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# Simulation study of phase change materials operating in thermoelectric devices

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Abstract. In this paper, a computerized analysis is performed to evaluate the effect of phase change materials on the performance of thermoelectric generators. This study was conducted using commercial OpenFOAM software. Analyze changes in temperature, potential and efficiency due to phase change materials. The study evaluated a variety of geometric and operational conditions, such as changes in material height and heat flux. The results obtained indicate that the presence of phase change material allows a significant increase in the temperature difference between the surfaces. The temperature difference is increased by 35% with a height of 3.25 mm. The temperature difference increases the potential of the thermoelectric generator and increases the maximum output voltage by 21%. Overall, phase change materials have been shown to improve thermoelectric efficiency by 23%. For test conditions, the maximum efficiency is 4.77%. From this result, it can be concluded that the phase change material is a promising alternative for improving the low efficiency of thermoelectric generators due to their heat storage capacity.

#### 1. Introduction

Thermoelectric generation devices (DTEG) have the ability to transform energy in the form of heat to electricity through the effect known as the Seebeck effect [1]. The electrical power and efficiency of DTEGs depend on the difference in temperature between their cold side and a hot side. The temperature of the hot side depends mainly on the type of heat source used. However, the cold side temperature is affected by various factors such as ambient temperature, cooling system, thermal conductivity, and bond strength of DTEG construction material. Achieving a more significant difference in temperature between sides implies an improvement in the DTEG efficiency [2,3].

The capacity of DTEGs allows them to be used in a wide range of applications where a residual heat source is available. This has encouraged the development of studies in which residual heat recovery through DTEGs has been sought [4-7] investigated by computational analysis the effect of input power on DTEG efficiency. Karana and Sahoo [8] evaluated the ability of DTEG to recover residual heat from vehicle exhaust gases using nanofluids. The conclusions indicate that the use of the nanofluid allows the production of electrical energy and the energy conversion efficiency to be increased by 11.38% and 10.95% compared to a common refrigerant.

Similarly, Mohamed [9] studied the performance of DTEGs for heat recovery in light diesel vehicles. The maximum efficiency of the system was reported to be 4.63% [10] used a multiphase numerical model to evaluate the efficiency of a water-air thermoelectric generation system [11] analyzed the effect of a load of a diesel generator on the potential of electricity production in a DTEG. The results showed an output of 1412 W in the DTEG when the engine load was 38 kW; different researchers point out the

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**2046** (2021) 012011 doi:10.1088/1742-6596/2046/1/012011

possibility of implementing DTEGs as a residual heat recovery system to use solar energy [12–14].

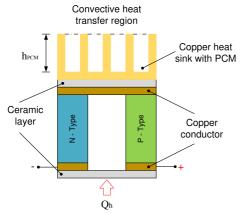
Despite the potential of these devices, the electrical power and efficiency can generally remain low today. This fact is directly related to the type of construction material and the thermal and electrical resistances inside DTEG. Due to this situation, researchers have sought strategies to achieve better performance. Phase change materials (PCM) have high potential as a heat storage medium, which has led to their use in refrigeration or heating applications in the commercial sector and thermal energy storage. Due to its ability to maintain a constant temperature condition, it is possible to improve DTEG efficiency [15] studied the performance of DTEGs in two-stage systems with phase-change materials.

This investigation shows that cold side temperature dropped considerably due to the presence of PCM. It is reported that this type of material can be used as a means of cooling and heating DTEG. Saha [16] noted an improvement in the heat dissipation process with the combined use of nanomaterials and PCM compared to pure PCM [17] reported that PCMs play an important role in improving power generation in DTEG.

In general, the energy conversion efficiency of DTEGs remains low, making it an unattractive solution for large-scale deployment. The state-of-the-art review shows that phase change materials are a promising solution for improving performance in DTEGs. However, further research is required to understand the capabilities of these materials. Due to the above, in this study, an evaluation of different geometric and operating conditions is carried out, such as variation in the height of the PCM and heat fluxes. The development of the numerical study is carried out using the OpenFOAM software. For performance evaluation, output parameters such as voltage, temperature difference, and DTEG efficiency are considered.

