Iranian Journal of Chemical Engineering

Journal Homepage: www.ijche.com

pISSN: 1735-5397
eISSN: 2008-2355

Regular Article

Simulation and Optimization of Energy in Oil Storage Tanks Using Nanocomposites of Phase Change Materials by Computational Fluid Dynamics

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ARTICLE INFO

Article history:
Received: 2023-05-27
Accepted: 2023-10-28
Available online: 2023-10-28

Keywords:
Phase change material,
Nanocomposite,
Tank,
Latent heat,
Thermal management

ABSTRACT

Current research has simulated polymer oxide/metal oxide nanofibers (nanocomposites) through the COMSOL Multiphysics software. The oil was placed inside a cylindrical tank covered with a thin layer of phase change material nanocomposites. A combination of polyethylene glycol (PEG) as a the phase change material (PCM) and polyamide 6 (PA6) as a support matrix for nanofibers were used. The effect of some parameters such as the type of metal oxide nanoparticles (Al_2O_3, Fe_2O_3, TiO_2, and CuO), the ratio of metal oxide to polymer (2% and 8% by weight), and time (600 and 4800 s) on some thermophysical properties such as changes in temperature, density and thermal conductivity were investigated. The simulation results showed that the most suitable system for thermal management is related to the presence of nanoparticles and PCM with the highest weight percentage. It was also found that the use of the nanofibers of phase change materials is very effective in improving thermal management and temperature control. As a result, they can be used as suitable materials for storing and transferring energy. The addition of 8% nanoparticles led to a 22.5% increase in thermal conductivity. Also, by providing the same initial and boundary conditions for all cases, the amount of melting in the presence of nanoparticles with a high percentage (8%) was higher than the with a low percentage (2%). As a result, the addition of nanoparticles to increase the melting rate can be very useful for various heat management purposes such as energy storage.

DOI: 10.22034/ijche.2023.399371.1491 URL: https://www.ijche.com/article_181947.html

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1. Introduction

Due to the increase in the need for energy, the limitation of fossil fuels as a depleting resource and the increase in environmental pollutants, it is necessary to use renewable energies. In recent decades, thermal energy storage systems have been used in heating and cooling applications and have a great scope for developing renewable energies [1]. Nowadays, Nano technology has emerged as one of the leading technologies in the world and storage Energy production using this technology and the use of phase change materials should be considered [2]. We can use phase change materials in the oil industry. The importance of using these materials, in addition to environmental and technical issues, is due to its economic justification, and the proper use of these materials will lead to a significant reduction in energy consumption [3]. Today, due to the environmental pollution and the non-renewability of fossil fuels, the need to use new methods to prepare clean and renewable fuels such as thermal energy is felt more [4]. One of the most important methods of the thermal energy storage is the use of phase change materials or PCM, which can be used in oil tanks to reduce the energy consumption to a great extent when necessary [5]. It changes phase and stores energy in different forms and releases this stored energy when needed, hence these materials are important especially in the oil industry. Phase change materials are organic and inorganic compounds that have the ability to absorb and store large amounts of heat [6]. Energy-heat storage in these materials occurs during the phase change process (phase change from solid to liquid and vice versa). When these materials change phase from solid to liquid or from liquid to solid, they absorb this heat from the environment or give it back to the environment [7]. Phase change materials store heat energy during phase change and release it when the temperature of the environment decreases [8]. Unfortunately, despite the existence of problems such as the non-optimization of the energy consumption in industries, power plants, buildings and thermal energy storages, the use of phase change materials has not yet been developed in Iran. It is important and has been the focus of many researchers [9]. The phase change material has the ability to maintain this latent heat energy without any change even after thousands of phase change cycles [10]. Considering the increase in population and economic growth, the demand for energy will double the current amount by 2050, this will lead to the need for excess energy storage and making the system more economical by reducing energy loss [11]. The main advantage of these materials is that they can store 3 to 4 times more energy per volume unit than sensible heat in solids and liquids at a temperature of approximately 20 ℃. Heat storage by PCMs occurs in the transition from one phase state to another phase state [12]. The ever-increasing demand for the energy consumption and the limitation of fossil fuels as depleting resources and the increase of environmental pollutants make the issue of the energy storage very important [13]. Using latent heat storage systems with phase change materials is an effective way to store energy [14]. Phase change materials have characteristics such as the high latent heat, appropriate phase transformation temperature, and small volume change during phase change, which have effects such as increasing the heat transfer coefficient, increasing the heat capacity, and thermal and chemical stability, which causes heat storage. Nano-technology and Nano-materials, meanwhile, with the ability to absorb and store high thermal energy, are one of the new methods of this technology [15].

Oil and gas units need a large number of tanks to store crude oil and gas as well as storing various petroleum products. The number of these tanks depends on factors such as the distance and proximity of the unit from crude oil supply sources, the number and capacity of refining units, the variety of produced products, and finally how the products are transported and distributed [16]. Produced products are also supplied to the domestic or foreign market in different ways. Several factors, such as ensuring product quality uniformity, accurate measurement of product volumes for sale, and the ability to load and transfer to a tanker or ship in the shortest possible time affect the selection of these delivery methods in order to enhance efficiency and cost savings [17]. The term tank is used for large storage containers with the application of moving, storing, measuring and transporting liquids [18]. As large oil fields are exploited, new operational conditions are required. It becomes imperative to establish a suitable platform that can stabilize operations, prevent time wastage, and facilitate the transfer of crude oil and petroleum products. In large exploitation units, storage tanks are strategically positioned, often integrated into pump houses at the locations of the crude oil transfer, and embedded within export terminals to streamline the overall process [19]. The creation of storage tanks in the oil extraction and refining industries, after purification and preparation for consumption, is one of the most important issues, because the materials that are the feed of many refineries and petrochemicals are not used immediately after production [20]. The number of tanks built for the storage of crude oil and gas and storage of petroleum products depends on the capacity of the refining units, variety of products, distance and proximity of the unit from the sources of crude oil supply and the way of transporting and distributing the products. Storage tanks in oil, refining and distribution industries and petrochemical companies are used to store a huge amount of hazardous materials, therefore, when an accident occurs, there is a possibility of losing a large amount of materials and causing a lot of damage to the tank, and global statistics confirm this[21].

According to the mentioned cases, research in the field of phase change materials has been conducted in research centers around the world, which has led to improvements in the energy optimization in the last few decades. According to the conducted research, there is still a fundamental gap in the field of the energy optimization in oil pipelines in oil and gas industries. In this research, the nanofibers of phase change materials (polyethylene glycol as a phase change material and polyamide6 as a preservative) and the nanoparticles of aluminum oxide, titanium dioxide, iron oxide and copper oxide within pipelines were investigated. Various conditions, including different weight percentages and exposure times, were studied and the simulations were conducted using the COMSOL Multiphysics software.For this purpose, oil is placed inside a tube and the chamber is covered with a thin layer of the nanocomposite of the phase change material. At first, the thermophysical properties of the multi-structured nanofibers of phase change materials in different weight percentages have been investigated. Despite all the advantages, these materials have problems such as leakage and the low coefficient of thermal conductivity. As a result, the use of metal nanoparticles can improve their properties.

In the continuation of this research, the melting of polyethylene glycol-polyamide containing nanoparticles of aluminum oxide, titanium dioxide, iron oxide and copper oxide with 2% and 8% wt in taft pipelines by means of the COMSOL Multiphysics software is simulated. And the effect of the presence of nanoparticles and phase change materials with different weight percentages and the effects of changes in temperature, density, viscosity and the thermal conductivity on them have been compared. The results of the research showed that the most suitable system for heat management is related to the Nanoparticles of phase change materials with the highest weight percentage of polyethylene glycol. Also, the use of nanofibers of phase change materials is very effective in improving thermal management and temperature control and they can be used as suitable materials for the energy storage and transmission. With the incorporation of 8% weight of nanoparticles, there has been a 22.5% increase in the thermal conductivity coefficient in the nanomaterial. By creating the same initial and boundary conditions for all states, it is observed that the extent of melting in the state containing 8% weight of nanoparticles surpasses that of both states of the 2% weight and pure polyethylene glycol-polyamide 6. This shows that adding nanoparticles to polyethylene glycol in order to increase the melting rate for various purposes of heat management such as the energy storage can be useful. The result of the simulation is a significant improvement in thermophysical properties; it shows the heat that can be used in optimizing the thermal management of various systems.

In 2007, Pesopadi and his colleagues [22] conducted extensive research on the application of phase change materials in buildings in the direction of energy management in commercial and construction units. In 2009, Wu and his colleagues [23] studied alumina-water Nano fluid as a new phase change material for the thermal energy storage in cooling systems. The results of their work show that the addition of alumina nanoparticles (aluminum oxide) significantly reduces the excessive temperature of water, on the other hand, it increases the initial freezing time and reduces the total freezing time. Given they showed that by adding alumina nanoparticles with a volume fraction of 0.2%, the freezing time of alumina-water Nano fluid can be reduced to 2.5%. In 2011, the effects of the water inlet temperature as well as the mass flow rate on the thermal performance and heat storage of phase change materials in shell and tube exchangers have been analyzed by Tau and Hay [24].

Their results showed that the melting time of the material is constant for one hour, it decreases with the increase of the initial water inlet temperature and the initial water inlet mass flow rate. In 2014, Yazichi and his colleagues [25] investigated the paraffin melting process in a shell-and-tube heat exchanger with increased eccentricity in an experimental work. The results of their investigation showed that increasing eccentricity improved the effects of natural displacement and this will have a significant effect on reducing the melting time. In a study conducted by Aziz Babapoor and his colleagues [26] in 2013 on the performance of the phase change material (paraffin) as a heat absorber, the results of this study showed that this material changes phase by absorbing the heat of the material. The battery prevents the excessive temperature rise even at the high discharge and improves the performance of the battery.

2. Modeling

2. 1. Geometric form of the problem

In the simulation carried out in this research, the thermal changes of the nanofibers of phase change materials (polyethylene glycol and polyamide 6) are located around a tank. The reason for choosing this chamber is that this condition is often observed in the oil industry and it is one of the parts where the energy loss is high. The thickness of the chamber wall in the tank is 10 mm and the height of the tank is 20 mm. Figure 1 shows the geometric shape modeled to check the thermal algorithm. The surrounding of the chamber in which the oil is located is covered with nanofibers of the phase change material.

