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Numerical Modeling for Thermal Investigations of Fuel Cell by Using TiO_2 , ZnO and SiO_2 Water Based Nanofluids

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Abstract: Thermal management of fuel cell is very much essential for its efficient and effective functioning. The present study involves a fuel cell which is encapsulated in a horizontal duct open at both the ends. The nanofluid as coolant is allowed to pass through the annular region between the fuel cell and duct. Three different water based nanofluids, namely Water- TiO_2 , Water- ZnO and Water- SiO_2 , are considered as coolants in the present investigations. The numerical studies are carried out to obtain the heat transfer behavior of encapsulated fuel cell for maintaining its temperature within the safe limit. For that, a 2D numerical model is being developed. The continuity, momentum and energy equations are solved to predict the thermal behavior. The simulations are performed to predict the temperature fields and temperature contours. The trends of results are along the expected lines. Then, the simulation results predicted with three different water based nanofluids are analyzed and compared for realizing the relative importance of the stated nanofluids. The model parameters considered are fuel cell heat flux of 10 W/cm^2 and nanofluid velocity of 9 m/s at duct inlet. The Water- ZnO is identified as the nanofluid giving the optimal fuel cell performance without any such thermal failure.

Keywords: Fuel Cell, Cooling, Simulation, Nanofluids, Water- TiO_2 , Water- ZnO , Water- SiO_2

I. INTRODUCTION

Fuel cells are devices that produce electricity through electrochemical reactions by transforming chemical energy (stored in the fuel) to electrical energy. Mostly hydrogen is used as fuel and the ambient air acts like an oxidant. However, in few cases methanol is also used as fuel and pure oxygen as oxidant. Fuel cells require a fuel source and will perform for infinite period of time if inflows of fuel are maintained. As the power generation takes place without burning of fossil fuels (or any other energy sources), fuel cells produce very less pollution since the byproduct involved in fuel cell is only heat and water. For the said reason it comes under green energy technology. The maintenance of fuel cell is simple since there are very few moving parts in the system as compared to any other energy sources. Fuel cells do not need conventional fuels such as oil or gas and can therefore reduce economic dependence on oil producing countries.

In case of batteries, they consume solid reactants such as lead, cadmium or other metal. Once these reactants are depleted, they must be discarded or recharged. Batteries can be regenerated either with electricity or by replacing the electrodes. Fuel cells maintain their popularity as efficient power generators. Considering their high energy conversion efficiency, zero emission potential, low noise and potential use of renewable fuels, the fuel cells are considered as future devices for mobiles, stationary and portable power applications. Researchers across the globe are still working for its implementation to some of the space programs and produce power for probes, satellites and space capsules. Fuel cells also have been used in various other applications due to its tremendous success. Fuel cells are successfully used to power fuel cell vehicles and are also used for primary and backup power for residential, industrial and commercial buildings.

II. LITERATURE REVIEW

Xuan and Roetzel [1] developed concepts of heat transfer correlations relating to nanofluids. S. Litster and McLean [2] described about the functioning of various proton exchange membrane (PEM) fuel cell electrodes. Min et al. [3] performed the parametric studies of proton exchange membrane fuel cell (PEMFC) numerically. Xuan et al. [4] reviewed about the contaminations in PEM type hydrogen fuel cells. Chaitanya et al. [5] investigated about the effects of anisotropic heat conduction in PEM type fuel cells. Nguyen et al. [6] used Al_2O_3 water nanofluid to enhance heat transfer in an electronic liquid cooling system. Sangseok and Dohoy [7] described about the various approaches for thermal management of proton exchange membrane fuel cell systems. Jong-Woo and

Song-Yul [8] investigated about the coolant control in PEM fuel cell systems. Zhang and Kandlikar [9] performed critical reviews of cooling techniques in PEM fuel cell stacks. Mohamed and Atan [10] analyzed about the excessive heating on thermal and electrical resistance of a polymer electrolyte membrane fuel cell. Keshavarz et al. [11] executed numerical studies on the influences of nanofluids on mini-channel heat sink. Houchang et al. [12] investigated about the performance characteristics of air-cooled proton exchange membrane fuel cell stacks at normal atmospheric conditions.

