tubes are made of stainless steel. The heat generation mechanism is located inside. The length of the heating surface is 1 m [16].

Fig. 8 shows the vertical annulus modelled in the CFD code which has been used in this paper for thermal hydraulic analysis.

Dependence of the wall temperature on the Reynolds number and nanoparticle volume fraction for experimental and the presented numerical simulation is illustrated in Figs. 9 and 10. It can be seen that in higher volume fractions, nanoparticles affect the wall temperature.

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**Fig. 13** – Temperature of the fuel center in terms of height of fuel rod at different concentrations and nanoparticle size of 20 nm.

**Fig. 14** – Temperature of fuel center at the nanofluid 1.5% TiO$_2$ with changing nanoparticle size.
By increasing nanoparticle concentrations, the wall temperature decreases. The reason behind this behavior is the higher thermal conductivity of the nanofluid in comparison to pure water. Increasing the Reynolds number decreases the wall temperature. A comparison of local heat transfer coefficients is illustrated in Fig. 11.

In the experimental study, it is assumed that heat generation is completely cosine and has a maximum in the center of the test section:

$$q^*(y) = \frac{P}{4r_{in}} \cos\left(\frac{\pi y}{l}\right)$$  \hspace{1cm} (18)

In this equation, $P$ stands for the total power of the test section heater which is $4$ kW, $r_{in}$ is the inner tube radius and $l = 1$ m is the length of the heating area.

In order to calculate the local and average heat transfer coefficient, the temperature of the wall and fluid bulk is needed. Wall temperature is measured through experiment. In order to obtain better results, the average measured temperature of the left and right sides of the wall is selected as the wall temperature.

The local heat transfer coefficient is obtained by:

$$h(y) = \frac{q^*(y)}{T_{wall} - T_{bulk}}$$  \hspace{1cm} (19)

In addition, the condition of the simulation is: $T_{in} = 25^\circ$ and system pressure $= 10$ bar.

The above results as shown in Figs. 9–11 demonstrate the validity of the presented CFD simulation code with written UDF. Therefore, we can rely on the results of the presented CFD simulation code.

Also, in order to confirm the accuracy and efficiency of the presented numerical method, relative errors between the experimental and numerical values are presented in Table 3, which confirm the accuracy and efficiency of the presented method.

2.3. Departure from nucleate boiling ratio calculation

Departure from nucleate boiling ratio (DNBR) is one of the important and fundamental parameters in nuclear safety issues of nuclear plants that limits the heat flux of a plant to prevent entering the film boiling region. To calculate this important parameter, the following formula is used [10]:

Fig. 15 – Temperature of the clad in terms of height of fuel rod at different concentrations and nanoparticle size of $10$ nm.

Fig. 16 – Temperature of the clad in terms of height of fuel rod at different concentrations and nanoparticle size of $20$ nm.
The $q^{\text{act}}$ is given by:

$$q^{\text{act}} = \frac{q^c A_f}{C_f}$$  

(21)

For DNBR calculation using the code used in this paper, the initial intended flux is gradually increased, and points at which the initial boiling points occur are obtained. Indeed, at any point, flux is gradually increased until near the saturated temperature of the bulk for that point. Critical heat flux ($q^c$) is also obtained at that point. It is notable that this method has been checked and validated with the following correlation presented by Jens and Lottes [17] for critical heat flux ($q^c$).

$$q^c = C \times 10^6 \left( \frac{G}{10^5} \right)^m \Delta T_{\text{sub}}^{0.22}$$  

(22)
where C and m are pressure-dependent parameters that are 0.441 and 0.5671, respectively. For the present model, G is the coolant mass flux in Kg/sec that is obtained from the CFD code for the outer and inner channels, and ΔTsub is the difference between the saturated and local temperatures of the bulk.

In any increase, the maximum fuel temperature is calculated. By obtaining the actual flux (initial flux) at that point and using Eq. (20), the results of DNBR are shown in Fig. 23 for nanoparticle size of 10 nm, which is more effective than a nanoparticle size of 20 nm and its minimum that is an important criterion in the heat-up rate of heat power has been achieved.