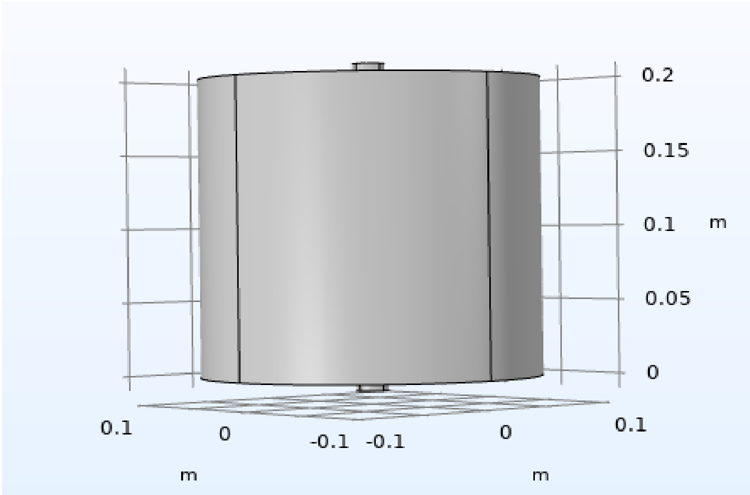


Figure 1. Geometric shape of the tank modeled to check the thermal algorithm of the nanofibers of phase change materials.

2. 2. Hypotheses of the model

To model the desired system, some hypotheses are applied for simplification as follows [27]:

- The liquid flow of the melted polyethylene glycol is layered and the losses due to viscosity are considered negligible.
- The physical properties of the nanocomposite mixture are considered a function of temperature.
- The heat transfer in this system takes place by both conduction and convection.
- The change in the volume of the whole system with the melting process of polyethylene glycol is considered insignificant.

2. 3. Governing equations in single-phase situations

The governing equations of the system are as follows [28]:

Continuity equation:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho U) = 0 \tag{1}$$

Momentum equation:

$$\frac{\partial \rho}{\partial t}(\rho U) + \nabla.(\rho UU) = -\nabla P + \rho g + \nabla.\tau + F \tag{2}$$

Energy equation:

$$\frac{\partial (\rho H)}{\partial t} \nabla.(\rho \mathrm{UH}) = \nabla.(\mathrm{K}\nabla\mathrm{T}) + \mathrm{S} \tag{3}$$

The unsteady conduction equation governs all layers in a single phase state. It is worth mentioning that due to the non-flow of the phase-changing material and the placement of these materials among other materials that do not change phase, the convection heat transfer has been omitted [29].

$$K_n \frac{\partial^2 T}{\partial X^2} = \rho_n C_n \frac{\partial T}{\partial t} \tag{4}$$

T_L is the temperature of the outside environment and T_0 is the temperature of the inside environment. The boundary conditions of the problem are considered as follows [30]:

$$T(0,t) = T_0 \tag{5}$$

$$T(L,t) = T_L(t) \tag{6}$$

C_n, ρ_n, K_n: They are the heat conduction coefficient, density and specific heat capacity respectively. By applying the finite difference method to the unsteady conduction equation, the central expansion for space and the leading expansion for time within each of the layers will be as follows [31].

$$T_i^{j+1} = T_i^j + \frac{K_n \nabla T}{\rho_n C_n \nabla X^2} K_{pcm}(T_{i+1}^j - 2T_i^j + T_{i-1}^j) \quad (7)$$

$$T_i^{j+1} = T_i^j + \frac{2\nabla t}{[(\rho c)_{ins} + (\rho c\ )_{pcm}]\nabla X^2} * [K_{ins}(T_{i-1}^j - T_i^j) + K_{pcm(}T_{i+1}^j - T_i^j)] \quad (8)$$

$$T_i^{j+1} = T_i^j + \frac{2\nabla t}{[(\rho c)_{ins} + (\rho c\ )_{pcm}]\nabla X^2} * [K_{pcm}(T_{i-1}^j - T_i^j) + K_{ins(}T_{i+1}^j - T_i^j)] \quad (9)$$

In the above equations, the subscript PCM indicates the phase change material and the subscript "ins" indicates the insulating layers.

2. 4. Modeling of the thermophysical properties of phase change materials

The thermophysical properties of phase change nanocomposite materials according to the properties of phase change materials and the nanoparticles used are obtained from Table 1 and the following equations [32].

$$\rho_{npcm=\varphi C_{np}+(1-\varphi)\rho_{np}} \quad (10)$$

$$K_{npcm} = \frac{K_{np} + 2K_{pcm} - 2(K_{pcm} - K_{np})\varphi}{K_{np} + 2K_{pcm} + (K_{pcm} - K_{np})\varphi} K_{pcm} + 5 * 10^4 \beta_k \xi \varphi \rho_{pcm} C_{p_{pcm}} \sqrt{\frac{BT}{\rho_{np} d_{np}}} f(T, \varphi) \quad (11)$$

$$\beta_k = 8/4407100\varphi^{-\frac{1}{07304}} \quad (12)$$

$$f(T, \varphi) = (2.8217 * 10^{-2}\varphi + 3.917 * 10^{-3})\frac{T}{T_{ref}}(-3.0669 * 10^{-2}\varphi + 0.00391123) \quad (13)$$

$$\beta = 0 \quad if \quad T < T_{solidus} \quad (14)$$

$$\beta = 1 \quad if \quad T < T_{liquidus} \quad (15)$$

$$\beta = \frac{T - T_{solidus}}{T_{liquidus-}T_{solidus}} \quad if \quad T_{solidus} < T < T_{liquidus-} \quad (16)$$

The difference between the starting point of the melting process and the end point of the melting process (melting temperature range) leads to the definition of a parameter called beta (β). β is the liquefaction fraction of paraffin, which is zero before the melting starts. And after the polyethylene glycol is completely liquefied, it is one and in the range of melting, it is a number between zero and one. B is the Boltzmann coefficient, which is equal to $1.381 * 10^{-23}\ J/K$. The heat conductivity coefficient is modeled according to both the Maxwell's model and the Brownian motion model, providing insights into the volume fraction of aluminum oxide within polyethylene glycol (∅) [33].

2. 5. Choosing physical models

In this software, various physical models are available to the user by default to investigate all kinds of problems. Also, in cases where the model of the system under consideration does not exist in the defaults of the software, it is possible for the user to enter a new model. In this research, the heat transfer model is selected [34].

2. 6. Initial and boundary conditions

In order to solve the mentioned relations, suitable initial and boundary conditions are needed to obtain the temperature distribution function. In the COMSOL Multiphysics software it is also needed to have appropriate boundary conditions to numerically solve this relationship and obtain the temperature of each point of the object, which the user must define

[35]. In this research, the most important boundary condition is related to the heat exchange through the walls and with the surrounding environment. When a hot plate is placed in the vicinity of a fluid, heat is exchanged by the convection method. As a result, the following boundary condition is established between the walls and the environment [36]:

$$n(k\nabla T) = hA(T_W - T_\infty) \qquad (17)$$

The initial conditions are also defined for this software. The boundary conditions are shown in Figure ۱ and the meshing done for this simulation is shown in Figure ۳. The type of the mesh used is triangular, the size of the largest element in the tank is equal to 0.0154 mm and that of the smallest element is equal to $8.2 * 10^{-4}$ mm and the total number of elements is ۸۷۴۶. The finite volume numerical solution method is used to solve the governing equations. The COMSOL Multiphysics software solves equations 1 to 16 numerically, according to the boundary conditions and meshing that was done in the previous steps, and the necessary indicators such as volumetric mass changes, the effective thermal conductivity coefficient, and how it shows the temperature distribution. The numerical method used by COMSOL Multiphysics to solve the partial differential equations in this simulation is the finite element method, which numerically solves the governing equations in three dimensions after meshing and applying the initial and boundary conditions.

7. 2. Simulation steps

The modeling methods in the COMSOL Multiphysics software and in fact the research method are as follows:

The choice of model depends on the number and type of phases, nanofibers, tank shape, tank material, characteristics of the oil, *etc*. In this research, the simulation is done in three dimensions. In this modeling, the geometry on which we want to perform the simulation and calculations is a cylindrical tank. The goal is to simulate changes in the temperature, density, viscosity and thermal conductivity coefficient within this geometry in the state covered with phase change materials. In this way, after determining the dimensions and characteristics of the material, the simulation is done in three dimensions. The flow is considered as a laminar flow, and in the physics section of the problem, according to the goal we have defined, we choose the options of the heat transfer as the heat transfer in solids and liquids. In the section of selecting the type of solvers, selecting any physics reveals the corresponding variables associated with that physics. Within this section, various methods, of which all are time-dependen, for analyzing the model are listed. The reason for using this method is that the nature of phase change systems is unstable. In the next step, we will also add a stationary stage, this stage will be based on the laminar flow mode, because laminar flow systems reach a stable state after a short period of time, and we do not need to involve unstable systems to solve them. Therefore, the stationary option will be a more convenient option and the amount and time of calculations will also be reduced. For the heat transfer, we consider the time dependent mode. In the geometry section, the capacity to delineate and visualize the intended geometry by its specified shape and dimensions is provided. The subject geometry for investigation pertains to a cylindrical oil tank. It is essential to observe the parameters employed for constructing this geometry and to adjust them according to requirements. It is recommended to make an early selection of the material for the body, implementing suitable labeling for each segment to ensure clarity in the subsequent analysis. At this stage, the chambers in which the phase change materials will be placed will also be drawn. Within the material section, the designation of the tank type and the selection of the phase change material take place. If the desired material is not pre-defined, COMSOL Multiphysics offers the capability to define a new material. In this section, the specifications for the input or stored fluid, pipe type, characteristics of both the oil and polyethylene glycol-polyamide, and container type for housing the phase change material are delineated. The properties of each material will be inputted, and subsequently, the geometry will be associated with the designated material to facilitate the desired analysis. In this part, we will apply the phase change, then enter the phase vaporization temperature, and the desired temperature will be determined between the solid and liquid phases. The rest of the properties are considered as default. We put the fluid velocity in the velocity field (spf) mode because the flow is considered as a laminar flow. In the next step, the geometry is meshed and calculations are performed.

