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Study of safety parameters of a PWR reactor using Cu nanofluids by molecular dynamics method

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HIGHLIGHTS

- The Molecular Dynamics and CFD methods are used for thermal hydraulics analysis of nanofluids.
- Using Molecular Dynamics, the required thermophysical properties are calculated in high pressure and temperature.
- Copper-Water nanofluid properties such as thermal conductivity and shear viscosity are calculated using MD method.
- The thermal-hydraulics of nanofluids in a WWER1000 reactor have been obtained by CFD method.
- The safety parameters of fuel and cladding are calculated by the Finite Difference Method.

ABSTRACT

In this analysis, nanofluid properties are evaluated by interaction correlations between particles using molecular dynamics (MD) method, and thermal-hydraulics characteristics of nanofluids in a WWER-1000 reactor is investigated by Computational Fluid Dynamics (CFD). This study conceptualizes power increase by changing the cooling from pure water to nanofluid without changing the safety parameters. The Copper nanoparticles are used in primary loop cooling system, to evaluate the heat removal from the core. Thermophysical properties such as thermal conductivity and shear viscosity of Cu-Water nanofluids are obtained by MD in operating pressure and temperature of the Bushehr reactor core. These properties have been used in thermal-hydraulics analysis and nanofluids are considered as a homogeneous fluid. Thermal hydraulic properties of coolant have been calculated for different volume fractions of nanofluids. Thermal hydraulic simulation illustrated enhancement of the thermal characteristics of the core, due to the increment in heat transfer coefficient and thermal diffusivity. The thermal-hydraulic analysis of the reactor core has been performed in steady state at different powers. The requirements for changing the reactor power are not to change the fuel center temperature and Outer Cladding Surface temperature compared to the current state.

KEYWORDS

Nanofluids
CFD
Molecular Dynamics
PWR rectors
Ansys-CFX

HISTORY

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Nomenclature

ρ	Density
C_p	Specific Heat Capacity
ϕ	Volume Fraction of nanoparticles
μ	Viscosity
K	Thermal Conductivity
V	Volume
K_B	Boltzmann Constance
T	Temperature
t	Time
j	Heat Current
η	Shear Viscosity
J_p^{xy}	Non-diagonal element of Stress Tensor
σ	Distance Parameter
Nu	Nusselt Number
h	Heat Transfer Coefficient
ε	Parameter expressing the strength of the interaction
Re	Reynolds Number
Pr	Prandtl Number
D	Hydraulic Diameter
f	Darcy Friction Factor
α	Thermal Diffusivity
T_f	Temperature of Fluid
T_s	Temperature at the Outer Cladding Surface
q	Heat
q''	Surface Heat Flux
q'''	Power Density
k_{gap}	Thermal Conductivity of Gap
k_{ave}	Thermal Conductivity of Fuel
r	Radius Distance
T_{fs}	Temperature of the Outer Surface of the Fuel
r_{fs}	Radius of the Outer Surface of the Fuel
A	Area of at the Outer Cladding Surface

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Subscribe

nf	Nanofluid
bf	Base Fluid
np	Nanoparticle
md	Molecular Dynamic
Exp	Experimental

1 Introduction

The thermal-hydraulics of a nuclear reactor describes the effort involving the coupling of heat transfer and fluid dynamics to accomplish the desired heat removal rate from the core under both normal operations and accidents. In nuclear power plants, the density of the energy generation is high. It puts demands on an efficient cooling system. The heat transfer enhancement technology refers to one that can increase the heat transfer coefficient under a determined temperature difference and heat transfer area. It aims to improve thermal efficiency, reduce power consumption, limit the component temperature, and reduce the size of the instruments (Lu et al., 2021).

The use of nanotechnology makes it possible to prepare fluids with high thermal conductivity called nanofluids that can be used in heat transfer systems. The nanofluids are dilutions of nanometer-sized particles in single-phase fluids (Sundar et al., 2022). Preliminary experimental results (Eastman et al., 1996; Choi and Eastman, 1995) showed that enhancement of thermal conductivity by up to 60% could be obtained by a 5% volume fraction of CuO nanoparticles in the water base fluid. The nanofluids offer the great advantage of heat transfer over single-phase fluids. The lower dispersion of nanoparticles in single-phase fluids can significantly improve the thermal transport properties. They have expected to be widely used in heat transfer due to their excellent thermophysical properties. The concentration range of nanoparticles is typically between 0.01-5 wt%, and the mean particle size is usually 10 to 100 nm. The nanoparticles can be metals, metallic oxides, carbides or carbon materials. Common base fluids are water and mineral oils. Due to their enhanced thermophysical properties, nanofluids have great potential for improving heat-transfer efficiency (Panduro et al., 2022).

Several investigations have revealed the enhancement of thermal conductivity and higher heat transfer rate of nanofluids. Significant improvement in the heat transfer rate have been reported by several researchers with the use of various nanofluids. Understanding of nanofluids properties, such as thermal conductivity, viscosity, and specific heat is very important for the utilization of them in various applications. Further study of the fundamentals for heat transfer and friction factors in the case of nanofluids is considered to be very important to extend the applications of nanofluids.

The different parameters such as volume fraction, dimensions, shape, nanomaterials, the pH of the fluids, surfactant, solvent type, hydrogen bonding, temperature, base fluids, and fluid stability significantly affect the thermal behavior of nanofluids. These parameters have been found to affect the thermal conductivity of the nanofluids directly and can either increase or decrease the thermal conductivity. In contrast, other parameters, such as the viscosity, have an "indirect" effect on the thermal conductivity (Younes et al., 2022). The experimental results of water-based Fe_3O_4 nanofluids with highly disaggregated nanoparticles show that the highest thermal conductivity can be achieved when nanofluids is at a highly disaggregated level with a volume fraction of 0.32%. When Fe_3O_4 particles are highly dispersed, the viscosity of nanofluids does not change with the shear rate. Once nanoparticles undergo uncontrolled aggregations, it could be difficult to predict the thermal conductivity and viscosity at a specific temperature and particle concentration (Liu et al., 2022).

There are two ways to analyze the thermal-hydraulics of a reactor coolant with nanofluids. First, one can conduct experimental studies with the desired loop configuration. Second one is using simulation software. Experimental studies are expensive. It has an environmental error that will increase costs even more. A simulation program improves accuracy and reduces costs. However, the accuracy in the calculation is depending on its numerical model. Many researches have been carried out on the behavior of various nanofluids in nuclear reactors; such as thermal conductivity and heat transfer enhancement, natural circulation, single and two-phase models, the effect of nanofluids in neutronics, safety and etc. (Kim et al., 2009). For instance, Buongiorno et al. (Alsammarraie et al., 2023) have examined the employment of nanofluids as the reactor coolant. According to studies in this field, nanofluids as the reactor coolant are effective in reactor power, reactor core size, and reactor safety parameters.