From the aforesaid literature, to the best of author’s knowledge, it is quite obvious that there is not a single comprehensive numerical investigation pertaining to the influences of water based nanofluids (namely Water-TiO₂, Water-ZnO and Water-SiO₂) on heat transfer behavior of fuel cells. With this perspective, the present paper demonstrates numerical investigations with the stated nanofluids on thermal characteristics of fuel cells. And also, the numerical model includes additional key factors like inertia, viscosity and gravity effects apart from the usual issues concerning the present physical problem. However, the stated model ignores both compressibility and viscous heat dissipation effects. The model is very well demonstrated for the detailed numerical investigations on the influences of the already stated nanofluids (as they significantly affect the cooling characteristics) by taking fuel cell heat flux and duct inlet nanofluid velocity as the important model parameters. Lastly, the predictions of the model pertaining to the different nanofluids are also along the expected lines.

III. DESCRIPTION OF PHYSICAL PROBLEM

The schematic and detailed representation of a typical fuel cell to be kept in a duct is depicted in the figure 1. The corresponding physical model as illustrated in figure 2, describes about the overall heat transfer from the fuel cell which is encapsulated in a horizontal duct open at both the ends. The coolants considered in the present investigations are three different water based nanofluids named as Water-TiO₂, Water-SiO₂ and Water-ZnO. A 2D model is considered to save computation/simulation time by ignoring end effects in the transverse direction. The model includes the viscosity along with the gravity effect as well. The fluid flow is considered to be laminar and incompressible. The no slip boundary condition is specified at the walls. The velocity inlet boundary condition is set at the entry to the duct from where water based nanofluids are allowed to pass through. A pressure outlet boundary condition is specified at the exit of the duct. The ambient condition is taken at the entry to the duct. For cooling of the fuel cell surface, a convective boundary condition in the form of heat flux is introduced to simulate the overall temperature variation inside the duct due to heat transfer. The thermo-physical properties of various nanoparticles together with the additional system parameters, are shown in table 1.

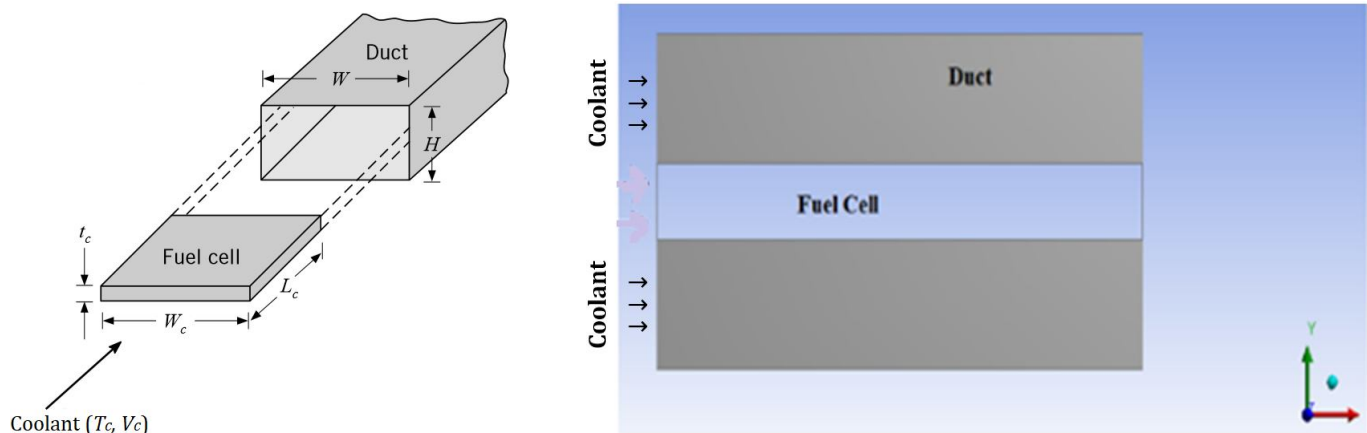


Figure 1. Schematic of fuel cell to be kept in a rectangular duct Figure 2. 2D computational domain of physical model