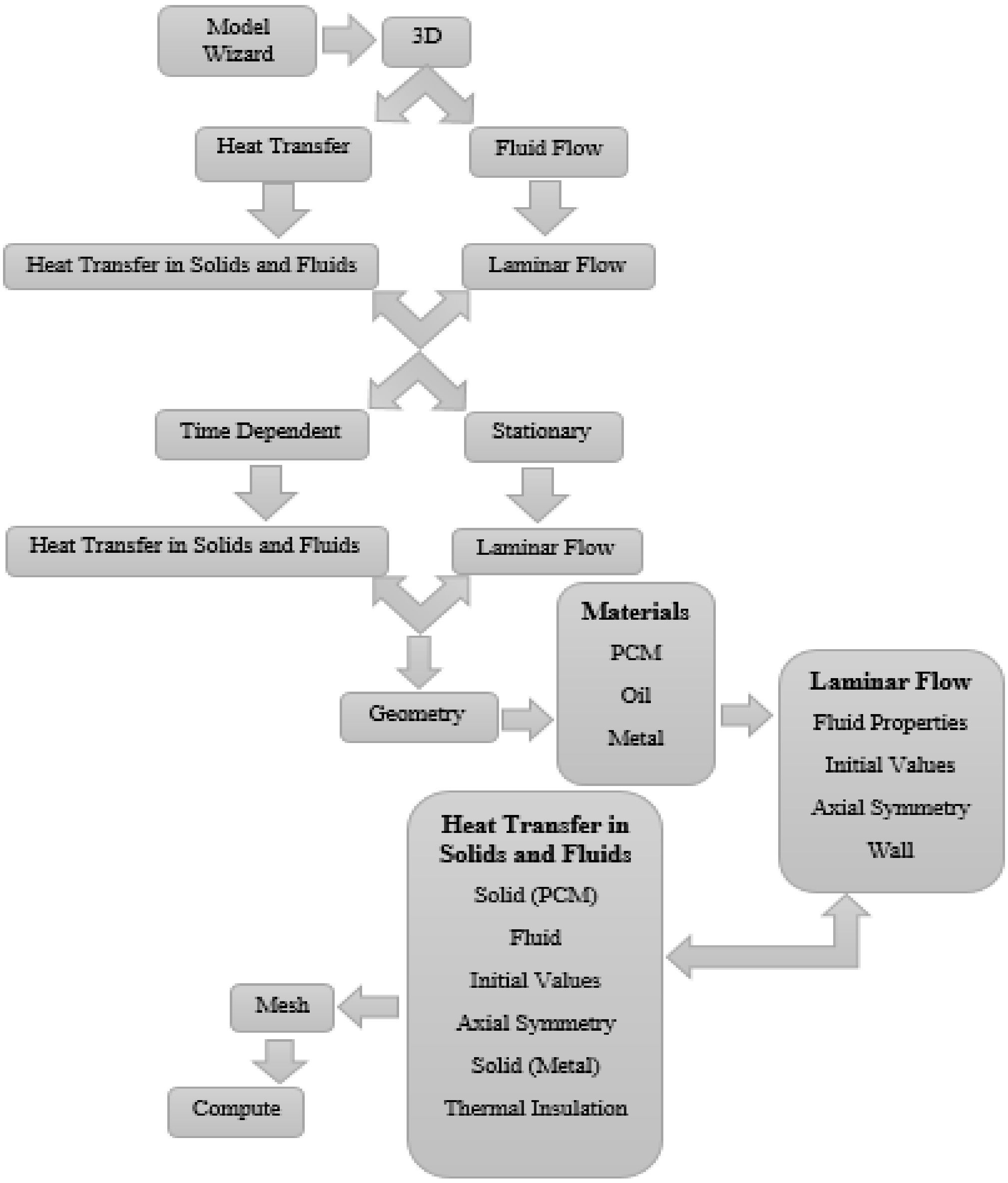


Figure 2. Simulation steps.

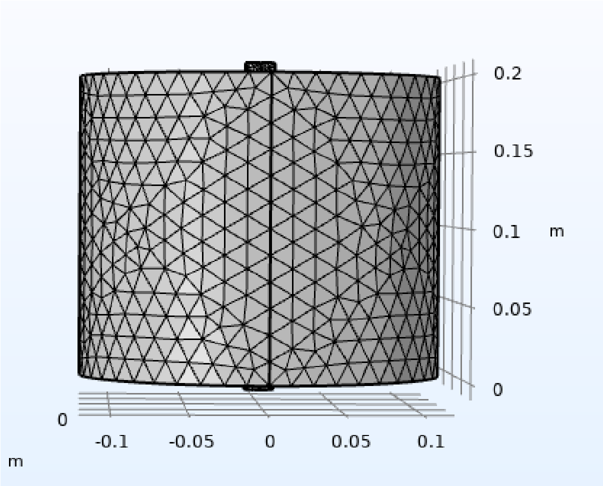


Figure 3. Model meshing in COMSOL.

The finite element method is a little different from the finite difference method in solving partial differential equations, but it has better efficiency when working with more complex physics problems. The most common method for solving engineering problems that have partial differential equations is the finite element method, which is used by many software, including COMSOL Multiphysics, to solve partial equations [37]. The governing equations in this research are time-dependent partial differential equations that are solved in three dimensions. The mesh independency is an important feature in simulation. The most important issue in numerical simulations is to achieve a suitable and sufficient number of grids to start the solution. Therefore, the calculations commence with the selection of a suitable grid, followed by the verification of solution independence through the evaluation of various mesh structures. A different size of the grid is used for solving. It can be said that in any modeling, the minimum number of cells required in the mesh structure for simulation is one of the key indicators in achieving accurate results, because using a mesh structure less desired than the optimal mesh leads to numerical errors. The results are accurate. Also, the further increase in the number of cells in the mesh structure leads to a significant increase in the solution time and a decrease in the calculation speed, and as a result, an increase in the calculation cost. In the modeling of chambers with phase change materials in order to achieve the optimal number of cells in the mesh structure, 3 different structures with different sizes and numbers of cells were used for simulation. Table 1 shows the information about the number of elements. The smallest and the largest mesh sizes in each grid for the pipe and the information related to the cylindrical tank are presented in Table 1. In order to evaluate the results in different mesh structures and to choose the optimal one, the temperature index along the vertical line on the wall which is created at the same position for all three meshing modes, has been averaged and compared. The purpose of choosing this vertical line is to cover the entire height of the chamber from the beginning to the end. Initially, the length of the wall line situated in the corner of the chamber, characterized by the enhanced heat exchange with the external environment, experiences a temperature decrease. This drop in temperature is more pronounced due to the shorter path of temperature propagation towards the middle sections. Meanwhile, the influence of the elevated temperature within the chamber persists, exhibiting an upward trend that extends until the termination of the line. This trend of the temperature change can be seen in all 3 types of grids. But by comparing the trend of the temperature change in different meshes, it can be seen that the mesh with the lowest number of meshes is very different from the rest of the meshes and especially from the mesh with the highest number of meshes. Due to the slight changes in the temperature trend in these three types of meshing, at the end, the least number of meshes that have higher accuracy will be selected from these three types of meshes; number 8746 in the cylindrical cone is selected. Also, according to the last column of Table 1, where the number of elements of the wall part is given, it can be concluded that the change of the number of elements and dimensions of the mesh in this part do not have significant effects on the pseudo-construction results.

Table 1
Specifications of different meshes in the tank.

	Number of elements	Largest element	Smallest element	Wall elements
Mesh type 1	9630	0.0112	2.6×10^{-4}	4738
Mesh type 2	7324	0.0438	1.8×10^{-3}	2605
Mesh type 3	8746	0.0154	8.2×10^{-4}	3892

To evaluate the results in the different mesh structure and to choose the optimal mesh, the temperature index, along the vertical line on the wall, which is created at the same position for all three meshing modes, has been averaged and compared. The purpose of choosing this vertical line is to cover the entire height of the chamber from the beginning to the end. To determine the effect of the meshing method on the results, we examine the temperature in the chamber in the line created in the diagram of figure 2. As depicted in Figure 2, at the initial segment of the wall length located in the chamber corner with superior heat exchange with the external environment, there is a decline in temperature. Owing to the relatively short path, the temperature experiences minimal changes upon reaching the middle sections. Subsequently, influenced by the elevated temperature within the chamber, the temperature begins to ascend and continues this trend until the conclusion of the line. This trend of temperature changes is seen in all 3 types of grids. But by comparing the trend of the temperature change in different meshes, it can be seen that the lowest number of meshes (8746 elements) is not much different from the rest of the meshes, especially the mesh with a higher number. In the following, due to the slight changes in the temperature trend in these three types of meshing, at the end, the smallest number of meshes that have higher accuracy will be selected from these three types of meshing, *i.e.* 8746. Also, according to the last column of Table 1 where the number of elements of the wall part is given, it can be concluded that changing the number of elements and dimensions of meshing in this part did not have significant effects on the simulation esults.

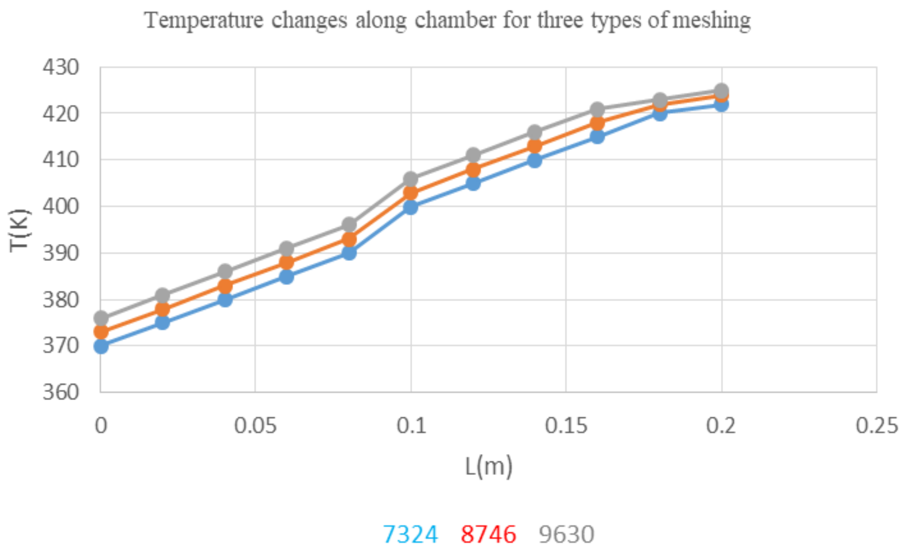


Figure 4. Temperature changes in the reservoir for three types of meshing in the nanocomposites of phase change materials.