#### 2. Methodology

Figure 1 depicts the geometric configuration of the DTEG used for the computational study. The phase change material selected was OM32. The properties of the material are shown in Table 1 [18].



**Figure 1.** DTEG geometry for computational analysis.

**Table 1.** Phase change material properties.

Properties	Unit	OM 32	
Latent heat	kJ/kg	191	
Melting point	°C	32	
		Solid	Liquid
Specific heat capacity	J/kg·K	3200	2800
Thermal conductivity	W/m·K	0.25	0.125
Density	kg/m <sup>3</sup>	915	880

The equations that govern the internal behavior of the DTEG are described in Equation (1), Equation (2), and Equation (3).

$$q = P \cdot J - k \cdot \nabla T, \tag{1}$$

$$Q = \left(\rho \cdot c_p \cdot \frac{\partial T}{\partial t}\right) + \nabla q, \tag{2}$$

$$J = -\sigma \cdot \nabla V - \sigma \cdot S \cdot \nabla T, \tag{3}$$

**2046** (2021) 012011 doi:10.10

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where S is the Seebeck coefficient,  $c_p$  is the specific heat capacity,  $\rho$  is the density, J is the electric current density, q is the heat flux by Fourier heat conduction and Peltier heat, P is the Peltier coefficient,  $\sigma$  is the electrical conductivity, Q is the internal heat generation, k is the thermal conductivity, V is the voltage and T is the temperature, respectively. The specific heat of the OM 32 material is determined by Equation (4).

$$c_{p} = c_{p,s} \cdot \left(1 - \alpha_{(T)}\right) + c_{p,l} \cdot \alpha_{(T)} + L \cdot \frac{d\alpha_{(T)}}{dT},\tag{4}$$

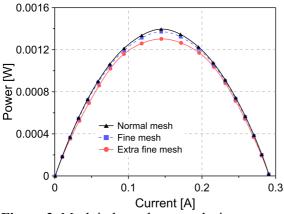
where  $c_{p,s}$  and  $c_{p,l}$  is the specific heat capacity in solid state and liquid state. L is latent heat, and  $\alpha_{(T)}$  is the thermal diffusivity, respectively. The efficiency  $(\eta)$  of DTEG is defined by Equation (5).

$$\eta = \left(1 - \frac{T_c}{T_h}\right) \cdot \left(\frac{\sqrt{1 + ZT_m} - 1}{\frac{T_c}{T_h} + \sqrt{1 + ZT_m}}\right),\tag{5}$$

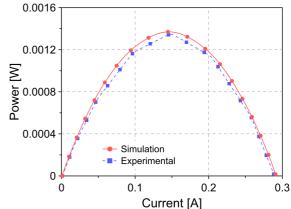
where  $ZT_m$  is the dimensionless figure of merit,  $T_c$  is the temperature in the cold side and  $T_h$  is the temperature in the hot side.

The solution of the dynamic process characteristics in the DTEG was carried out using the open-source CFD software OpenFOAM. For the boundary conditions, constant heat input and a convection condition were established. Additionally, it is considered transient heat conduction, and that the thermoelectric properties depend on the temperature. To ensure the reliability of the results obtained through the simulation, a mesh independence analysis was performed, and later an experimental validation. The results of these analyzes are shown in Figure 2 and Figure 3.

In the case of the mesh analysis Figure 2, the variation of the electrical power concerning the current was observed for three mesh configurations: normal, fine, and extra fine. It was observed that from a fine mesh, the variation of the results was less than 2% compared to the extra fine mesh. Therefore, the fine mesh was chosen for the rest of the study. Figure 3 shows the comparison between the electrical power predicted by the simulation and the one obtained experimentally. The results show that the maximum relative error between both behaviors was less than 5%. Additionally, it was observed that both behaviors maintain the same trend.