Table 1. Thermophysical properties of nanoparticles and model data

| Nanoparticle Properties | TiO ₂ | ZnO | SiO ₂ |
|--------------------------------------|------------------|------|------------------|
| Density, ρ (Kg/m ³) | 4175 | 5606 | 2648 |
| Specific heat, C_p (J/kg-K) | 692 | 667 | 745 |
| Thermal conductivity, k (W/m-K) | 8.4 | 13.0 | 10.4 |
| Model Data | Values | | |
| Height of duct (H) | 26 mm | | |
| Length of fuel cell (L_c) | 50 mm | | |

| | |
|-----------------------------------|----------------------|
| Thickness of fuel cell (t_c) | 6 mm |
| Width of fuel cell (W_c) | 50 mm |
| Width of duct (W) | 50 mm |
| Ambient air temperature | 300 K |
| Fuel cell heat flux | 10 W/cm ² |
| Velocity of coolant at duct inlet | 9 m/s |

IV. MATHEMATICAL FORMULATION

The present physical problem is transformed into a set of governing transport equations which are solved through the present numerical techniques concerning both modeling and simulation. The related continuity, momentum and energy equations in 2D for a fully developed hydrodynamic and thermal flow situations are described in equations from (1) to (4), respectively. The compressibility and the viscous heat dissipation effects are neglected in the existing physical situation.

Continuity equation:
$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{1}$$

X-momentum equation:
$$\rho \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} \right) = -\frac{\partial P}{\partial x} + \mu \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \tag{2}$$

Y-momentum equation:
$$\rho \left(\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\partial P}{\partial y} + \mu \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) + \rho g \tag{3}$$

Energy equation:
$$\left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} \right) = \alpha \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) \tag{4}$$

V. NUMERICAL PROCEDURES

The schematic and detailed representation of a typical fuel cell to be kept in a duct is depicted in the figure 1. The corresponding physical model as illustrated in figure 2, describes about the overall heat transfer from the fuel cell which is encapsulated in a horizontal duct open at both the ends. The coolants considered in the present investigations are three different water based nanofluids named as Water-TiO₂, Water-SiO₂ and Water-ZnO. A 2D model is considered to save computation/simulation time by ignoring end effects in the transverse direction. The model includes the viscosity along with the gravity effect as well. The fluid flow is considered to be laminar and incompressible. The no slip boundary condition is specified at the walls. The velocity inlet boundary condition is set at the entry to the duct from where water based nanofluids are allowed to pass through. A pressure outlet boundary condition is specified at the exit of the duct. The ambient condition is taken at the entry to the duct. For cooling of the fuel cell surface, a convective boundary condition in the form of heat flux is introduced to simulate the overall temperature variation inside the duct due to heat transfer. The thermo-physical properties of various nanoparticles together with the additional system parameters, are shown in table 1.

A. Numerical scheme and solution algorithm

The aforementioned governing transport equations are transformed into generalized form as follows.

$$\frac{\partial}{\partial t}(\rho \phi) + \nabla \cdot (\rho \mathbf{u} \phi) = \nabla \cdot (\Gamma \nabla \phi) + S \tag{5}$$

The transformed governing transport equations are discretized with the second order upwind scheme using a pressure based finite volume method with the SIMPLER algorithm, where Γ represents a transport property (k or μ), ϕ denotes any conserved variable and S is a source term.

B. Choice of grid size, time step and convergence criteria

A comprehensive and complete grid-independence test is carried out to establish a suitable spatial discretization, and the levels of iteration convergence criteria to be used. As an outcome of this test, we have used 50 × 20 uniform grids for the final simulation. Corresponding time step taken in the simulation is 0.0001 seconds. Though we checked with smaller grids of 30 and 40 in numbers for 20 mm height of the computational domain, it is observed that a finer grid system does not alter the results significantly. In other words, the statistical data reveals that the finer grids have minor effect in the simulation results which is quite obvious from the definition of grid-independence test. And also, the smaller grid pertains to more computational time involving more evenness in results of different contours/fields.

Convergence in inner iterations is declared only when the condition $\left| \frac{\varphi - \varphi_{old}}{\varphi_{max}} \right| \leq 10^{-4}$ is satisfied simultaneously for all variables, where φ stands for each variable u , v , and T at a grid point at the current iteration level, φ_{old} represents the corresponding value at the previous iteration level, and φ_{max} is the maximum value of the variable at the current iteration level in the entire domain.