2. 8. Properties of polyethylene glycol 10000

Polyethylene glycol is produced by the reaction of mixing ethylene oxide gas with monoethylene glycol or diethylene glycol. The general formula of polyethylene glycol is $C_{2n}H_{4n}+2O_{n+1}$, where n is the average number of ethylene oxide groups. PEG is a type of phase change materials that has high latent heat, suitable phase change temperature and low heat loss [38]. According to the molecular mass, polyethylene glycols can be available as liquid or solid under standard conditions. The different molecular weight of polyethylene glycol allows them to have different properties in average molecular weight. One of their types is polyethylene glycol with grade 10000, the properties of PEG 10000 are listed in Table 2. As the molecular weight increases, the phase change temperature and latent heat of PEG also increase[39].

Table 2

Properties of polyethylene glycol 10000.

Polyethylene Glycols (PEG)	Melting Process		Freezing Process		Reference
	(◦C)T_m	**(J/g)ΔH_m**	**(◦C)T_f**	**(J/g)ΔH_f**	
PEG-10000	63.7	189.2	39.1	167.3	**[40]**

2. 9. Thermal and physical properties of used nanoparticles

Nowadays, extensive progress has been made in the field of the preparation and use of nanoparticles. The significant increase in the thermal conductivity of these nanoparticles has proved their merit for further research and studies. Adding different nanoparticles as well as changing the physical conditions can contribute to increasing the thermal conductivity in these nanoparticles [41]. One of the important physical properties that are investigated is their thermal properties. In the study of thermal properties, things such as thermal conductivity, coefficient of thermal expansion, specific heat of matter, melting point and things like that are examined. Like showing many other characteristics, nanomaterials show special thermal properties, which are affected by various factors [42, 43]. Table 3 shows the thermal-physical properties of aluminum oxide, iron oxide, titanium dioxide and copper oxide nanoparticles.

Table
Thermo-physical properties of nanoparticles [44].

Nanoparticle	Purity	Particle size (nm)	Specific surface area (m^2/g)	Morphology	Thermal conductivity (W/m K)	Density (g/cm^3)
AL_2O_3	>99%	20	138	nearly spherical	41.1	3.890 Bulk density: 1.20
Fe_2O_3	>99.5%	20	40-80	spherical	6.4	True density: 5.24 Bulk density < 0.10
TiO_2	>99%	20	180-600	spherical	8.3	4.3
CuO	>99%	20	65	nearly spherical	13.51	6.315

3. Results

3. 1. Temperature distribution

Figures 5, 6, 7 and 8 show the contours of the temperature distribution respectively in the presence of nanoparticles of aluminum oxide, iron oxide, titanium dioxide and copper oxide with 2% wt (a , b) and 8% wt (c , d). They show the inside of polyethylene glycol in the tank at 600 and 4800 seconds. As it can be seen in the contours, with the increase in the weight percentage of nanoparticles in polyethylene glycol-polyamide 6 (the reason for the addition of polyamide 6 is to increase the melting temperature of polyethylene glycol), the nanofibers are initially solid and gradually melt over time. And they store more heat in themselves. The appropriate size and homogeneous distribution of nanoparticles can also affect these temperature changes. There are also temperature changes in most parts of the system. The presence of air does not have a great effect on the thermal management of the chamber. By placing a thin layer of nanocomposite on the chambers, the temperature inside the chamber decreases due to the high heat capacity of the nanoparticles of phase change materials and their good ability to store and absorb heat. The comparison of different modes shows that the higher the weight percentage of nanoparticles, the higher the amount of the heat absorption and the faster the decrease of the temperature. According to the contours, by increasing time, the temperature distribution has become uniform, which shows that as time passes, due to the presence of phase change materials, the temperature of the system decreases and the phase change material stores more energy in itself. On the other hand, with an increase in the percentage of polyethylene-glycol, the temperature distribution is improved. It can be said that in terms of temperature changes, titanium-dioxide and copper oxide nanocomposites are the best ones and can be used in the heat transfer of various systems.

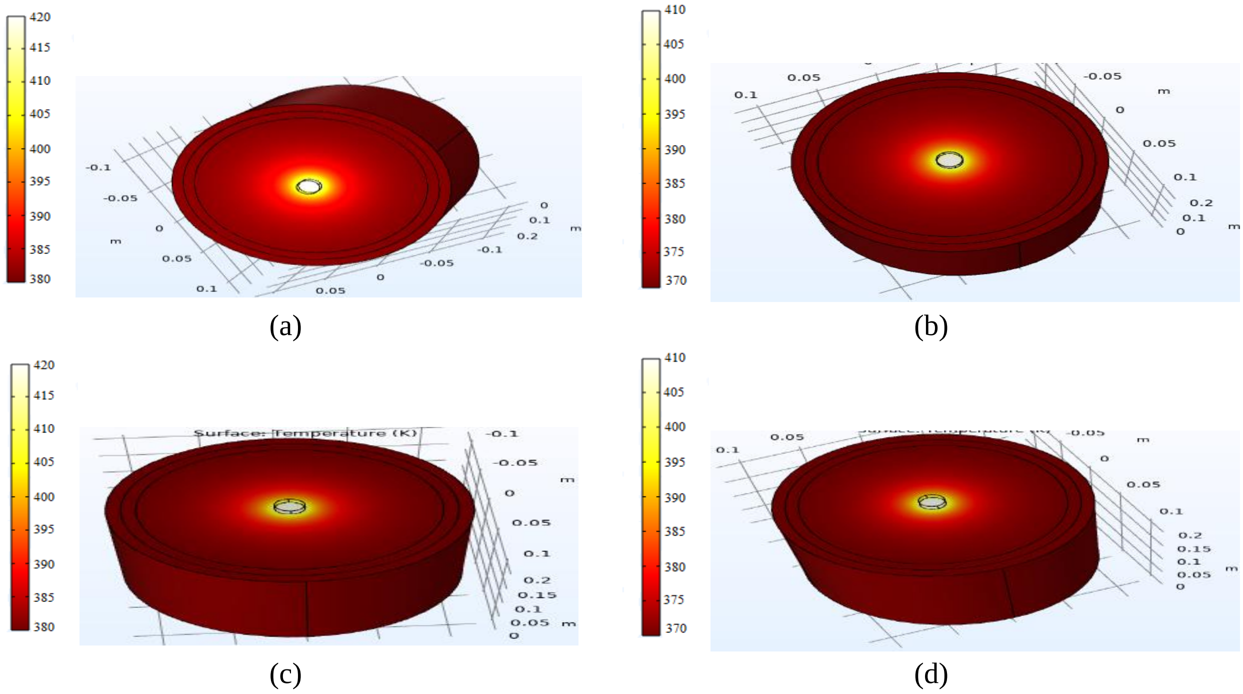


Figure 5. Temperature distribution in the tank with 2% wt (a , b) and 8% wt (c , d) of the aluminum-oxide nanocomposite at the times of 600 and 4800 seconds.

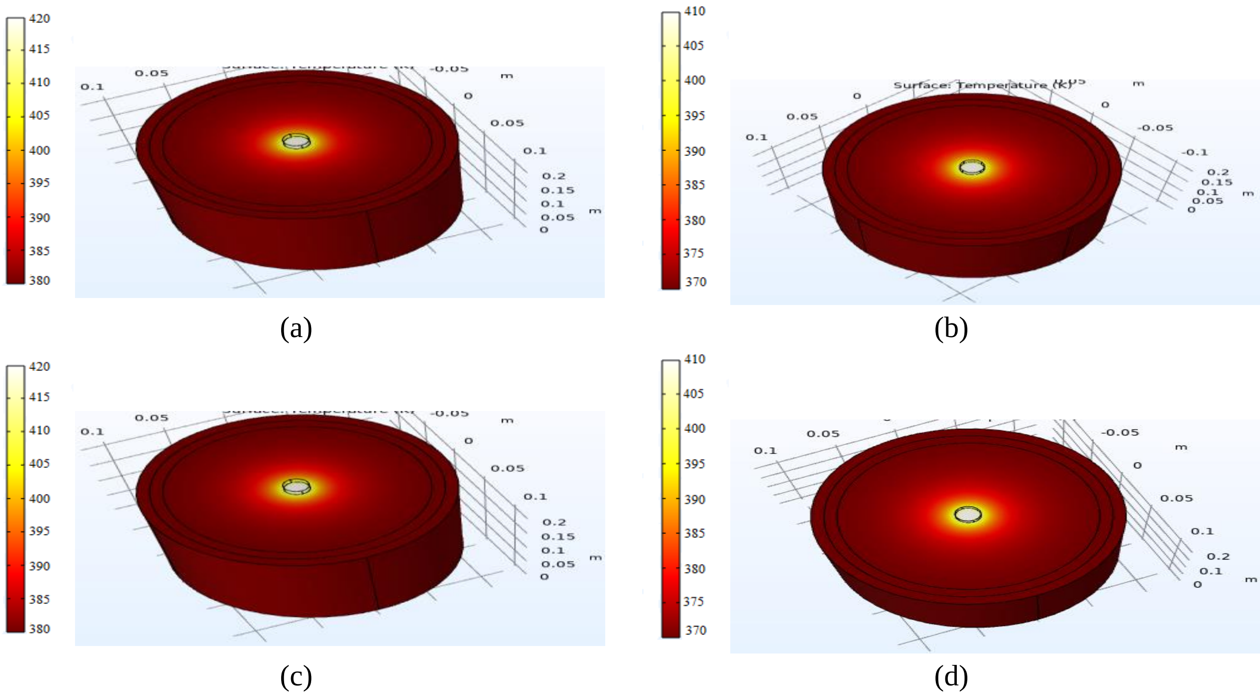


Figure 6. Temperature distribution in the tank with 2% wt (a , b) and 8% wt (c , d) of the titanium dioxide nanocomposite at the times of 600 and 4800 seconds.