Some properties such as thermal conductivity and dynamic viscosity of nanofluids are needed for thermal hydraulics evaluation. To calculate these parameters, one has to be employed empirical experiments or to simulate the motion of the particles in a molecular domain. The molecular dynamics simulation can calculate material properties. Molecular dynamics (MD) simulation is based on a general physics model that governs interatomic interactions. It predicts how every atom in a molecular system will move over time (Karplus and McCammon, 2002). These simulations can capture a wide variety of molecular processes, revealing the positions of all the atoms at femtosecond temporal resolution. MD simulations are not new. The first MD simulations of simple gasses had performed in the late 1950s (Alder and Wainwright, 1957; Rudyak et al., 2021). MD simulations have become much more powerful and accessible over the past few years. The physical models underlying MD simulations are inherently approximations, they have become significantly more accurate (Loya et al., 2022). The basic idea behind an MD simulation is straightforward. Given the positions of all the atoms in a system, one can calculate the force exerted on each particle by all the other particles (Rudyak, 2019). In molecular dynamics, one can determine the macroscopic properties of a system, such as diffusion coefficient, viscosity, thermal conductivity, etc. Numerous papers have been presented on the molecular dynamic simulation of nanofluids to investigate the properties of nanofluids.

Computational Fluid Dynamics (CFD) is a branch of

fluid mechanics that uses numerical analysis and data structure to solve and analyze subjects involving fluid flows. The underlying foundation for most CFD subjects is the Navier-Stokes equations, which define most single-phase fluid flows (gas or liquid, but not both). Computational Fluid Dynamics (CFD) has witnessed tremendous progress in the past two decades. The advancement of CFD in reactor design and analysis can be characterized by two major trends: (*i*) the ever-growing simulation capability (Kraus et al., 2021) and (*ii*) the expanding variety of applications (Yuan et al., 2020; IAEA, 2022). Ikeda (Ikeda, 2014) utilized CFD analysis in the design of a high-efficiency spacer grid to increase the critical heat flux (CHF) performance. It has also been well-recognized that the best practices should be complied within CFD analysis to obtain the high-fidelity results (Mahaffy et al., 2007). In addition, many investigations have been submitted by CFD coupling with kinetic models to study the behavior of the reactor core (Sharifian et al., 2020).

In this work, using molecular dynamics for Cu-Water nanofluids simulation, the thermal conductivity and shear viscosity of coolant in a WWER1000 reactor have been obtained. These parameters are calculated at operating pressure and temperature of this reactor for different volume fractions. The results are used in CFD simulation to investigate the behavior of nanofluids as a coolant, and the heat transfer characteristics are evaluated. Finally, to examine the effect of nanofluids on heat removal, the variation of heat flux has been studied and the safety parameters are assessed.

2 Methodology

In this work, the neutronics are neglected and the Cu-Water nanofluid with volume fraction range of 0 to 2.55% has been selected.

The calculation method has three parts:

1. The physical properties, such as thermal conductivity and dynamic viscosity of nanofluid, have been calculated by LAMMPS code version 8Aug2014. LAMMPS is a classical molecular dynamics code with a focus on materials modeling.

2. The dynamic behavior of homogeneous nanofluid in the fuel assembly geometry of the Bushehr reactor has been calculated by Ansys-CFX software. The Ansys-CFX is a high-performance computational fluid dynamics (CFD) software.

3. The thermal-hydraulic criteria e.g. maximum fuel temperature and maximum Outer Cladding Surface temperature, have been calculated by solving the heat transfer equations.

In order to analyze improved heat removal, thermal-hydraulic calculations have been performed in steady-state mode at different powers.

2.1 Molecular Dynamics

Loya et al. provided a good description of molecular dynamics simulation "The simulations that are implemented to simulate the virtual reality dynamics at an atomic or molecular level, are Molecular Dynamics Simulations (MDS)" (Loya et al., 2014). In molecular dynamics, with a certain number of particles and a numerical solution of Newton's laws of motion for each particle at each time step, the goal is to get the velocity and position of the particles in each time step. The resulting trajectory is, in essence, a three-dimensional movie that describes the atomic-level configuration of the system at every point during the simulated time interval. The forces in an MD simulation are calculated using the molecular mechanics force field model, which is fit to the results of quantum mechanical calculations and, typically, to certain experimental measurements. For example, a typical force field incorporates terms that capture electrostatic (Coulombic) interactions between atoms, spring-like terms that model the preferred length of each covalent bond, and terms capturing several other types of interatomic interactions. Such force fields are inherently approximate. The comparison of simulations to a variety of experimental data indicates that force fields have improved substantially over the past decade (Lindorff-Larsen et al., 2012), but the uncertainty introduced by these approximations should be considered when analyzing simulation results. In molecular dynamics, the energy level is obtained by solving Newton's laws of motion for the system (Hollingsworth and Dror, 2018).

2.1.1 Nanofluids in Molecular Dynamics

Nanotechnology provides high thermal conductivity fluids can be used in reactor cooling system. To obtain the properties of nanofluids in high pressure and temperature domains, the MD method can be employed. Physical properties of the nanofluids could be calculated with this method. The density of coolant increases by adding the nanoparticles to the base fluid. It behaves according to the relationship of ideal gases (Xuan and Roetzel, 2000):

$$\rho_{nf} = (1-\phi)\rho_{bf} + \phi\rho_{np} \tag{1}$$

The behavior of specific heat capacity of nanofluids is adapted to the thermal equilibrium theory (2). The base fluid and nanoparticles are considered in the thermal equilibrium. This model has been chosen as a basic formula in many nanofluid equations (Rajabpour et al., 2013):

$$C_{p_{nf}} = \frac{[(1-\phi)\rho_{bf}C_{p_{bf}} + \phi(\rho_p C_{p_{np}})]}{(1-\phi)(\rho_{bf}) + \phi(\rho_{np})} \tag{2}$$