VI. RESULTS AND DISCUSSION

Numerical simulations are performed to investigate the influences of three different water based nanofluids (such as Water-TiO₂, Water-SiO₂ and Water-ZnO) on cooling characteristics of fuel cell in terms of temperature distributions (i.e. temperature contours/fields) and surface temperatures of fuel cells. At the outset, the height of the duct is considered to be 26 mm, besides, the thickness and the length of the fuel cell as 6 mm and 50 mm respectively. In addition, the heat flux associated with the fuel cell is taken to be 10 W/cm² and the velocity of nanofluid at the duct inlet is chosen to be 9 m/s.

A. Case study with Water-TiO₂ nanofluid as coolant

With the stated model conditions, in order to investigate the influence of Water-TiO₂ nanofluid on the thermal behavior of the fuel cell, the numerical simulations are performed, by taking into account the thermophysical properties of the stated nanofluid.

Figure 3 illustrates the simulated results of the temperature field (together with the colored scale bar displaying the temperature values in terms of K) as obtained at the stated model conditions by considering Water-TiO₂ nanofluid as coolant. The surface temperature of fuel cell is found to be 353 K (which is very close to the safe limit of 356 K temperature as desired in order to avoid the thermal failure of the fuel cell). As expected, the temperature of the Water-TiO₂ nanofluid is maximum near the vicinity of fuel cell. And also, the temperature of the Water-TiO₂ nanofluid gradually decreases with the increase in the distance from the fuel cell and then it becomes equal to the atmospheric temperature in the far field region. The corresponding temperature contour is also demonstrated in figure 4. Here also, the trends of results are along the expected lines.

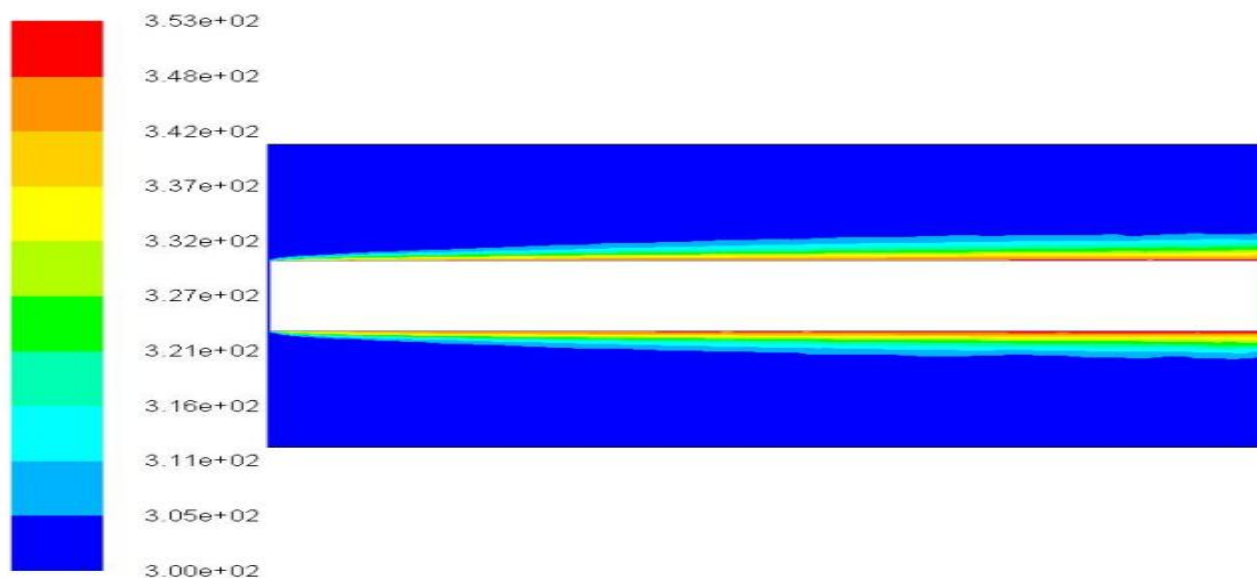


Figure 3. Temperature field with Water-TiO₂ nanofluid as coolant.