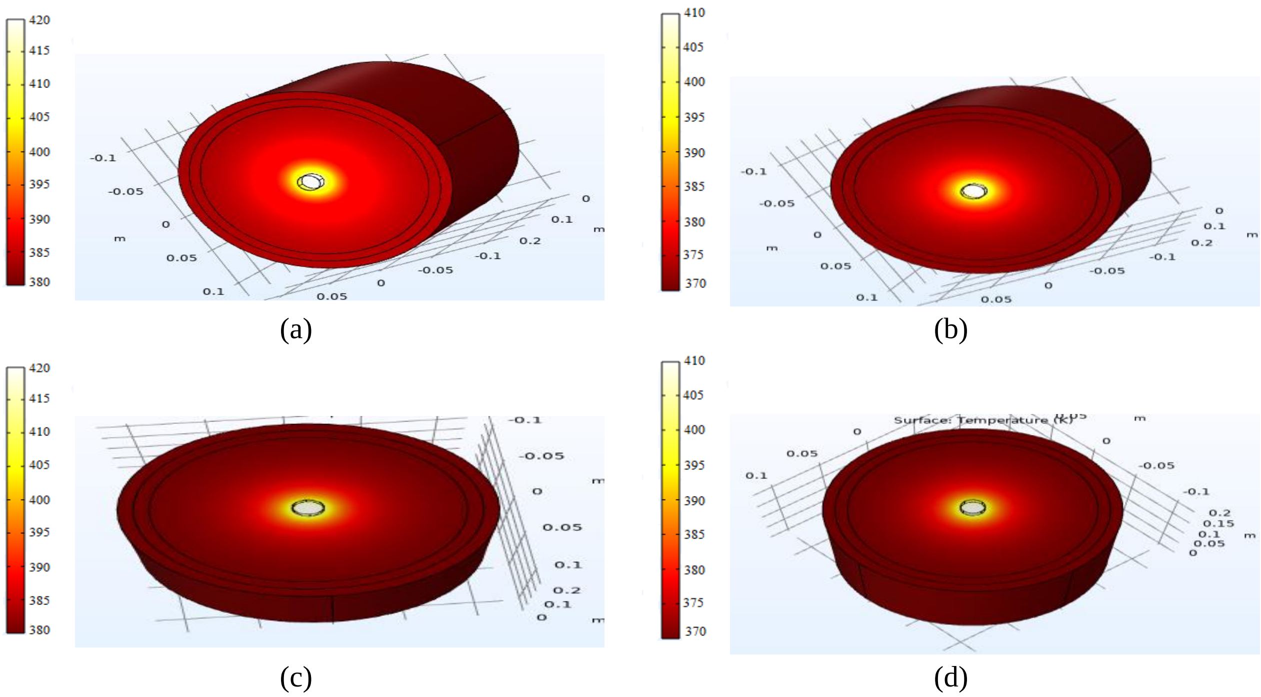


Figure 7. Temperature distribution in the tank with 2% wt (a , b) and 8% wt (c , d) of the iron oxide nanocomposite at the times of 600 and 4800 seconds.

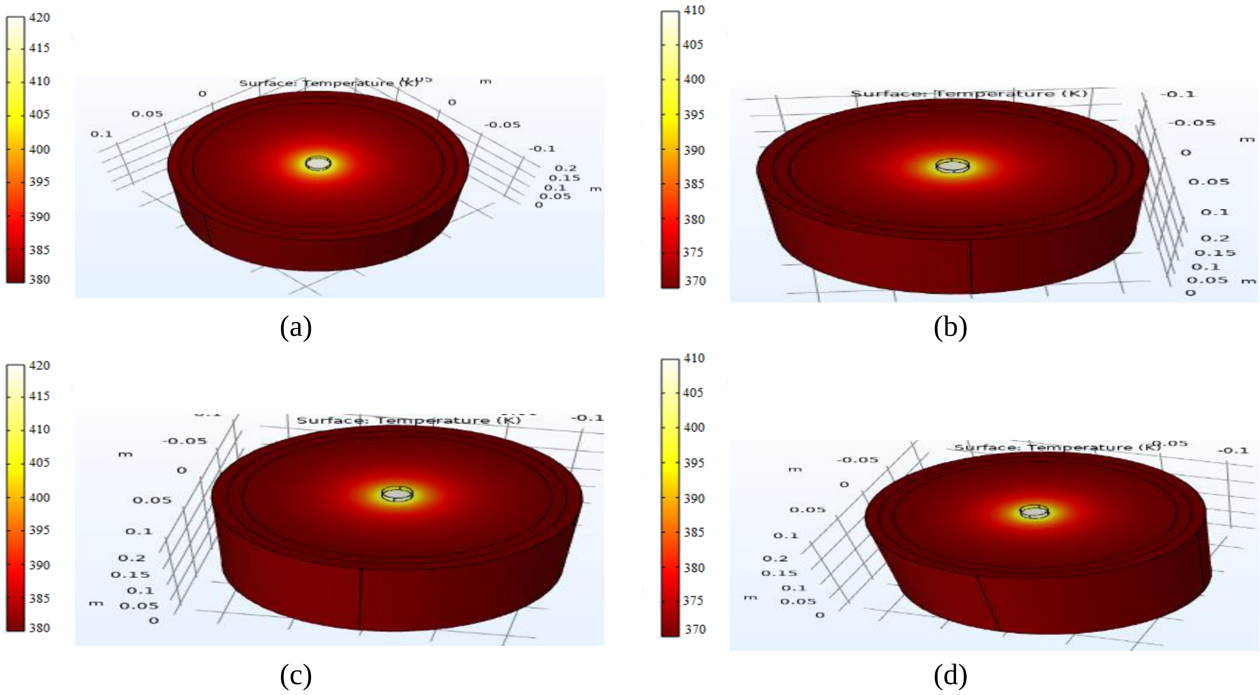
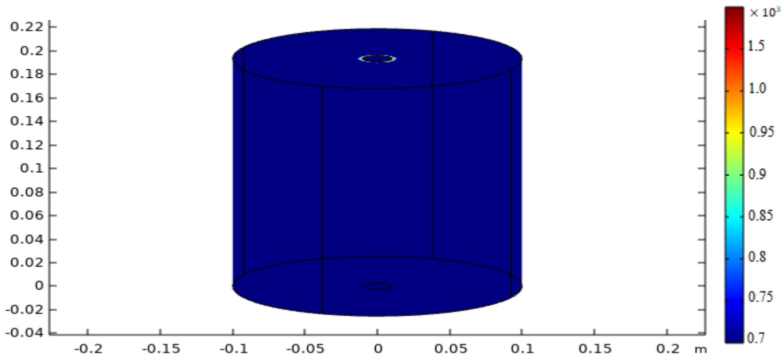


Figure 8. Temperature distribution in the tank with 2% wt (a , b) and 8% wt (c , d) of the copper oxide nanocomposite at the times of 600 and 4800 seconds.

3. 2. Density changes

Figures 9, 10, 11 and 12 respectively show the contours of density changes in the presence of the nanoparticles of aluminum oxide, iron oxide, titanium dioxide and copper oxide with 2% wt (a and b) and 8% wt (c and d). They show the contents of polyethylene glycol in the tank at 600 and 4800 seconds. By adding nanoparticles to the phase change material, the density increases, it can also be seen that with the increase in the percentage of nanoparticles, the temperature inside the phase change material first increases and then decreases, the reason for this is the thermal diffusion coefficient that is resulted from the division of the thermal conductivity coefficient by density and heat capacity obtained, as the percentage of the nanoparticle increases, the increased density causes the thermal diffusion coefficient to increase and the thermal conductivity coefficient to increase, and the heat transfer rate at 8% wt is more than the same at 2% wt. Among the used nanoparticles, the highest increase is related to the nanocomposites of titanium dioxide and copper oxide.



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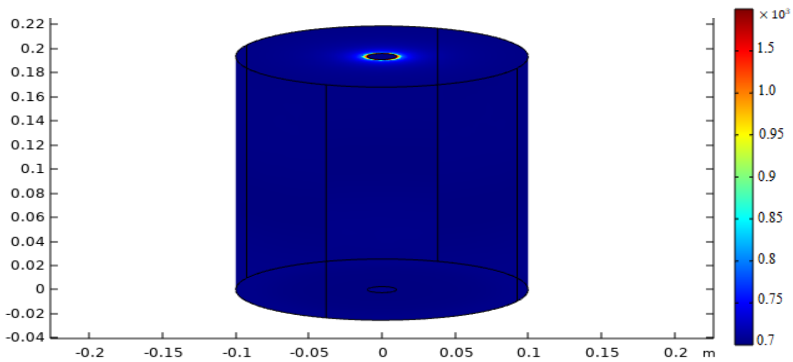

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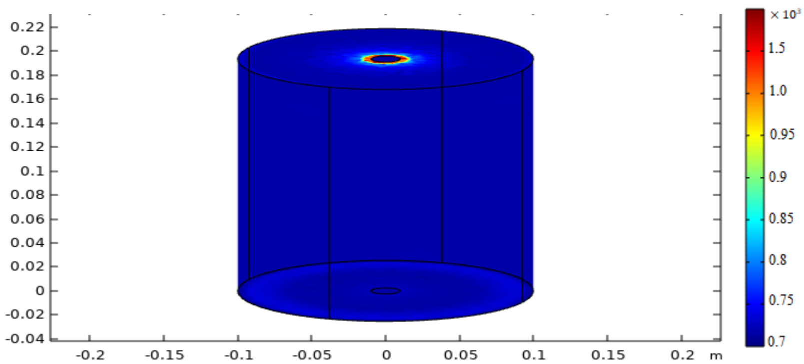

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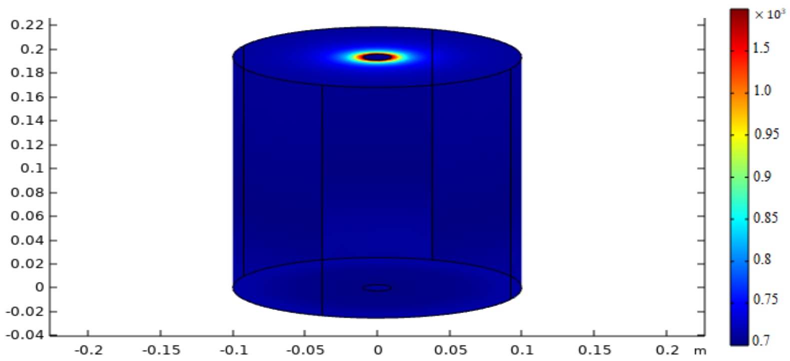
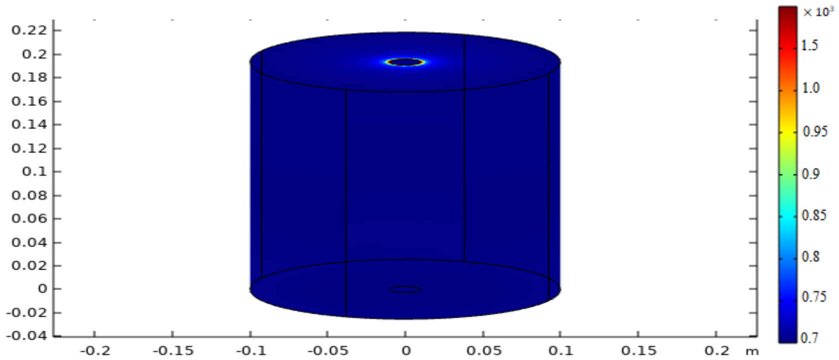


(d)

Figure 9. Density distribution in the tank with 2% wt (a , b) and 8% wt (c , d) of the aluminum oxide nanocomposite at the times of 600 and 4800 seconds.