**Figure 2.** Mesh independence analysis.



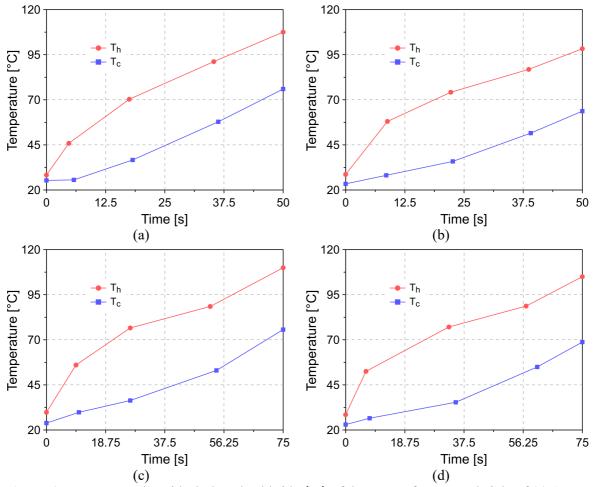
**Figure 3.** Validation of the results predicted by the simulation.

**2046** (2021) 012011

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#### 3. Results

Figure 4 shows the effect of the PCM height (see Figure 1) on the temperature in the sides (hot and cold) of the DTEG. The results show that the PCM allows maintaining a high difference between the extreme sides of the DTEG. An average temperature difference of 27°C was obtained for the simulated conditions, which can be maintained over time. This behavior is due to the latent heat storage capacity of the PCM. In general, increasing the height of the PCM allows more significant temperature differences to be achieved. The maximum temperature difference recorded was 41°C for a PCM height of 3.25 mm.



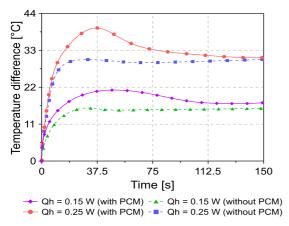
**Figure 4.** Temperature hot side  $(T_h)$  and cold side  $(T_c)$  of the DTEG for a PCM height of (a) 1 mm, (b) 1.75 mm, (c) 2.50 mm and (d) 3.25 mm.

Figure 5 shows the effect of PCM on the change in a temperature difference ( $\Delta T$ ) over time for different input heat flow ( $Q_h$ ) conditions. It was observed that the presence of higher heat fluxes leads to an increase in  $\Delta T$ . For a 67% increase in  $Q_h$  there was a 65% increase in  $\Delta T$ . The use of PCM allows a significant improvement in  $\Delta T$ . In general, an 11% increase in  $\Delta T$  was observed due to the use of PCM in the DTEG.

This behavior is a consequence of the additional decrease in temperature on the cold side of the DTEG due to the heat stored in the PCM during its phase change. Additionally, the presence of PCM in DTEG has the ability to reduce temperature fluctuations between the sides (hot and cold), which allows maintaining the temperature difference over time. Similar results are reported in experimental investigations [17].

**2046** (2021) 012011 doi:10.1088/1742-6596/2046/1/012011

Figure 6 shows the changes in  $\Delta T$  for different height conditions in the PCM. The results indicate an improvement in  $\Delta T$  with increasing PCM height, directly related to the greater heat retention capacity. It was observed that for a height of 1 mm, 1.75 mm, 2.50 mm, and 3.25 mm, the maximum temperature difference increases by 11%, 22%, 27%, and 35% compared to a DTEG without PCM. In general, increasing the height allows a higher concentration of temperature on the hot side, which causes an increase in the temperature difference in the DTEG.