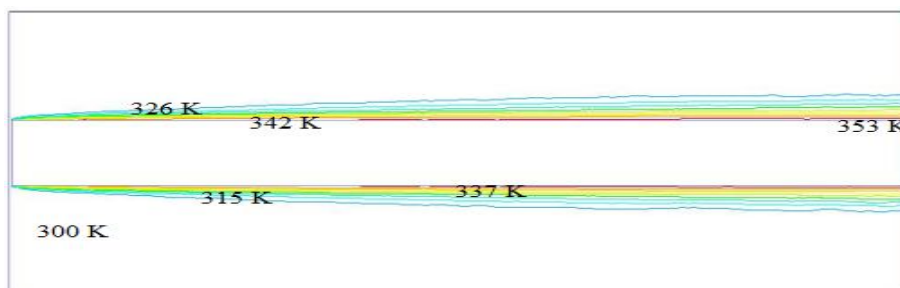


Figure 4. Temperature contour with Water-TiO₂ nanofluid as coolant.

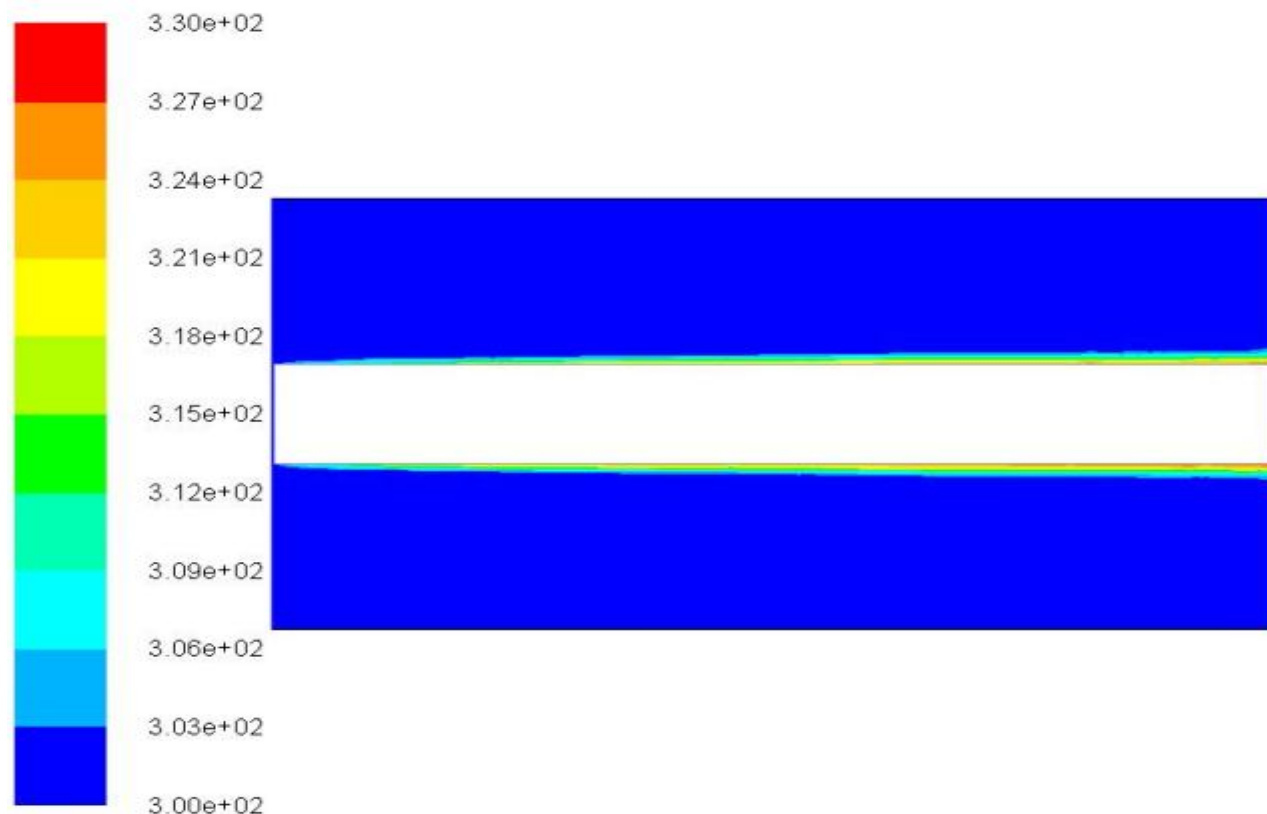


Figure 5. Temperature field with Water-ZnO nanofluid as coolant.

B. Case study with Water-ZnO nanofluid as coolant

With the stated model conditions, in order to investigate the influence of Water-ZnO nanofluid on the thermal behavior of the fuel cell, the numerical simulations are performed, by taking into account the thermophysical properties of the stated nanofluid.