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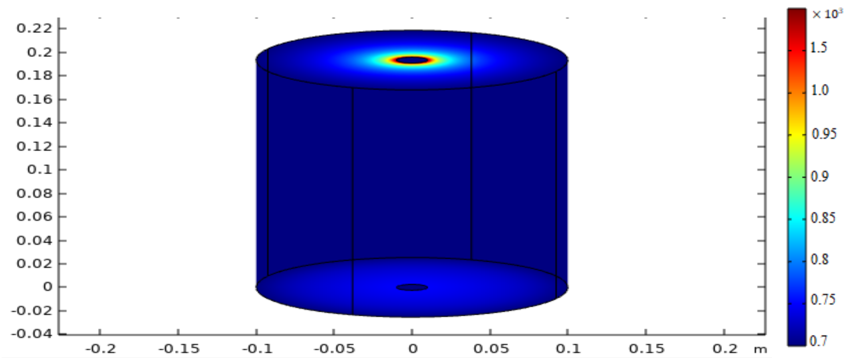

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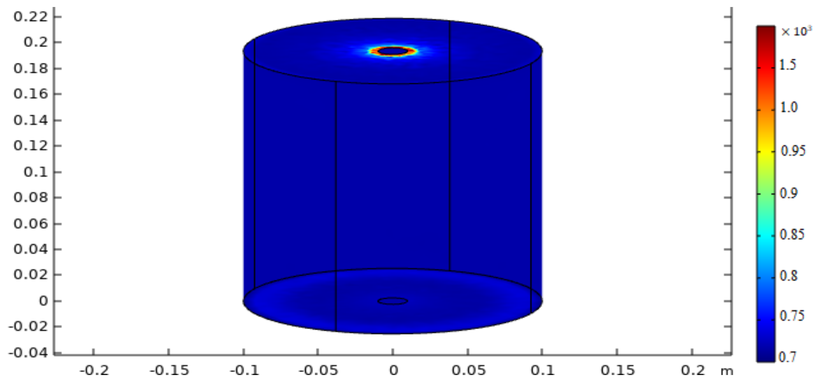

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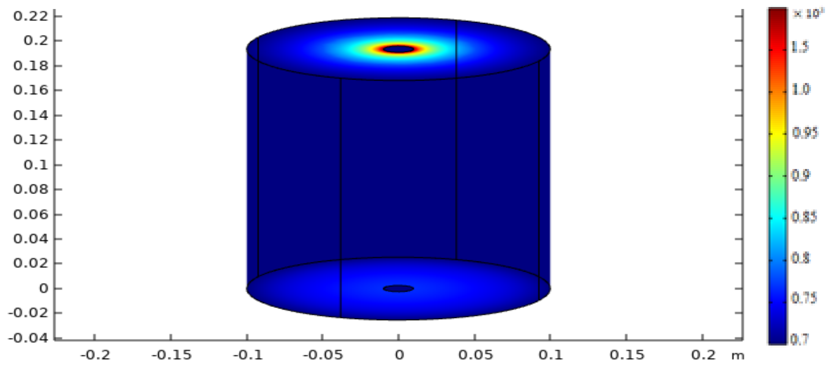
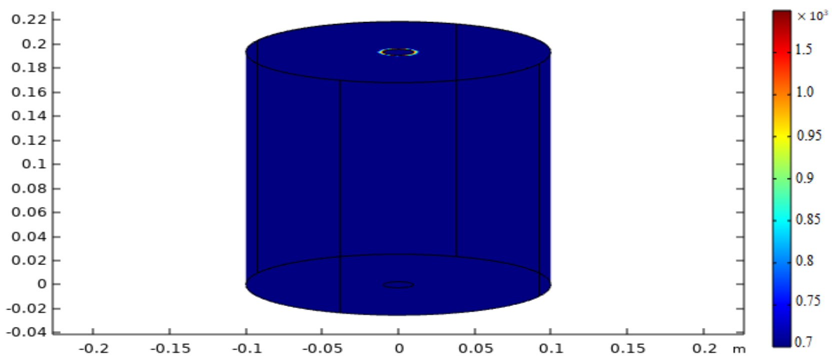


(d)

Figure 10. Density distribution in the tank with 2% wt (a , b) and 8% wt (c , d) of the titanium dioxide nanocomposite at the times of 600 and 4800 seconds.



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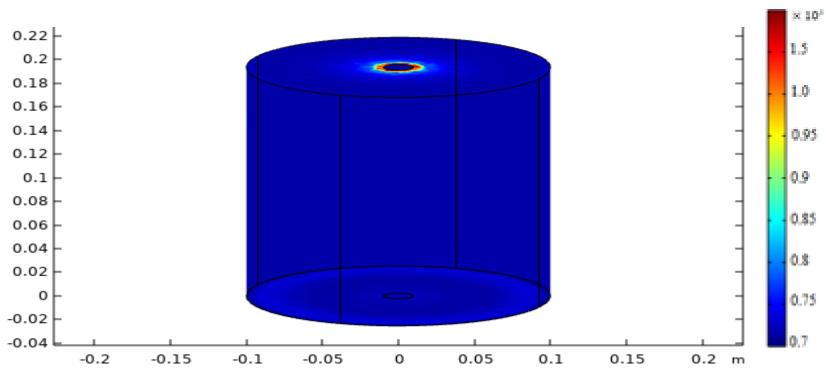

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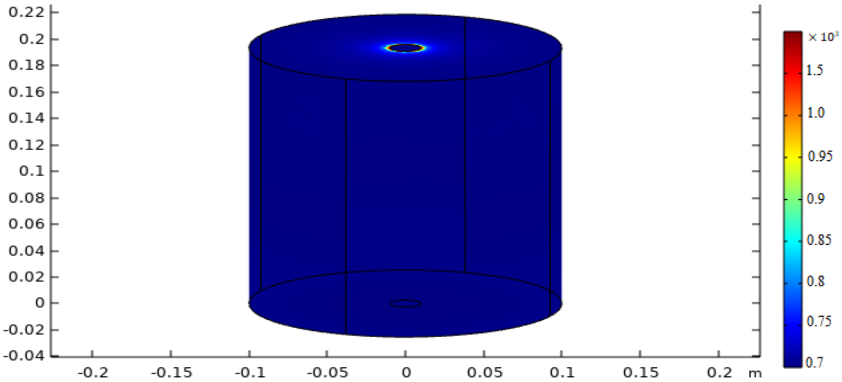

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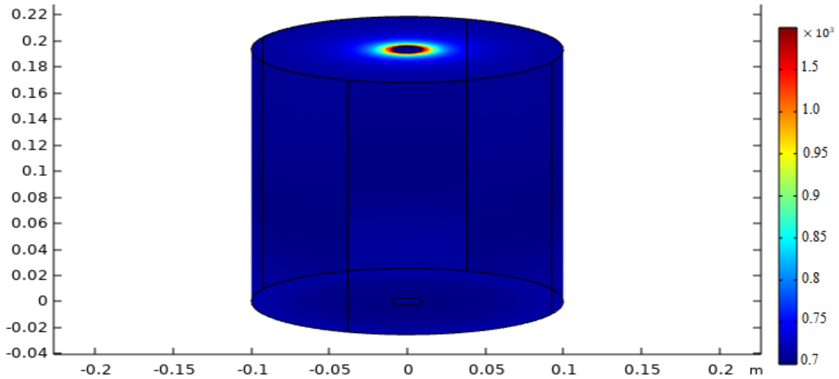
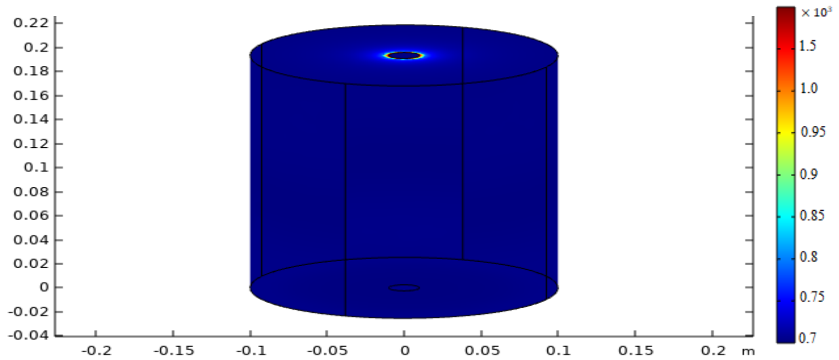


(d)

Figure 11. Density distribution in the tank with 2% wt (a , b) and 8% wt (c , d) of the iron oxide nanocomposite at the times of 600 and 4800 seconds.