Various theoretical relations are presented to model the viscosity ratio of a nanofluids by the base fluid. In the Einstein model (3), the nanofluids is the composition of the suspension of rigid and spherical particles in the base fluid. It is the first reliable theoretical formula for estimating viscosity, which is valid for a specific volume fraction ($\phi < 0.02$):

$$\mu_{nf} = \mu_{bf}(1 + 2.5\phi) \tag{3}$$

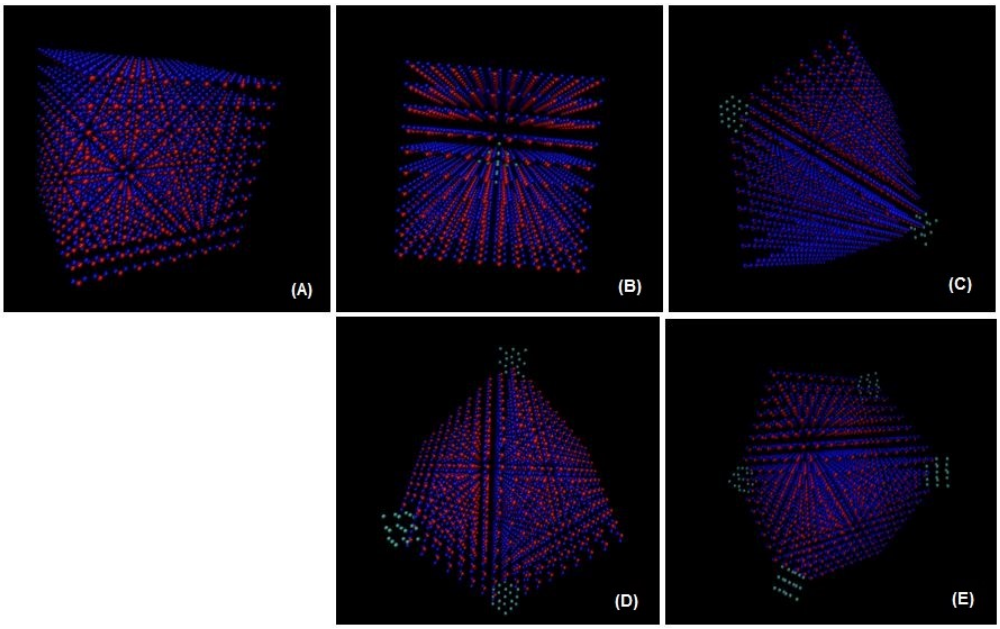

Figure 1: Schematics of initial structures for Molecular Dynamics simulations.

The Brinkman model (4) is a modification of the Einstein model, which is applicable for less than 4% volume fraction:

$$\mu_{nf} = \mu_{bf}\left(\frac{1}{(1-\phi)^{2.5}}\right) \tag{4}$$

The increase in viscosity is undesirable. According to theoretical formulas and empirical results (Udawattha et al., 2019), it should be noted that to have an acceptable increase in viscosity, volume fraction less than 4% is favorite.

According to (Mao and Zhang, 2012), between the three-site models employed in the simulation of the water molecule, the variation in the SPC is not correct. They compared the thermal conductivity variations of SPC/E and TIP3P models with experimental data and it is demonstrated that the SPC/E has proper agreement. So, the SPC/E model is chosen for this work since it has good agreement with experimental results in the water 3-site models.

MD simulations are carried out in two methods. These methods are the equilibrium and non-equilibrium molecular dynamics. The equilibrium molecular dynamics simulation gives better results for nanofluids with a multi-atomic fluid. In the equilibrium molecular dynamic, the Green-Kubo correlation is applied to calculate thermal conductivity and dynamic viscosity (Habershon et al., 2009; Kubo, 1957):

$$K = \frac{1}{3VK_BT^2}\int_0^\infty < j(0)j(t) > \mathrm{d}t \tag{5}$$

From a microscopic point of view, the shear viscosity is obtained by integrating the correlation function of non-diagonal elements of the stress tensor J_p^{xy}.

$$\eta_s = \frac{V}{K_BT}\int_0^\infty < J_p^{xy}(0)J_p^{xy}(t) > \mathrm{d}t \tag{6}$$

In molecular dynamics simulation of Cu-Water nanofluids, the non-bonding potentials of Lennard-Jones (LJ) have been used (See Table 1). Define of non-bonding potential between base fluid and nanoparticles is done by combination rules of Lorentz-Berthelot.

$$\sigma_{sl} = \frac{\sigma_{ss}+\sigma_{ll}}{2}, \quad \varepsilon_{sl} = \sqrt{\varepsilon_{ss}\varepsilon_{ll}} \tag{7}$$

The initial structure in molecular dynamics simulation is defined by 1000 water molecules in a cubic with sides of 34 angstroms that showed in Fig. 1-A. Boundary conditions have been assumed periodic. Also, for nanofluids, nanoparticles are scattered in this volume. The nanoparticles have a diameter of 10 angstroms. The Face Centered Cubic (FCC) crystal structure and the lattice constant equal to 3.597 angstroms are considered for Cu nanoparticles. As seen in Fig. 1, 1 to 4 copper nanoparticles are included in this volume of water, respectively Fig. 1-B to Fig. 1-E. The LAMMPS code provides several methods for controlling temperature and pressure. Depending on which state variables (for example, the energy E, volume V, temperature T, pressure P, and number of particles N) are kept fixed, different statistical ensembles can be generated. A variety of structural, energetic, and dynamic properties can then be calculated from the averages or the fluctuations of these quantities over the ensemble generated. The system must reach the equilibrium state to use the Green-Kubo correlations. To obtain an equilibrium state, the minimizing energy, NVT, NPT, and NVE ensembles have been applied to the system, respectively.

Table 1: LJ parameters for non-bonding interactions.

Interaction type	ε (kcal/mole)	σ (Å)
H_2O-H_2O	0.1553	3.5533
Cu-Cu	9.4390	2.3377
H_2O-Cu	1.2107	2.9455

Table 2: Parameters defined in the input of CFD simulations.

	Volume fraction (%)	a	b
Thermal Conductivity (K)	0	-0.001959000	1.681736000
	0.62	-0.001793771	1.743333367
	1.27	-0.001294255	1.645914305
	1.87	-0.002873467	2.808325469
	2.55	-0.003733504	3.574849692
Shear Viscosity (μ)	0	-3.96740E-07	0.000315894
	0.62	-6.402040E-07	0.000466172
	1.27	-4.720960E-07	0.000374420
	1.87	-4.19670E-07	0.000345604
	2.55	-5.490120E-07	0.000424804

2.2 Computational Fluid Dynamics

Obtaining thermal-hydraulic parameters of coolant requires the thermodynamic and thermal-physical properties, including density, specific heat capacity, thermal conductivity, and dynamic viscosity of the nanofluids. There are two ways to obtain the nanofluids properties with experiments and simulations. In many cases, preparation of experimental facility in high temperature and pressure is not possible. The heat transfer in nanofluids investigates from two viewpoints. In the first view, the base fluid and the nanoparticles are considered homogeneous fluids, and nanoparticles could not move relative to the base fluid and thermo-physical properties are dependent to the mixture temperature. In the second view, the nanofluids have been assumed as a two-phase fluid; the nanoparticle can slip through the base fluid (Kuznetsov and Nield, 2010).