Figure 5 illustrates the simulated results of the temperature field (together with the colored scale bar displaying the temperature values in terms of K) as obtained at the stated model conditions by considering Water- ZnO nanofluid as coolant. The surface temperature of fuel cell is found to be 330 K (which is also within the safe limit of 356 K temperature as desired in order to avoid the thermal failure of the fuel cell). As expected, the temperature of the Water- ZnO nanofluid is maximum near the vicinity of fuel cell. And also, the temperature of the Water- ZnO nanofluid gradually decreases with the increase in the distance from the fuel cell and then it becomes equal to the atmospheric temperature in the far field region. The corresponding temperature contour is also demonstrated in figure 6. Here also, the trends of results are along the expected lines.

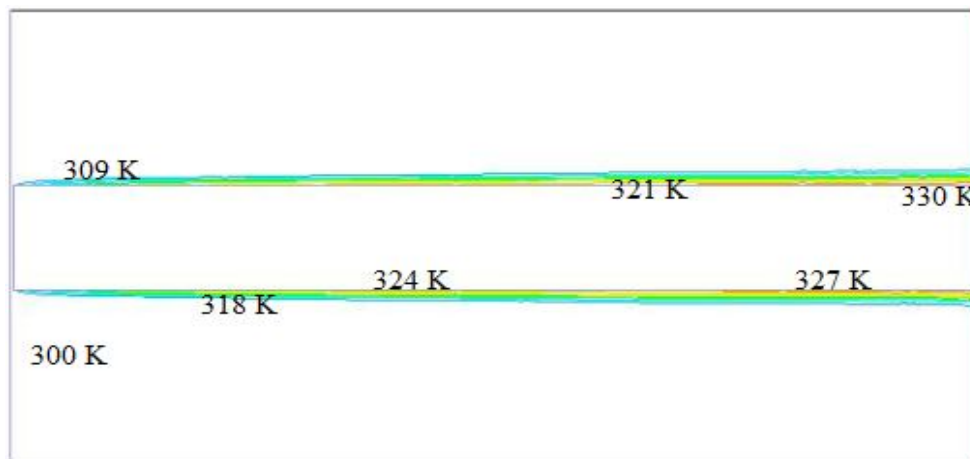


Figure 6. Temperature contour with Water-ZnO nanofluid as coolant.

C. Case study with Water- SiO₂ nanofluid as coolant

With the stated model conditions, in order to investigate the influence of Water-SiO₂ nanofluid on the thermal behavior of the fuel cell, the numerical simulations are performed, by taking into account the thermophysical properties of the stated nanofluid.

Figure 7 illustrates the simulated results of the temperature field (together with the colored scale bar displaying the temperature values in terms of K) as obtained at the stated model conditions by considering Water-SiO₂ nanofluid as coolant. The surface temperature of fuel cell is found to be 342 K (which is also within the safe limit of 356 K temperature as desired in order to avoid the thermal failure of the fuel cell). As expected, the temperature of the Water-SiO₂ nanofluid is maximum near the vicinity of fuel cell. And also, the temperature of the Water-SiO₂ nanofluid gradually decreases with the increase in the distance from the fuel cell and then it becomes equal to the atmospheric temperature in the far field region. The corresponding temperature contour is also demonstrated in figure 8. Here also, the trends of results are along the expected lines.