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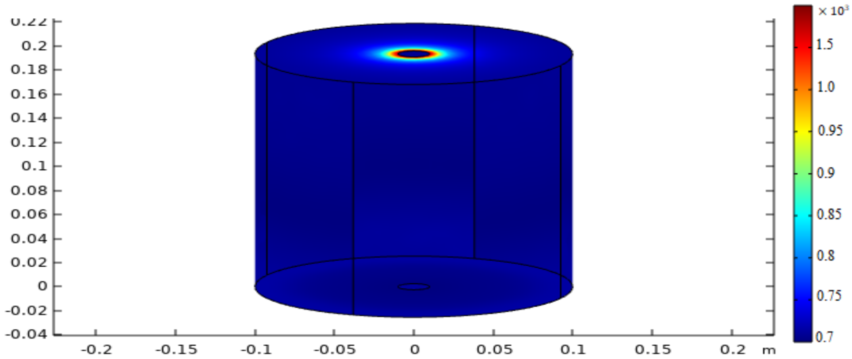

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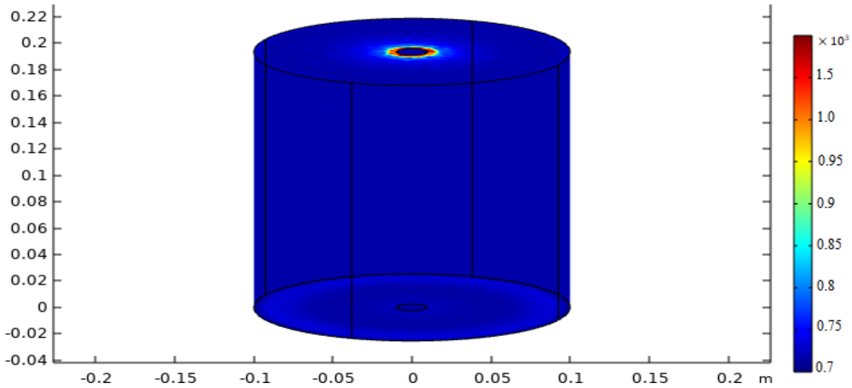

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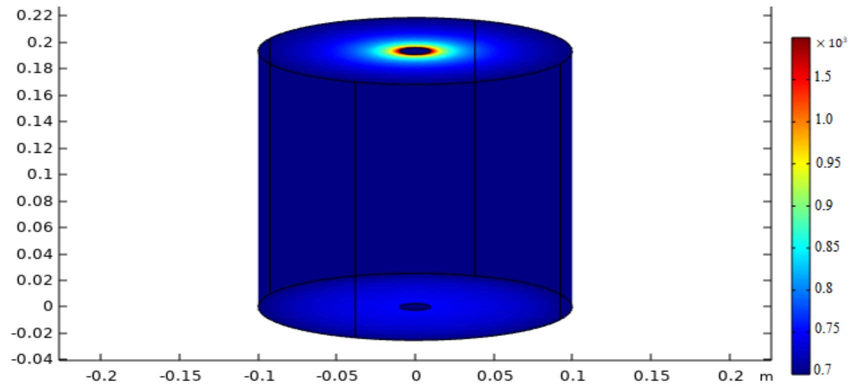
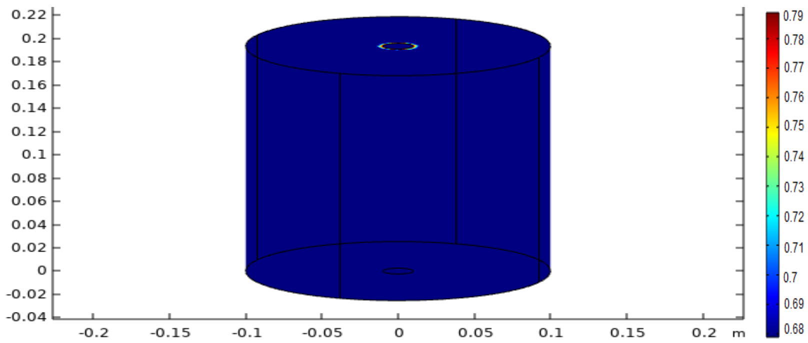


(d)

Figure 12. Density distribution in the tank with 2% wt (a , b) and 8% wt (c , d) of the copper oxide nanocomposite at 600 and 4800 seconds.

3. 3. Changes in the heat transfer coefficient

Figures 13, 14, 15 and 16 show the contours of thermal conductivity coefficient changes in the presence of aluminum oxide, iron oxide, titanium dioxide and copper oxide nanoparticles with 2% wt (a and b) and 8% wt (c and d inside the polyethylene glycol in the tank at 600 and 4800 seconds. Phase change materials inherently exhibit lower thermal conductivity than nanocomposites. Consequently, the incorporation of nanoparticles has enhanced various properties of polyethylene glycol, notably improved the heat transfer coefficient. The simulation results show that the heat transfer coefficient increases with the addition of ـanoparticles and this increase in the heat transfer coefficient happens when the percentage of nanoparticles is higher and also with the passage of time we will have an increase in the heat transfer coefficient. Among the used nanoparticles, the biggest increase is related to the nanocomposites of aluminum oxide and copper oxide. For example, adding 2% of copper oxide to polyethylene glycol causes a 20% increase in thermal conductivity. This nanoparticle is chosen as the optimal nanocomposite due to the significant increase in the heat dissipation coefficient.



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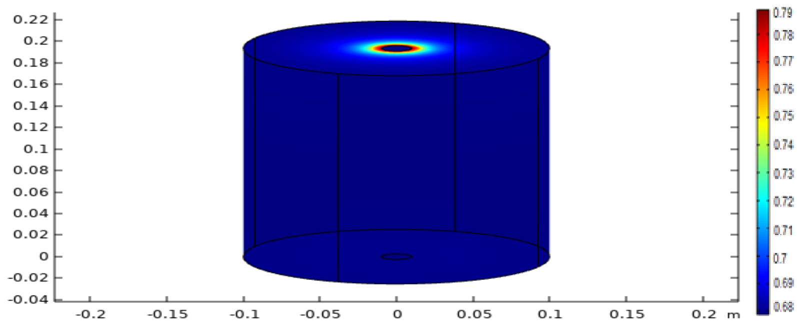

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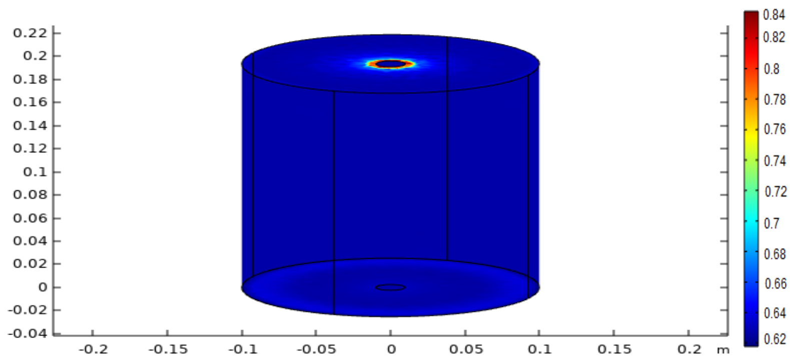

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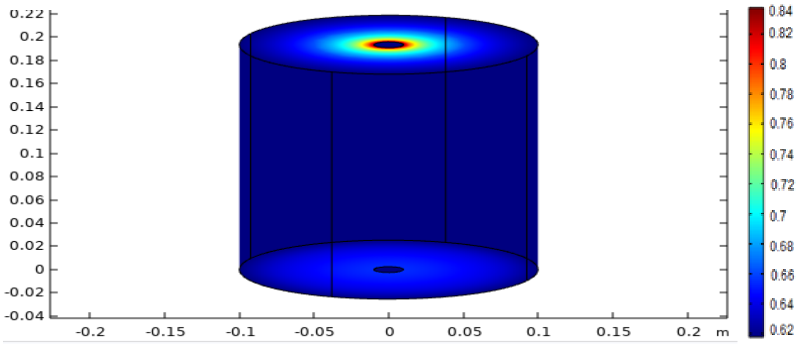

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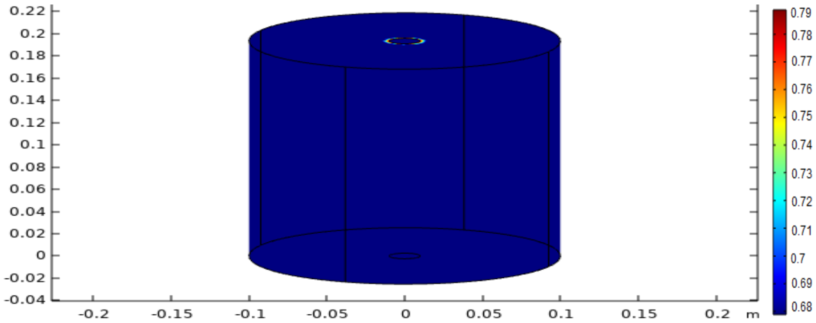
Figure 13. Thermal conductivity coefficient in the tank with 2% wt (a , b) and 8% wt (c , d) of the aluminum oxide nanocomposite at the times of 600 and 4800 seconds.



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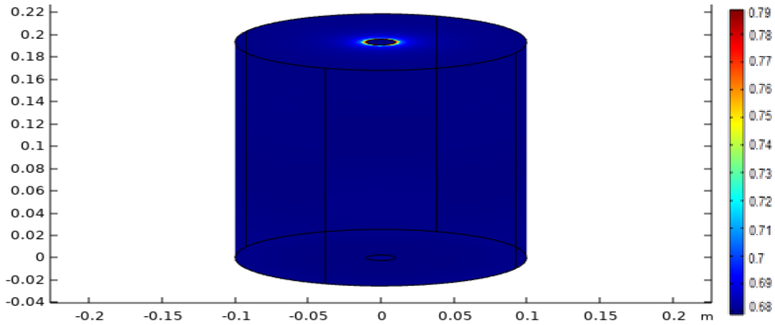

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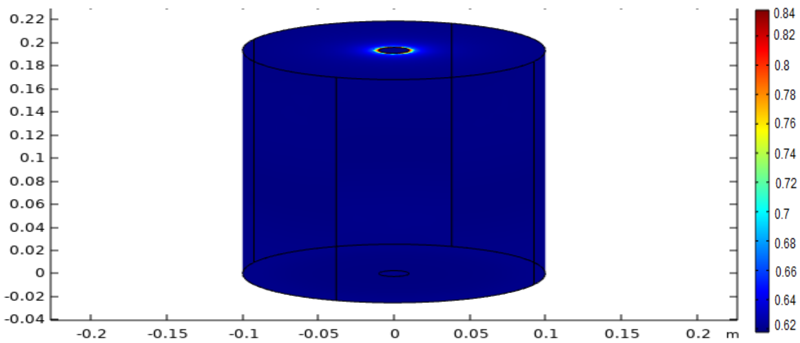

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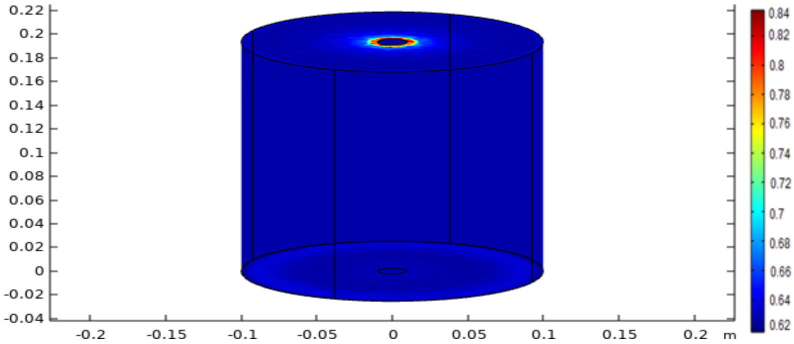
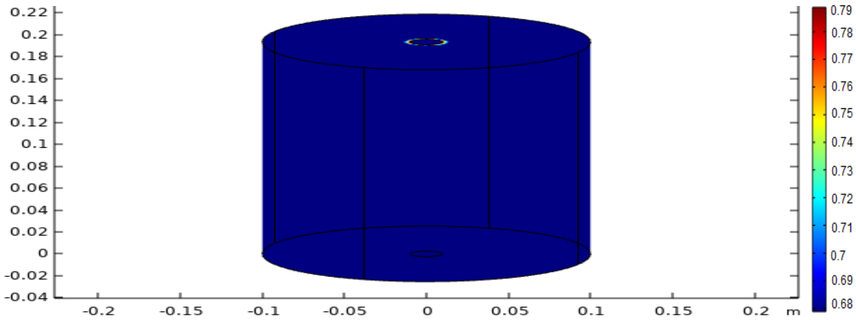


(d)

Figure 14. Thermal conductivity coefficient in the tank with 2% wt (a , b) and 8% wt (c , d) of the titanium dioxide nanocomposite at the times of 600 and 4800 seconds.