To obtain heat transfer coefficient of fluid (h) and temperature distribution, computational fluid dynamic (CFD) simulations have been used.

For CFD simulation, the fluid properties have to be defined individually. So, the molecular dynamics results are not applicable directly. To employ the results, the following relationship are used:

$$(\frac{K_{nf}}{K_{bf}})_{md} \times (K)_{exp} = (K)_{nf} \tag{8}$$

$$(\frac{\mu_{nf}}{\mu_{bf}})_{md} \times (\mu)_{exp} = (\mu)_{nf} \tag{9}$$

The (md) subscript describes the relative properties of nanofluids calculated by MD. These properties are obtained by equilibrium molecular dynamics simulation. The (exp) subscript for base fluid describes the properties of pure water according to thermal-dynamic tables (Borgnakke and Sonntag, 2020). The nanofluid properties such as thermal conductivity and dynamic viscosity are used in the CFD simulation to define the heat transfer coefficient and distribution temperature of fluid. Experimental results and most analytical correlations have shown that these properties have a linear behavior against temperature changes. These relations for thermal conductivity and dynamic viscosity are defined in the form of $(aT + b)$ for CFD simulation, which is shown in Table 2. Also, ρ and C_p are calculated according to Eqs. (1) to (2), respectively.

In this study, for CFD simulations, coolant is considered a homogeneous fluid. The thermal-hydraulic analysis of the reactor core is performed in steady-state. The geometrical data of fuel assemblies of the WWER1000 reactor is obtained from the Final Safety Analysis Report (FSAR) of BNPP. The fuel assembly of the WWER1000 reactor has the one-sixth symmetry. Figure 2 shows the top view of the geometry design.

In the regions of inlet and outlet of fuel assembly irregular volumetric meshes have been used and in other areas regular volumetric meshes have been applied. According to the Safety Analysis Report(SAR) of the Bushehr reactor, the boundary conditions have been shown in Table 3. The implemented shape of heat flux in the fuel rods that extracted from the Safety Analysis Report of Bushehr nuclear reactor, has shown in Fig. 3. It is clear that the Fig. 3 shows the shape of linear heat rate generated by nuclear fission along fuel assembly height.

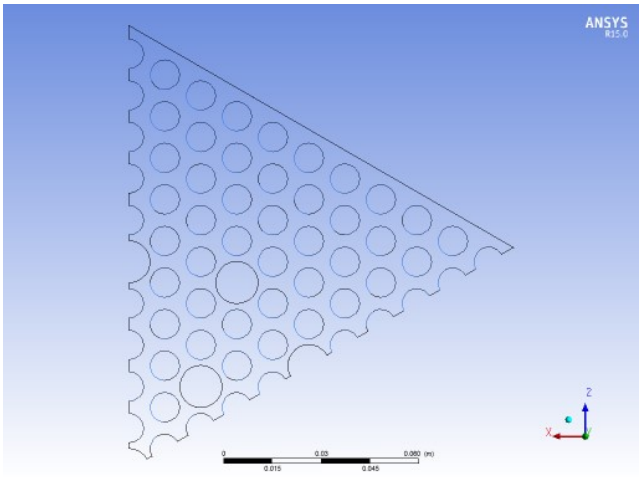

Figure 2: The top view of the designed geometry in CFD simulations.

Table 3: The boundary conditions applied in CFD simulations.

Boundary Surface	Boundary Type	Boundary Condition
Inlet	Temperature (K)	564
	Velocity (m.s^{-1})	5.6
Outlet	Pressure (MPa)	15.7
Fluid Outlet Surface	Periodic	-
Guide Tube Wall	No Slip Wall	Adiabatic
Fuel Rod Wall	No Slip Wall	Heat Flux

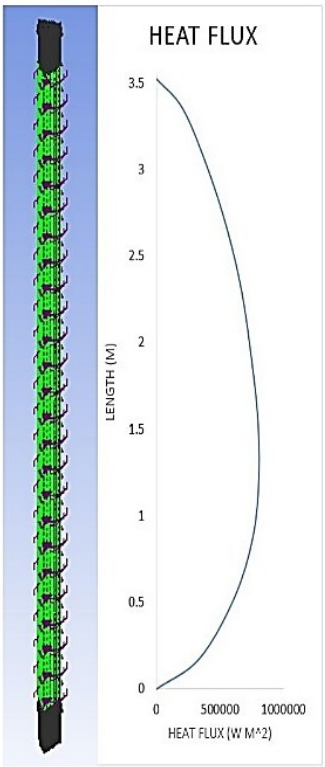

Figure 3: The distribution of heat flux applied on fuel rods in CFD simulations.

The Gnielinski correlation is known as a modern heat transfer equation. This correlation is encompassed a wide range of the Reynolds and Prandtl numbers. According to (Bejan and Kraus, 2003), the error of the Gnielinski method is ±10%. The Gnielinski correlation is presented by Eq. (11) (Gnielinski, 1975) and the thermal diffusivity of fluid is defined as the ratio of heat transferred to heat stored by the unit volume (see Eq. (13)).

$$h = \frac{Nu\,K}{D} \tag{10}$$

$$Nu = \frac{(f/8)(Re - 1000)Pr}{1 + 12.7\sqrt{f/8}(Pr^{2/3} - 1)} \tag{11}$$

$$f = \frac{1}{(1.82\log(Re) - 1.64)^2} \tag{12}$$

$$\alpha = \frac{K}{\rho\, C_p} \tag{13}$$

2.3 Investigation of the Thermal-hydraulic Parameters

It should be noted that theoretically there is no limit to the reactor thermal power. The capability to heat removal is the main limit and there is a direct proportionality between thermal power density and the neutron flux in a nuclear reactor. To study the heat removal capabilities from the reactor core, the reactor safety parameters should be investigated. The main reactor safety parameters in this case are the maximum fuel temperature and maximum Outer Cladding Surface temperature. It is expected that safety parameters by nanofluids were better than pure water. According to heat transfer equations the Outer Cladding Surface temperatures can be calculated by below relations (El-Wakil, 1971):

$$q'' = h(T_s - T_f) \tag{14}$$

$$q'' = k_{gap}\frac{\partial T}{\partial r} \tag{15}$$

The analytical solution of the heat transfer equation in the radial direction for fuel pellets is Eq. (16), which described the radial distribution of fuel temperature:

$$T_{(r)} = \frac{q'''}{4k_{ave}}(r^2 - r_{fs}^2) + T_{fs} \tag{16}$$

In this work, the one-dimensional finite difference method (FDM) has been employed in the heat transfer calculations (the coolant to the fuel center).

