Numerical simulation of segmented ratio in bismuth telluride and skutterudites for waste heat recovery

K W Cheong¹, J H Lim*¹

¹ School of Computer Science and Engineering, Faculty of Innovation and Technology, Taylor’s University Lakeside Campus, No. 1, Jalan Taylor’s, 47500 Subang Jaya, Selangor, Malaysia.

* E-mail: joonhoong.lim@taylors.edu.my

Abstract. The thermoelectric performance of the segmented annular thermoelectric generators with the bismuth telluride and skutterudites has been investigated. The effect of the length ratio of the hot-segment leg to total length leg on the thermoelectric performance of the segmented annular thermoelectric generators is analysed and discussed and the optimization design of the annular thermoelectric generator with bismuth telluride and skutterudites as the materials with high thermoelectric performance is obtained. The result of the thermoelectric performance with the manipulated variable of the increase of length ratio, the output power, output voltage and efficiency of the segmented annular thermoelectric generators increase at the beginning then decrease afterwards. Additionally, to compare with the single bismuth telluride and skutterudites annular thermoelectric generators, the output voltage, output power and the conversion efficiency of the segmented annular thermoelectric generators can be improved twice. Lastly, the thermoelectric performance of the segmented annular thermoelectric generators operating in the changes of the temperature. The result has proved that as the temperature increase, the thermoelectric performance of the annular thermoelectric generator will also increase. Hence, the acquired results may be given some useful applications of the bismuth telluride and skutterudites on the segmented annular thermoelectric generators for waste heat recovery.

1. Introduction
Thermoelectric generators is a device that can transmit from the heat energy to electrical energy through the concept of the Seebeck effect. The thermoelectric generator also has several of advantages in real life such as the simple design, long-lasting, the replacement and the maintenance are unnecessary as well as environmentally friendly, which means it does not have any chemical products. The thermoelectric generator usually made up for several thermopiles where the purpose is to increase the output power [1]. The thermopiles on the thermoelectric generators are made of thermocouples where it connected with the electric sources while the parallel orientation is with the thermal sources [2]. Besides that, there are two types of the design for the thermoelectric generator, which are a planar thermoelectric generator, vertical thermoelectric generators and the annular thermoelectric generator [2]–[4]. In spite the thermoelectric generators provide the Seebeck effect, the Peltier effect is also a phenomenon that the cooling junction and the heating on the other junction when the electric current is stabilized in the circuit where it consists of two dissimilar thermoelectric conductors, the effect will be increase as the thermoelectric materials are the semiconductor due to the high figure of merit (zT) [5].
The first thermoelectric generators design is applying with the lateral thermocouples orientation to produce the lateral heat flow on the TEG, where the thermocouple is established and printed on the surfaces. It is known as the planar TEG. The advantages for this TEG is to control the thickness of the length of the thermocouple arms to compatibility towards the thin film, which has cause high temperature gradient and as the result the voltage will be increased. The second design of the thermoelectric generator design is the vertical thermoelectric generator, which it is arranged vertically along with the hot-segment to the cold-segment [6]. Hence, the heat flow will transmit vertically to the thermoelectric materials to provide electrical energy [7]. It is same to the Peltier based module for refrigeration. However, this TEG is also given a high density and as because of the simplicity of the design. The last design of the TEG is the annular thermoelectric generators, this TEG mostly applies on the heat engine on the cylindrical pipe. The system and the structural is almost similar to the vertical thermoelectric generators, but the shape is an annular ring shape.

As the semiconductors are the best thermoelectric materials for every thermoelectric generators due to the high figure of merit and high efficiency, the bismuth telluride (Bi2Te3) is the most suitable semiconductor for the thermoelectric system [8]. This is because the bismuth telluride has highest figure of merit among all of the semiconductor as well as the highest power factor with respect of the Seebeck coefficient (S) and the electrical resistivity (ρ) and the thermal conductivity (K), which is ZT > 1 as the highest is around ZT = 1.06 while at the room temperature in p-type thermoelectric leg. Another synthesized thermoelectric material, the skutterudites also have a high figure of merit which is at around ZT = 1.7 at the temperature of 850 K in p-type thermoelectric leg. As for the n-type thermoelectric leg, the figure of merit is about ZT = 1.4 at room temperature while for skutterudites the figure of merit is 1.3 at the temperature of 800 K.