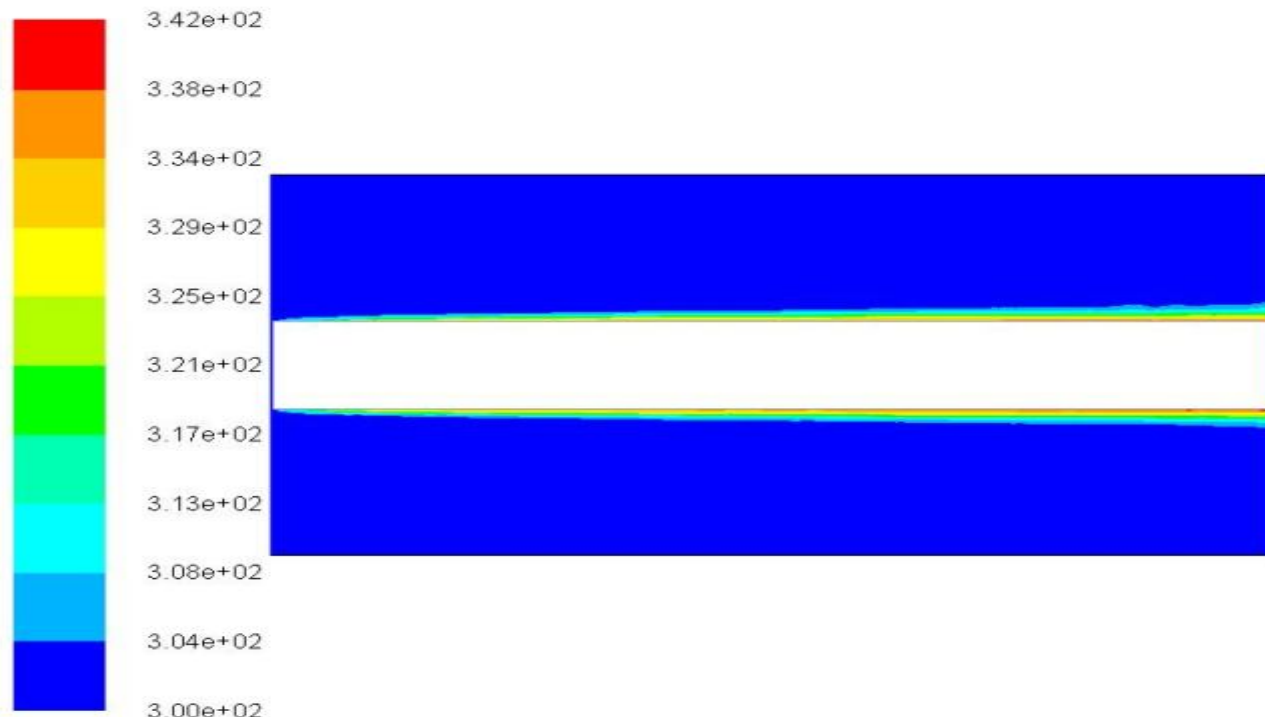


Figure 7. Temperature field with Water- SiO₂ nanofluid as coolant.

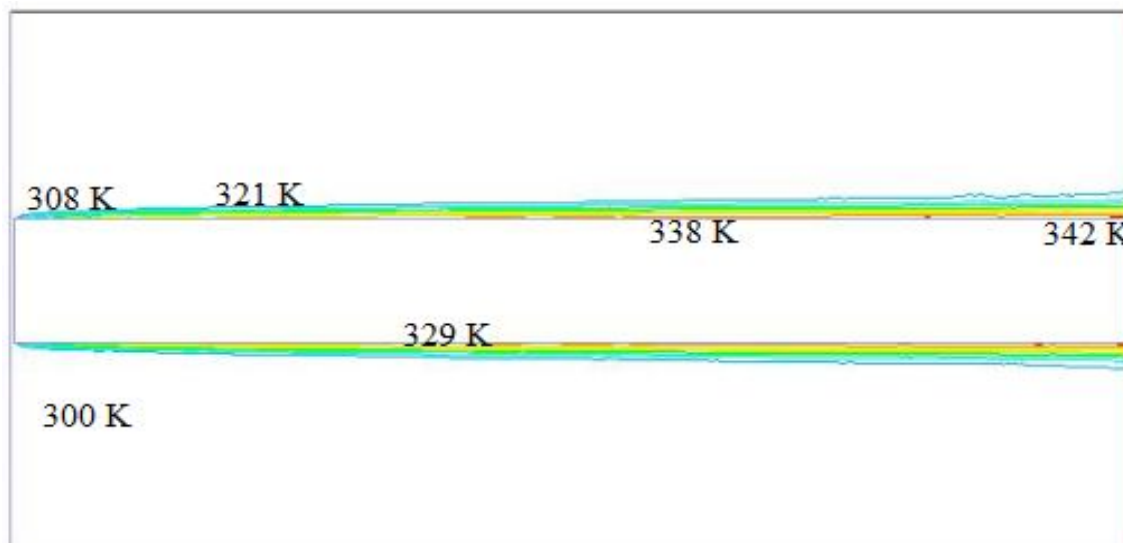


Figure 8. Temperature contour with Water- SiO₂ nanofluid as coolant.