3 Results

3.1 Results of Molecular Dynamics

The coolant in the Bushehr nuclear reactor has a high temperature and high pressure. To study the nanofluids behavior, the physical properties of nanofluid in reactor condition are necessary. Reported experimental analysis have not been performed for Cu-water nanofluids as a reactor coolant. Also, the experimental data are available in room conditions. In this work, the molecular dynamics simulation is carried out to obtain the properties. The simulation requires validation of the model and interaction potentials. So, first the simulation is performed under room conditions and the experimental data (Xuan and Li, 2000; Xian-Ju and Xin-Fang, 2009) have been used to verify the result of thermal conductivity and dynamic viscosity. These experiments were performed in several volume fractions. Experimental results demonstrate the linear relations. The comparison of the linear trend lines obtained from the experimental results and MD results has shown the maximum error for thermal conductivity equal to 5.84% and a maximum error for dynamic viscosity equal to 4.86%. Diagrams and obtained linear equations have been shown in Figs. 4 and 5. The simulations have been performed by pressure 15.7 MPa in temperatures 564, 574, 584, and 594 K. The results obtained for the considered volume fractions are shown in Figs. 6 to 7. According to the experimental and the theoretical results (Al-Sharafi et al., 2016; Guo et al., 2018; Alawi et al., 2018), It was observed that behaviors of thermal conductivity and dynamic viscosity versus temperature have linear equations. Therefore, linear equations derived from the molecular dynamics simulation. The results were compared in a temperature range of 564 to 594 K. In the simulation of nanofluids by equilibrium molecular dynamics, always the ratio of property is used to compare the results for thermal conductivity and dynamic viscosity (Kakaç and Pramuanjaroenkij, 2009; Prasher et al., 2005). So, these behaviors have been reported.

For validation, MD results at room conditions was compared with experimental results (Figs. 4 to 5). The errors are based on the comparison of the line equations of experimental and MD results in the considered range.

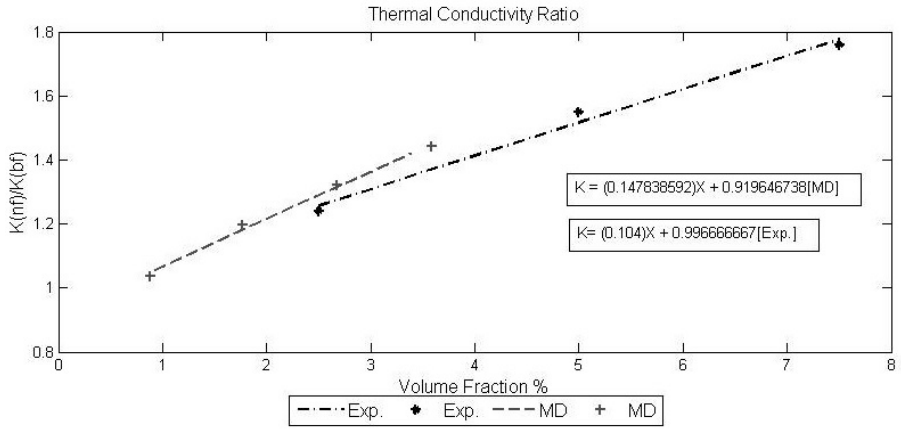

Figure 4: Thermal conductivity ratio (nanoparticles and base fluid).

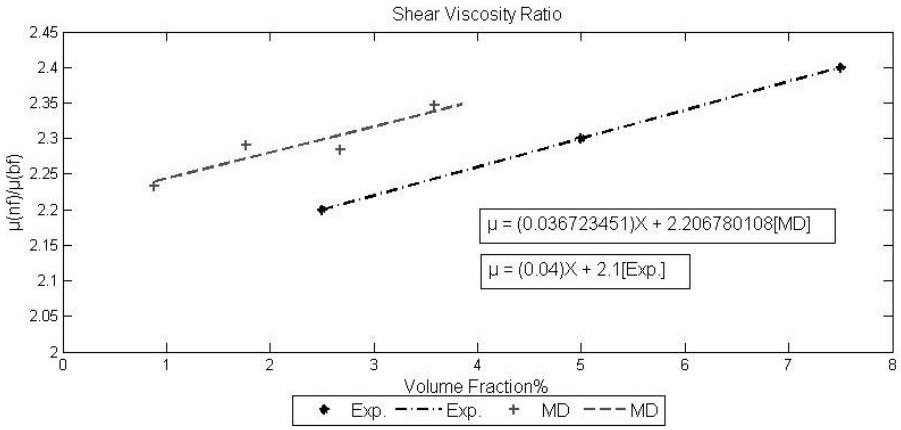

Figure 5: Shear viscosity ratio (nanoparticles and base fluid).

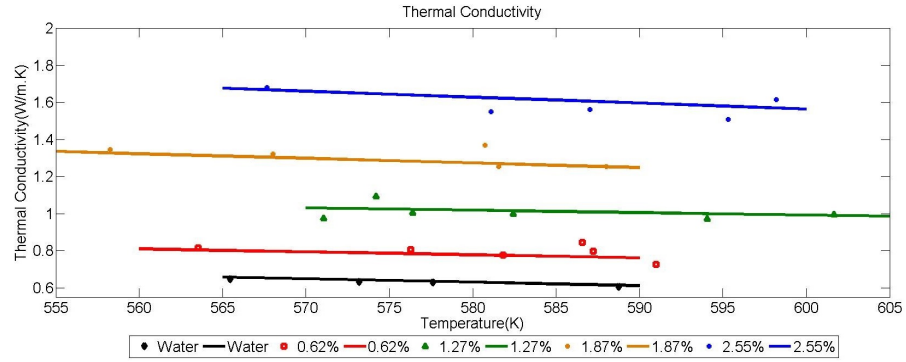

Figure 6: The thermal conductivity (MD).

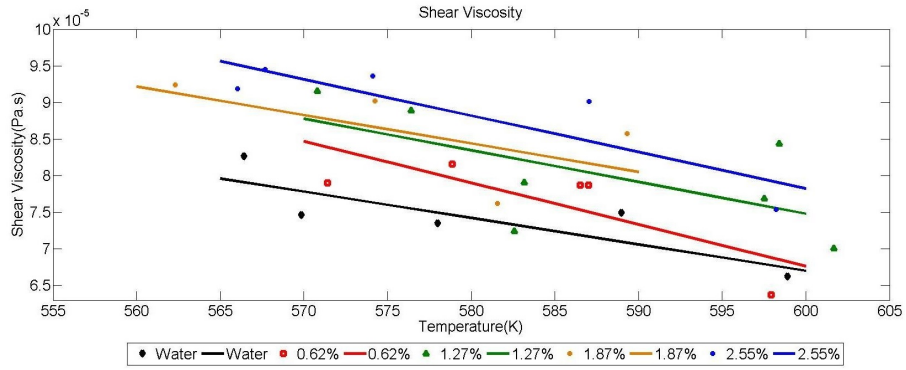

Figure 7: The shear viscosity (MD).