Waste heat recovery (WHR) is the system that can transfer the heat through the heat output process to another process for several purposes and mostly increased its efficiency of the system [9]. The purpose of operating the waste heat recovery system is to decreasing the emission of the greenhouse gases and increase the efficiency of the system [10]. Nowadays, the waste heat recovery system has become one of the major fields in industries especially for the automotive [11]. It also has become the major area of research which is to reduce the fuel consumption, decrease the emission of harmful gases and improve the efficiency of the production. As for the application of the waste heat recovery, it used it for the recovery of waste heat on the automotive vehicles from the exhaust gas and the solar energy through the heat pipes on the vehicles [12]. For example, the design of the heat sources on the vehicle is cylindrical. The annular thermoelectric generator is suitable for reduce the heat loss on the heat section area of annular thermoelectric generator.

Based on the research, the heat transfer of the cylindrical shape heat exchanger has the better performance than the traditional heat exchangers for the automotive vehicles in some specific situations. From the other research, it stated that the energy efficiency of the annular thermoelectric generators decreases due to the affection of the Thomson effect as it founded that the transient pulse heating enhanced the performance of the SATEG for all heat input functions [13]. The heat source of the waste heat recovery is mostly at the temperature of 867 K or even higher [14]. As a result, the SATEG can improve the recovery rate of the waste heat. Besides the automotive vehicles can be apply on the waste heat recovery process, the heat engines are also used for waste heat recovery system with applying the first law of thermodynamics with the maximum efficiency acquired which is known as the Carnot efficiency [15]. The thermoelectric materials for heat engines are represent as the figure of merit. Based on the theory from the reference, the higher thermoelectric figure of merit and the temperature changes, the higher the output power that release from the TEG [16]. To identify the temperature region, the high temperature region of the waste heat recovery has including the recovering waste heat of 400°C, while the medium temperature range is around 100°C to 400°C [17]. Basically, the waste heat process carried out with the high temperature region to provide the combustion process as in the medium temperature region is from the exhaust gas of the combustion unit as well as for the low temperature region, is to making products and the equipment with the unit of process [18].
2. Methodology

2.1. Mathematical Model

The conversion efficiency of the segmented annular thermoelectric generator (SATEG) was determined with respect to the length ratio of the thermoelectric leg with the cold temperature bismuth telluride and medium temperature skutterudites as the materials for automotive exhaust as the waste heat recovery [19], [20]. To building the stationary SATEG from the two-dimensional mathematical model for the numerical analysis, several of assumptions were made for the numerical simulation of the SATEG module and simplify it. The conditions are:

- The difference between of the surfaces on the hot side and cold side are similar and fixed.
- The resistance of the thermal and electrical energy on the SATEG is negligible.
- The heat loss due to the convection on the surface of the SATEG is negligible.
- The heat sink is the temperature surrounding on the SATEG.
- The steady state heat transfer is employed, and the transfer of the heat energy is flow in one-dimensional towards the direction of the SATEG legs.
- Considering the hot side and cold side are the heat insulators and no convection around the SATEG.
- The material properties of the welding layer are negligible where it had the purpose to prevent the error during the numerical analysis.

![Figure 1. Schematic view of the SATEG.](image)

Based on the Fig. 1 shown, the schematic of the SATEG has consisted of the ceramic, copper layers, welding layers and the thermoelectric legs, where the hot side junction is the skutterudites while the cold side junction is the bismuth telluride. These thermoelectric can be represented by \( L_c \) and \( L_h \) respectively. The optimization of the parameter with the annular thermoelectric generator has been carried out. Hence, in this experiment, the length of the thermoelectric legs has been studied to observe the performance of the SATEG. Therefore, the overall length of the thermoelectric legs can be calculated as:

\[
L_t = L_h + L_c
\]

Where the \( L_t \) is the total length of the thermoelectric legs. The ratio of the hot-segment thermoelectric leg (skutterudites) with respect of total length can be determined as:

\[
\theta_1 = \frac{L_h}{L}
\]
As the ratio increased, the length of the hot-segment skutterudites also increases, while the length of the cold-segment bismuth telluride decrease. Where the $\theta_1$ and $\theta_2$ are representing as the ratio of hot-segment and cold-segment to the total length of thermoelectric legs respectively. To prevent the factors occur in a same time, the length of the thermoelectric must be fixed for this research. Therefore, the allowable ratio of the overall thermoelectric leg length to the specific hot-segment skutterudites of the thermoelectric legs must be assumed as:

$$0 < \theta_1 < 1$$

As for the analysis of the thermoelectric performance, the governing equation of the thermoelectric effect has considering about the concept of the Fourier and the Joule effect, where if the thermoelectric module was in a transient condition [22], the equation can be determined as:

$$\rho C \frac{\delta T}{\delta t} = \nabla \cdot ([\lambda] \nabla T - [I] J) + E \cdot J$$