Fig. 20 – Temperature of cooling fluid with different nanoparticle sizes in nanofluid 1.5% TiO2.

Fig. 21 – Local heat transfer coefficient in terms of height of fuel rod with concentration changes of nanofluids. (A) 10 nm nanoparticle. (B) 20 nm nanoparticle.

Fig. 22 – Local heat transfer coefficient at the nanofluids of 1.5% TiO2 with changes in nanoparticle size.

3. Results and discussion

In this section, calculated parameters are presented. The parameters are: temperature distribution of different parts of the cell and coolant, local heat transfer coefficient, and DNBR.

3.1. The temperature distribution of different parts of the cell and coolant

Figs. 12–17 show the temperature distribution of the different parts of the cell and coolant to compare the effects of the volume concentration and size of nanoparticles.

Fuel center temperature using the nanofluid state is less than that of the water state. The reason behind this behavior is the higher thermal conductivity of nanofluid in comparison to pure water. By increasing the nanofluid concentration, the central temperature of the fuel degrades more.

Fig. 14 shows that as nanoparticle size became smaller, the fuel center temperature decreases. Figs. 15 and 16 show that with increasing concentrations of nanofluid, clad temperature will decrease. As shown in Fig. 17,
smaller nanoparticle size causes a decrease in the clad temperature.

Figs. 18 and 19 show that with increasing concentrations of nanofluid, output coolant temperature will increase, which is important to enhance the thermal efficiency of nuclear power plants. Also, Fig. 20 demonstrates that nanoparticle size has no considerable effect on outlet temperature and mean temperature of the nanofluid.

3.2. Heat transfer coefficient

Calculated local heat transfer coefficients in this research are illustrated in Figs. 21 and 22 to compare the effects of the volume concentration and size of nanoparticles.

Fig. 21 demonstrates the considerable effect of nanoparticles in increasing the heat transfer coefficient. As shown in Fig. 22, smaller nanoparticle size causes an increase in convection heat transfer.

3.3. DNBR

According to Eq. (20) and the performed simulation, the DNBR is calculated as shown in Fig. 23.

Actual heat flux of the fuel rod \( (q_{\text{rod}}) \) obtained from fluent. In order to perform the critical heat flux \( (q^*_{\text{rod}}) \) calculation, at any point, Flux is gradually increased until near the bulk saturated temperature for that point.

Using nanofluid causes a minimum decrease of DNBR and decreasing nanofluid causes improvement in the DNBR.

4. Conclusions

In this paper, the effects of a nanofluid (TiO\(_2\)/water) on the heat transfer characteristics, such as the thermal conductivity coefficient, heat transfer coefficient, fuel clad and fuel center temperatures in a VVER-1000 reactor have been investigated. First, the cell equivalent for a fuel rod and its surrounding coolant fluid were obtained in the hexagonal fuel assembly of a VVER-1000 reactor. Then, a fuel rod was simulated in the hot channel using CFD simulation codes. Thermohydraulic calculations (maximum fuel temperature, fluid outlet, MDNBR, etc.) were performed and compared with a VVER-1000 reactor without nanoparticles. By investigating the effects of nanofluids on a VVER-1000 reactor and comparing them with a cooling fluid without nanofluid, the following results were obtained. (1) By increasing nanoparticle concentrations, temperature decreases. The reason behind this behavior is higher thermal conductivity of nanofluid in comparison to pure water. (2) As nanoparticle size became smaller, the following results were obtained: (i) convection heat transfer coefficient increased; (ii) no effect was observed on special heat capacity, density, and viscosity; (iii) fuel center and clad temperatures decreased; (iv) outlet temperature and mean temperature of the nanofluid were unaffected; (v) no effect was seen on outlet temperature and mean temperature of the nanofluid; (vi) considerable increase was observed in convection heat transfer; and (vii) usage of the nanofluid reduced MDNBR.

Conflicts of interest

All authors have no conflicts of interest to declare.

References