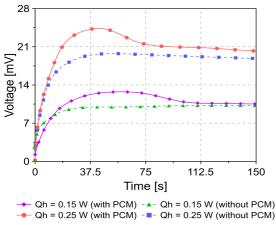


**Figure 5.** Comparison between the temperature difference without and with PCM.

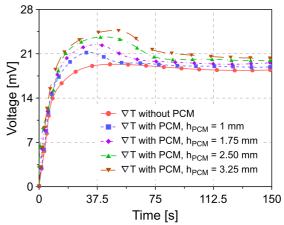
**Figure 6.** Temperature difference for PCM heights.

Figure 7 presents the DTEG voltage behavior with different heat flux inputs. The trend of the curves obtained shows that the voltage tends to increase with the heat flux increase. Additionally, an increase in voltage was observed with the use of PCMs. A 21% increase in the maximum voltage reached when using the PCM in the DTEG was observed from the results. The increase in voltage due to the use of PCMs is directly related to the increase in the temperature difference, as observed in the results shown in Figure 5. The theoretical analysis shows that the output voltage of the DTEG is a linear function that depends on the Seebeck coefficient and the temperature difference between the sides (hot and cold) of the DTEG [19].

Figure 8 depicts the variation of the voltage produced in the DTEG for various PCM heights. It was observed that the DTEG voltage improves with the increase in the height of the PCM, which is due to the greater different temperatures that can be reached, as shown in Figure 6. The previous result shows that the process of phase shift of PCMs is beneficial to improve DTEG thermal performance.



**Figure 7.** Comparison between the voltage without and with PCM.



**Figure 8.** Voltage difference for PCM heights.

**2046** (2021) 012011 doi:10.1088/1742-6596/2046/1/012011

Figure 9 describes the effect of PCM on DTEG efficiency for different heat flow conditions; in general, the results show that the presence of PCM allows for improving DTEG efficiency regardless of the heat flow condition. The increase in efficiency becomes more evident with the increase in the input heat flux.

On average, is observed in Figure 9 that a 30% increase in heat flux causes a 37% increase in DTEG efficiency. For the simulated conditions, it was possible to obtain maximum efficiency of 3.87% and 4.77% without PCM and with PCM, respectively. The higher efficiencies due to PCM use are the consequence of different factors that allow improving the energy conversion process in DTEG. Among the main factors is its heat storage capacity, which produces less uninterrupted electricity generation than DTEG without PCM. This characteristic is crucial when considering the practical applications of DTEG since, in general, thermal conditions are unstable or intermittent.

Additionally, the heat absorbed by the PCM material reduces energy losses due to the flow of heat transferred to the environment by conduction and convection processes. In general, the energy conversion efficiency reported in the literature for DTEGs is approximately 3%, 4% [20]. This low energy efficiency overshadows the broad benefits of DTEGs. Therefore, the use of PCM and geometric optimization methodologies is a tool with a high potential to improve the efficiency of DTEGs.

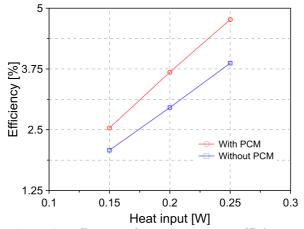


Figure 9. Influence of PCM on DTEG efficiency.

#### 4. Conclusions

In the present investigation, computational analysis is carried out to study the effect of phase change materials on the thermal performance of DTEG. The analysis involves the study of the conditions of temperature, electric potential, and efficiency. In general, it was observed that the presence of PCM in DTEG allows a significant decrease in the temperature difference between the sides. This is due to the ability of the material to maintain a constant temperature on the cold side due to its property of storing heat.

The results demonstrate that a 35% increase in temperature difference is possible with a PCM height of 3.25 mm. The greater temperature difference due to the use of the PCM has a positive influence on the electrical potential. A 21% increase in the maximum DTEG voltage was evidenced when using the PCM from the results obtained. Additionally, it can be deduced that the increase in the heat flux allows the increase of the electric potential in the DTEG. The analysis shows that PCM increases the efficiency of DTEG by 23%.

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