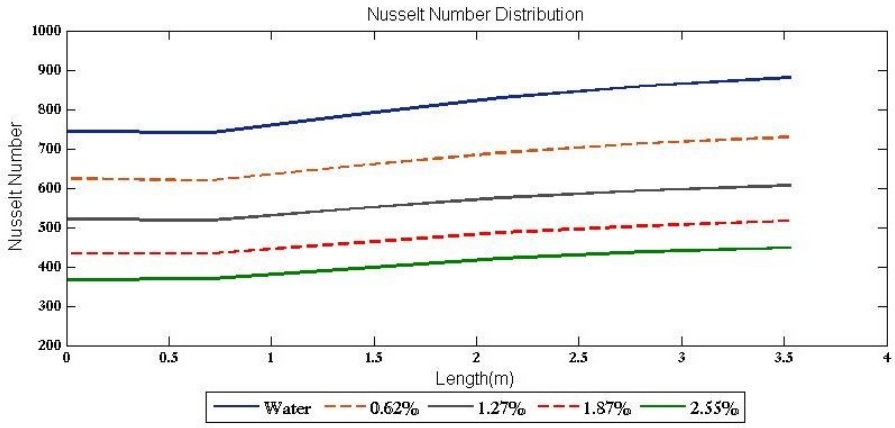

Figure 8: The distribution of the Nusselt number along coolant channel.

The symbols are values that calculated from MD simulations for various coolants, and lines are linear trend lines of symbols. The linear equations of thermal conductivity are presented as described in Table 4.

The linear equations of shear viscosity are presented as described in Table 5.

As depicted in the results, the thermal conductivity and shear viscosity have decreased with increasing temperature. Also, by increasing the volume fraction at a constant temperature, thermal conductivity, and shear viscosity have increased. Increasing the shear viscosity causes to increase in the pump's work. Generally, results demonstrate good agreement with published data.

Table 4: Linear equation of Thermal Conductivity [$K = A(T) + B$].

Volume fraction (%)	A	B
0	-0.001959000	1.681736000
0.62	-0.001793771	1.743333367
1.27	-0.001294255	1.645914305
1.87	-0.002873467	2.808325469
2.55	-0.003733504	3.574849692

Table 5: Linear equation of Shear Viscosity [$K = A(T) + B$].

Volume fraction (%)	A	B
0	-3.96740E-07	0.000315894
0.62	-6.402040E-07	0.000466172
1.27	-4.720960E-07	0.000374420
1.87	-4.19670E-07	0.000345604
2.55	-5.490120E-07	0.000424804

3.2 Results of Computational Fluid Dynamics

According to FSAR, the outlet temperature of reactor core is 594 K. So, to verify the simulations, the fuel assembly with the pure water as the coolant has been simulated and average outlet temperature of 594.24 K is obtained. The CFD simulation results have been obtained for the WWER1000 reactor at 3000 MWth. The results of CFD modeling for several volume fraction of Cu-Water nanofluids are presented in Tables 6 to 7.

It can be observed (see Table 6) that the outlet temperature did not change significantly while thermal conductivity is doubled and C_p has been reduced. This is due to the low variation of ρC_p while the fluid temperature depends on it. This term expresses the amount of heat that must be given to the fluid to increase the fluid temperature by one degree. With the increase of the volume fraction, the heat transfer coefficient (h) and thermal diffusivity (α) have increased. This case shows that the heat diffusion in the nanofluids is faster than in the pure water. For more certainty, these properties have been investigated for fuel assembly (Table 7).

In Table 7, the results show the trends are maintained and faster heat diffusion in the fluid by increasing the volume fraction of the nanofluid.

As shown in Fig. 8, Nusselt values decreased with increasing volume fraction. The Nusselt number represents the ratio of convective to conduction heat transfer. Therefore, by increasing the volume fraction of nanoparticles in the base fluid, the contribution of conductive heat transfer has become more prominent.

As depicted in Fig. 9, the heat transfer coefficient has increased with the increasing volume fraction of nanoparticles. The heat transfer coefficient performs the main effect on cooling of solid surfaces contacting with fluid.

As it is clear from Fig. 10, by increasing nanoparticles volume fraction up to 1.27%, the coolant temperature increases, but it has a downward trend from this point up to 2.55%, and fluid temperature decreases with the growth of volume fractions. This is due to changes in ρC_p. This term represents the amount of heat can be stored in the fluid to increase the temperature by one-degree. Usually, using nanofluids reduces ρC_p, while the specific heat capacity of nanoparticles is lower than water, their density is higher than water. The distribution of coolant temperature for pure water (Fig. 11-A) and Cu-Water with 0.62% to 2.55% volume fractions (Figs. 11-B to 11-E) have been provided in Fig. 11.

3.3 Results of Thermal-hydraulic Parameters

Steps to analyze the effect of nanofluid in increasing heat removal:

Table 6: Average properties at the fuel assembly outlet.

Properties	Volume fraction				
	0.00%	0.62%	1.27%	1.87%	2.55%
T (K)	594.239	594.444	594.931	594.648	594.319
K ($W.mK^{-1}$)	0.517628	0.677037	0.875922	1.09962	1.35596
μ (Pa.s)	8.01368e-5	8.56066e-5	9.35555e-5	9.60482e-5	9.85155e-5
ρ (kg/m3)	678.885	724.876	768.732	824.394	854.191
C_p (J/kg K)	6134.57	5706.04	5343.18	5083.31	4905.43
ρC_p (Pa/K)	4.16364e+6	4.13514e+6	4.10619e+6	4.18955e+6	4.1886e+6
h ($W.m^2K$)	39888.2	43245.8	46490.6	49685	53235.5
α ($m^2.s^{-1}$)	1.24341e-7	1.63749e-7	2.13351e-7	2.62533e-7	3.23802e-7

Table 7: Average properties in the fuel assembly.