D. Comparison of temperatures of fuel cells obtained with different nanofluids as coolants

Table 2 summarizes the numerically predicted temperatures of the fuel cells as obtained with the use of three different water based nanofluids (namely, Water-TiO₂, Water-ZnO and Water-SiO₂) as coolants. It is observed that the numerical predictions/results are comparable with each other. As expected, the variations in the numerically predicted temperatures of the fuel cells are witnessed very clearly with the use of the stated water based nanofluids as coolants. This is because of the variations in the thermal conductivities of the corresponding nanoparticles as mentioned in table 1.

Table 2: Comparison of numerical predictions of fuel cells temperatures with different nanofluids as coolants.

| Name of Nanofluid | Numerically Predicted Temperature of Fuel Cell (K) |
|------------------------|--|
| Water-TiO ₂ | 353 |
| Water-ZnO | 330 |
| Water-SiO ₂ | 342 |

Correspondingly, figure 9 also illustrates the plot representing the variations in the fuel cells temperatures with three different water based stated nanofluids as coolants. It is quite obvious that the trends of the variations in the numerically predicted results are along the expected lines.

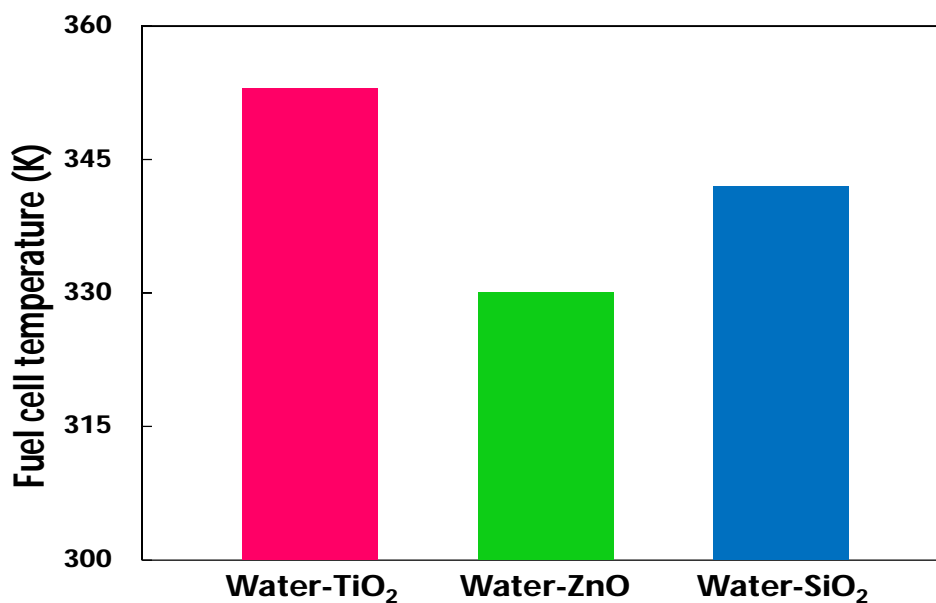


Figure 9. Variations in fuel cells temperatures with different water based nanofluids as coolants.

VII. CONCLUSIONS

A numerical model relating to the fuel cell is developed to predict the thermal behavior with three different water based nanofluids, namely Water-TiO₂, Water-ZnO and Water-SiO₂ as coolants. The model includes additional key factors like inertia, viscosity and gravity effects apart from the usual issues concerning the present physical problem. However, the stated model ignores both compressibility and viscous heat dissipation effects. The model is very well demonstrated for the detailed numerical investigations on the influences of the already stated nanofluids (as they significantly affect the cooling characteristics) by taking fuel cell heat flux of 10 W/cm² and duct inlet nanofluid velocity of 9 m/s as the important model parameters. The predictions of the model pertaining to the different nanofluids are along the expected lines. Direct comparison with other numerical models of fuel cells is not possible because of the absence of such models in the literature. However, the experimental comparison with an in-house experimental setup is planned for the future. With the said model conditions, it is observed that the Water-ZnO nanofluid renders appropriately effective cooling behavior without any such thermal failure and is the optimum one as the fuel cell temperature is very far below the safe

limit. Hence, the stated model together with the nanofluid can be utilized directly in industries to enhance heat transfer and for cooling of fuel cells.

VIII. ACKNOWLEDGMENT

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