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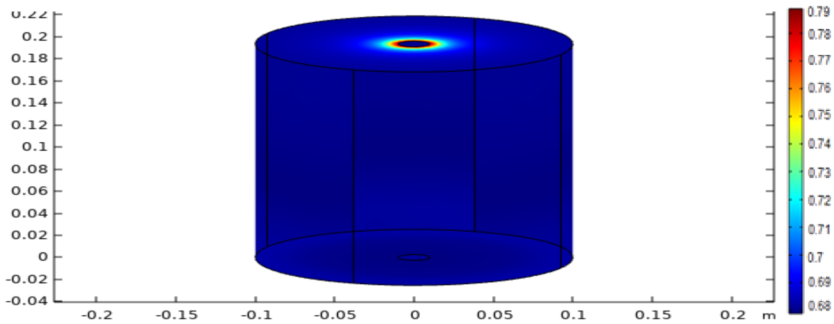

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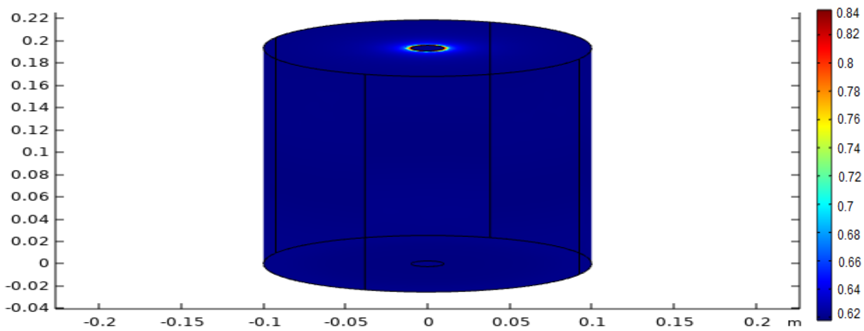

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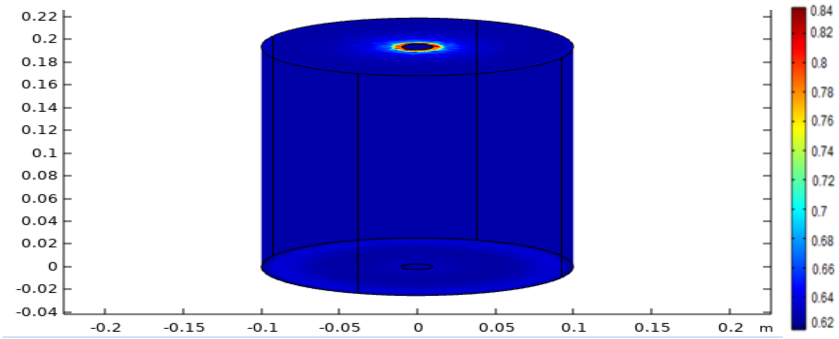
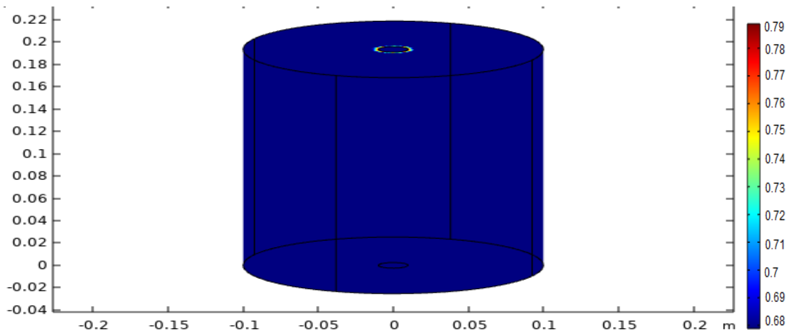


(d)

Figure 15. Thermal conductivity coefficient in the tank with 2% wt (a , b) and 8% wt (c , d) of the iron oxide nanocomposite at the times of 600 and 4800 seconds.



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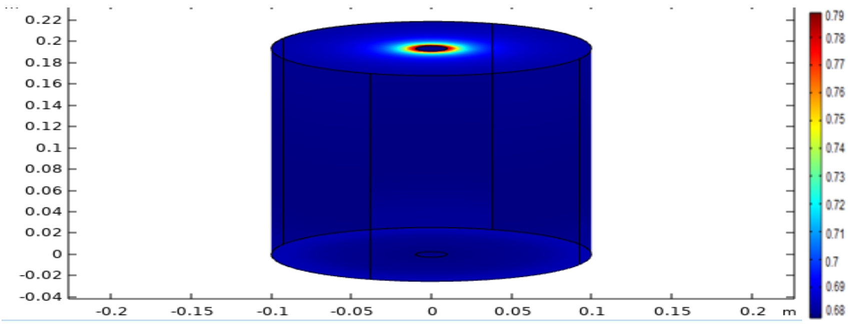

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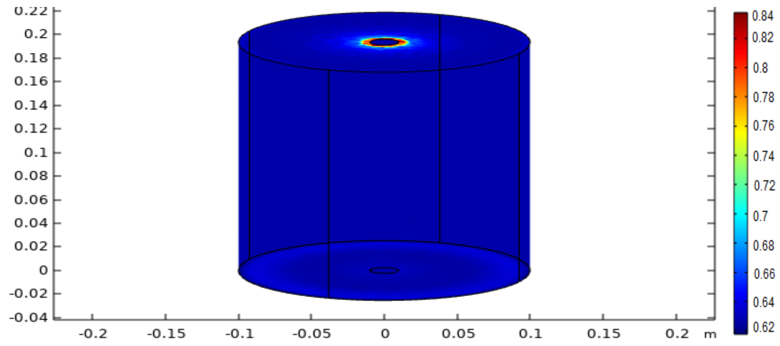

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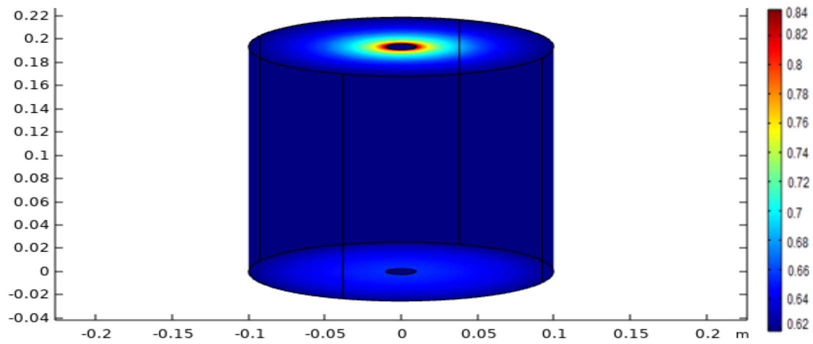

(d)

Figure 16. Thermal conductivity coefficient in the tank with 2% wt (a , b) and 8% wt (c , d) of the copper oxide nanocomposite at the times of 600 and 4800 seconds.

4. Effect of the different weight percentages of nanoparticles and the geometric shape of the problem

One of the ways to increase the heat transfer rate is to use phase change materials. The type and concentration of nanoparticles as well as the diameter of the designed chambers have great effects on the heat transfer rate. Netabaj showed that adding nanoparticles, with percentages and concentrations of up to certain levels, to the phase change material increases the heat transfer coefficient and improves it, but increasing the concentration and percentage of nanoparticles has a negative effect and causes a decrease in the heat transfer rate. In fact, at an optimal concentration for nanoparticles, the amount of heat transfer increases.

5. Conclusion

In this research, the behavior of nanocomposite phase change materials in a three-dimensional cylindrical tank has been investigated. The simulation results show an increase in the density, heat transfer coefficient, temperature and better energy storage of the nanocomposite of phase change materials compared to those of pure phase change materials due to increase in the thermal conductivity and decrease in latent heat. This simulation study shows the great potential of nanoparticles for being used in phase change materials in thermal energy storage applications. Adding nanoparticles to the phase change material increased the effective heat conductivity of the phase change material. However, the specific heat and latent heat of phase change materials are reduced. The advantage of increasing the effective thermal conductivity causes proper temperature distribution and density increase.

The results show that increasing the thermal conductivity coefficient has a great effect on reducing the tank temperature, that is, by increasing the nanoparticles with a higher thermal conductivity coefficient, it improves the heat transfer rate and reduces the melting time of the phase change material.

Nomenclature

T_L Temperature of the outside environment [K]

T_0 Temperature of the inside environment [K]

K Coefficient of thermal conductivity [$^W/_{mK}$]

C_p Specific heat capacity [kJ/(kg K)]

ins Insulating layers

PCM Phase change material

β Liquefaction fraction [$^1/_K$]

B Boltzmann coefficient [K/J]

∅ Volume fraction [m^3]

q The rate of energy produced per unit volume by the heat source [W/m^3]

ρ Density [kg/m^3]

T_m Temperature of the cooling medium [K]

g The acceleration of gravity [m/s^2]

θ Melting fraction of the phase change material

L Latent heat [kJ/kg]

u Fluid velocity [$^m/_s$]

F Buoyancy force per unit volume [N]

T_{ref} Reference temperature [K]

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