Properties	Volume fraction				
	0.00%	0.62%	1.27%	1.87%	2.55%
T (K)	581	581.125	581.455	581.293	581.164
K ($W.mK^{-1}$)	0.543557	0.700929	0.893363	1.138	1.40507
μ (Pa.s)	8.53881e-5	9.41337e-5	9.99172e-5	0.000101653	0.000105738
ρ (kg/m3)	708.198	756.224	804.423	857.138	897.776
C_p (J/kg K)	5730.44	5328.17	4925.12	4694.15	4482.79
ρC_p (Pa/K)	4.05094e+6	4.02193e+6	3.95257e+6	4.01558e+6	4.01296e+6
h ($W.m^2K$)	38291.2	41147.9	43750.2	46978.5	49874.6
α ($m^2.s^{-1}$)	1.34371e-7	1.74484e-7	2.26374e-7	2.84031e-7	3.50975e-7

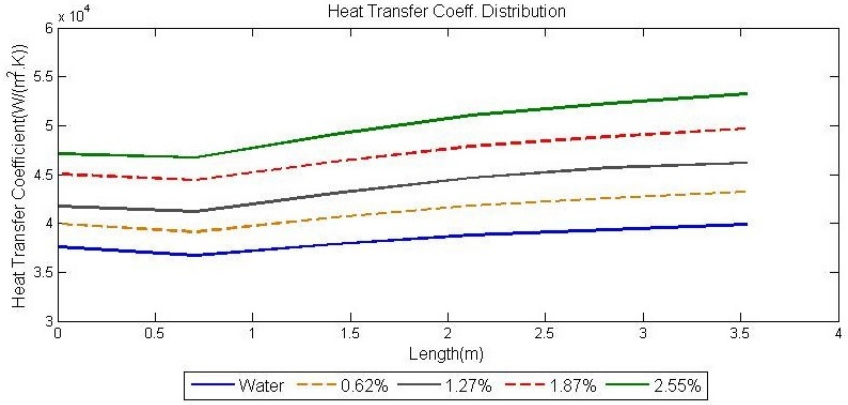

Figure 9: The distribution of the heat transfer coefficient along coolant channel.

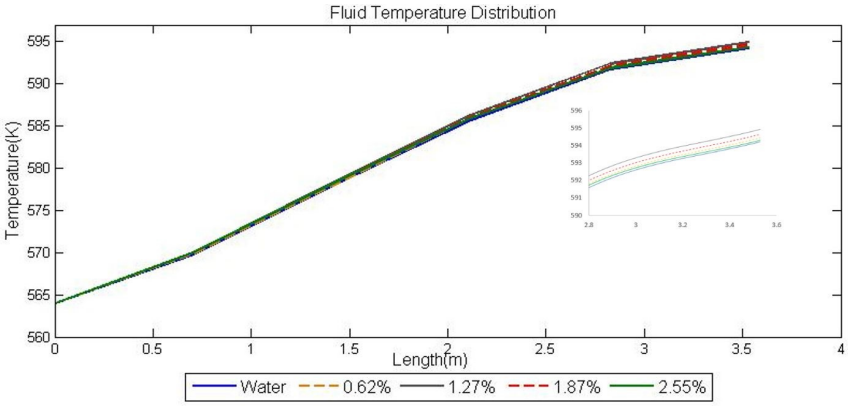

Figure 10: The temperature distribution along coolant channel.

- Calculation of the maximum fuel temperature and the maximum Outer Cladding Surface temperature at the power of 3000 MWth and pure water as a coolant.
- Calculation of the maximum fuel temperature and the maximum Outer Cladding Surface temperature at powers higher than 3000 MWth and Cu-Water nanofluids as coolant.

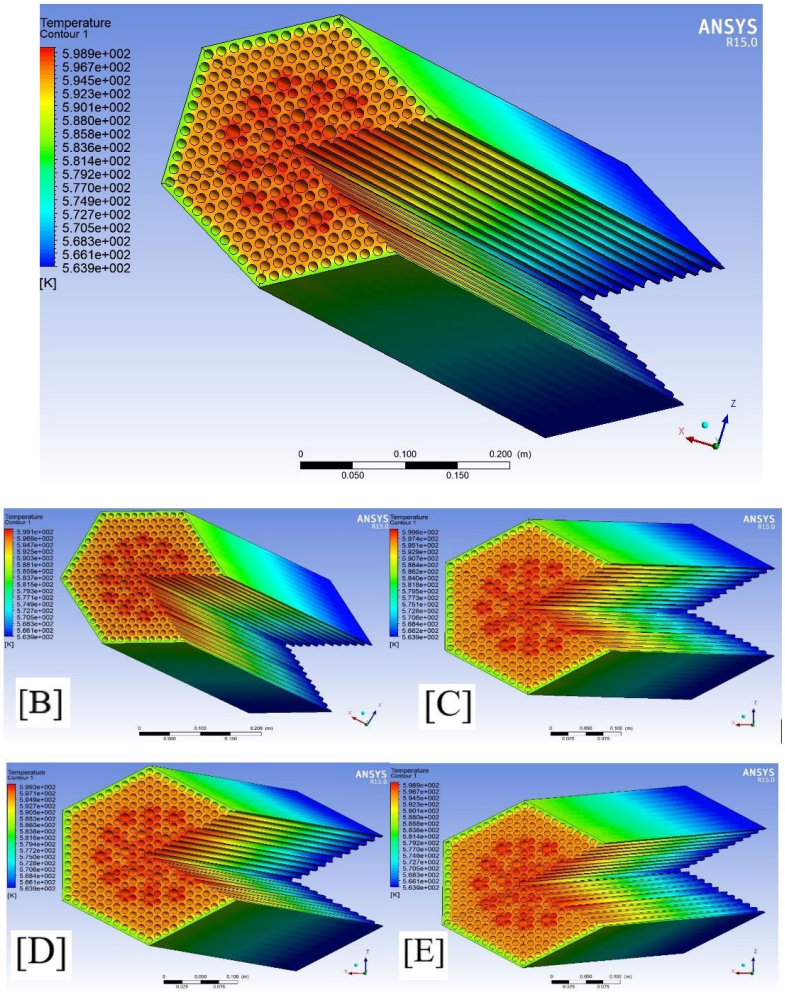

Figure 11: The temperature distribution along coolant channel by CFD.

- Comparison of the maximum fuel temperature between pure water at 3000 MWth and nanofluids at higher powers.
- Comparison of the maximum sheath temperature for pure water at 3000 MWth and nanofluids at higher powers.
- Determining the maximum power of the reactor in such a way that the maximum fuel temperature and the maximum Outer Cladding Surface temperature by nanofluid as a coolant do not exceed the corresponding temperature at the power of 3000 MWth and pure water.

By increasing the reactor power to 3050 MWth, the heat flux increasing factor in fuel rods will be 1.0166. The temperatures distribution for nanofluids as coolants compared with pure water at 3000 MWth have been provided in Figs. 12 to 13.

As it is shown in the Figs. 12 to 13, the highest and lowest temperatures of the fuel centerline along the reactor height are volume fractions of 0.62% and 2.55%, respectively. It is clear that the increase in nanoparticles concentration leads to reduction in the maximum fuel temperature and maximum Outer Cladding Surface temperature (See Fig. 14).

The maximum fuel temperature at 3050 MWth by 2.55% Cu-Water nanofluid as a coolant is higher than the corresponding temperature at 3000 MWth by pure water. By analyzing data, the coolant with a volume fraction of 2.55% has shown more favorable results. In Table 8, the results for safety parameters are obtained for water-copper nanofluid with a volume fraction of 2.55% as coolant.

In this way, other powers have been investigated in order to achieve the maximum fuel temperature, the results are presented in Table 8. Therefore, the use of nanofluids to increase heat removal from the reactor core is not very economical.

Table 8: Safety parameters by Cu-Water with 2.55% as the coolant at different reactor powers.

Safety Parameters		
Reactor Power	maximum fuel temperature (°C)	maximum cladding surface temperature (°C)
3000 (Water)	1204.8	602.5546
3050	1211.4	600.611
3020	1205.1	600.2505
3019	1204.8	600.2385

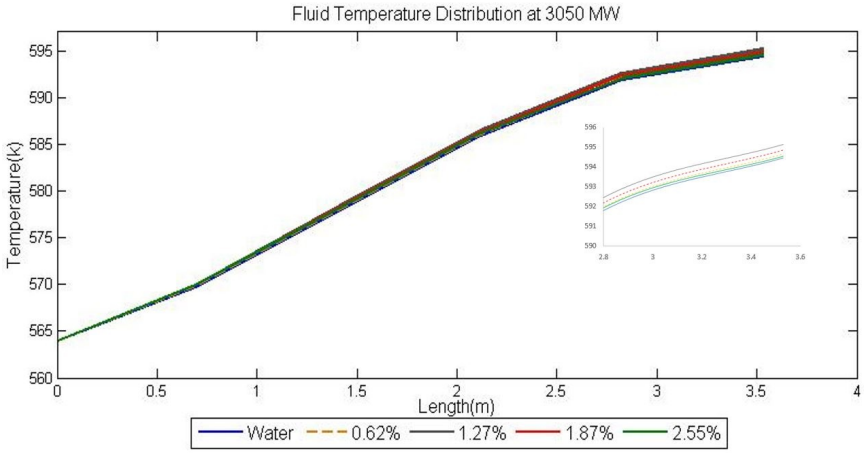

Figure 12: The temperature distribution of coolants along the channel.

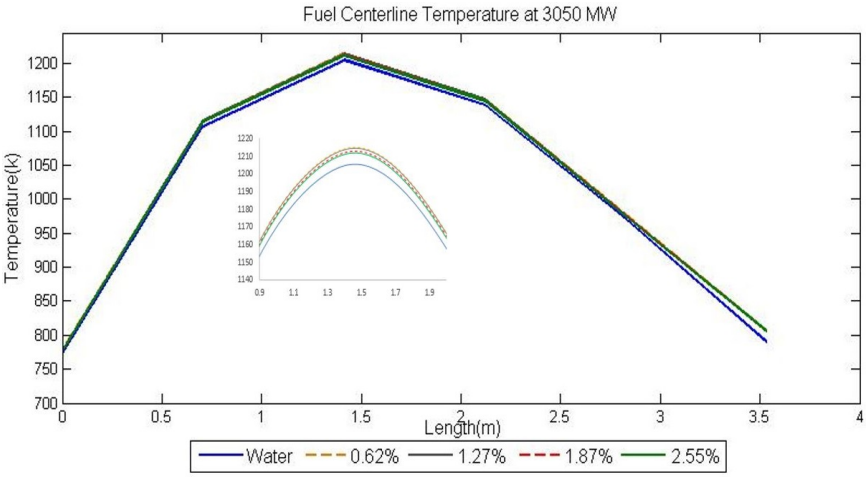

Figure 13: The temperature distribution of the fuel centerline for along the coolant channel.

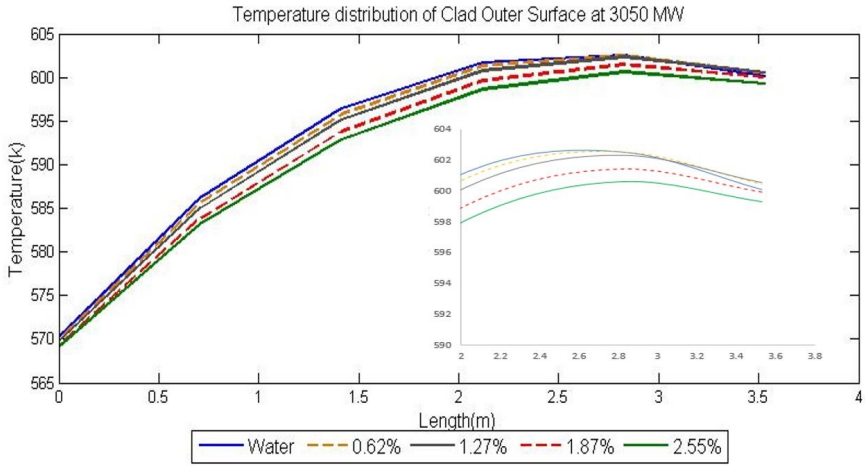

Figure 14: The temperature distribution of cladding surface for coolants along the channel.

4 Conclusions

This research showed that for safety analysis of nuclear reactors molecular dynamics simulations, computational fluid dynamics, and heat transfer calculations in the fuel assembly can be applied. This method needs improvement and development to achieve more precise results. In addition, it concludes that, nanofluids as a coolant in the reactor increase the heat transfer coefficient and thermal diffusivity while ρC_p does not change significantly. In addition, nanofluids increase undesirable viscosity. Nanofluids increase heat removal capability so that the safety

parameters, like the maximum fuel temperature, are not weakened. Due to the increase in heat transfer coefficient, nanofluids can be used to improve reactor safety. Molecular dynamics simulation can be used to obtain the thermal-physical properties of reactor coolants. Also, for future works, it is recommended to study the use of nanofluids in high-temperature reactors such as SCWR that can lead to further increase in heat removal and for molecular dynamics simulation, the use of different interaction potential parameters can lead to increase the accuracy of results.

Conflict of Interest

The authors declare no potential conflict of interest regarding the publication of this work.

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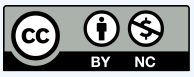

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