While for the steady state thermal, the equation can be defined as:

$$0 = \nabla \cdot ([\lambda] \nabla T - [I] J) + E \cdot J$$

Besides the definition for the thermal state for the thermoelectric module, some of the equation can investigate the performance of the SATEG. To simplify the equation of the thermoelectric effect, the ANSYS is the suitable software to find out the results. The cold segment of the thermoelectric module must be flawless and the temperature of the cold segment must be fixed which the temperature is fixed at 298.15 K. The temperature of the hot segment is also fixed as it follows the assumptions shown above, in which the thermoelectric module is in a steady state [23]. While for the analysis of the transient state, the heat flux will be shown on the hot-segment of the SATEG module, which can be defined as:

$$\dot{q} = \alpha \sin(2\pi t - t_0) + b$$

Where the $\dot{q}$ is the rate of heat transfer per unit mass on the thermoelectric module, while $b$ is a constant value. To stop and avoid several of variable factors simultaneously, the overall heat flow is in constant value in advance. The potential of the copper layers on the SATEG module where it locates at the cold-segment of the $p$ thermoelectric legs is zero, while the whole thermoelectric module is act as an open circuit. Therefore, the operated potential voltage of the thermoelectric module under the environment with the difference of the temperature can be defined as:

$$V_0 = a(T_H - T_C)$$

Where the $T_H$ and $T_C$ are represented as the temperature of the hot-segment and cold-segment. Besides that, the open circuit voltage can be determined as:

$$V = -RI + V_0$$

The power output of the SATEG module can be defined as:

$$P = VI = I^2 R_L$$

The conversion efficiency of the SATEG module can be calculated as:

$$\eta = P/Q_{in}$$
2.2. Simulation

The dimension of the SATEG must be at fixed parameter except for the thermoelectric legs on the hot-segment skutterudites and cold-segment bismuth telluride in order to investigate the performances occur as the result of the experiment. The experiment will goes on the finite element analysis as the numerical simulation of the SATEG. As the ANSYS software and Solidworks software are used to investigate the research, the pre-processing steps and post-processing steps are provided to test the performance of the SATEG. For the pre-processing steps, the preparation for the design of the SATEG is the most crucial steps in Finite Element Analysis. In FEA, the surfaces on the design can be separated to the small parts and multiples of elements which are known as the finite element. In short, this process is called as the meshing. Each of the different surfaces must have apply with the different mesh, where it was to provide more accurate result. But before the meshing, the selection of the material properties of the whole SATEG. The material for this thermoelectric module are bismuth telluride (Bi₂Te₃), Skutterudites, copper and the ceramic.

For the dimension of the SATEG, the annular thermoelectric module will be made into the segmented part which is around 6 degrees. The length of the ceramic, copper layer are the 0.7 mm and 0.3 mm respectively. As for the thermoelectric legs, it included p-leg and n-leg. Each of the thermoelectric legs length are 2mm while the gap angle of the SATEG is 2 degrees. Prior to the post-processing steps, the adjustment of the meshing process is needed to acquire the result of the SATEG more accurate. The faces of the whole SATEG has been selected for meshing in which the dimension of the element sizes are 0.2 mm. Besides the face meshing on the SATEG, the edge meshing is apply on the edge of the ceramic layer since the shape of the thermoelectric module is annular. Later on, the setup of the boundary condition is also needed for the research methodology, the temperature of the cold-segment of the SATEG is about 298.15 K (25°C) whereas the hot-segment is about 573.15 K (300°C) and it is considered as the medium range temperature. Besides the setup of the temperature of the SATEG, the initial voltage of the annular thermoelectric module is 0 V where it has applied onto the side of the copper layer along with the n-leg skutterudites. For the verification of the SATEG model in this numerical simulation, some of the cases had been examined on the similar conditions, such as the length of the SATEG leg is 6 mm and the temperature of the cold-segment was always constant, which is 298.15 K (25°C). As the boundary conditions of the SATEG are mostly symmetrical, the performances of the segmented annular thermoelectric module is simulated.

3. Results and Discussion

3.1. Analysis of thermoelectric performance

![Figure 2](image_url)

**Figure 2.** Comparison between the length ratio of the hot-segmented leg to the total length and the output voltage in different temperature difference
In the thermoelectric analysis, the voltage, material selections, and the temperature must include to find out the results of the numerical simulation of the SATEG. The figure below shows the average output voltage with respect of the ratio of the hot-segmented skutterudites leg length to the total length of the SATEG leg with different temperature difference. The Fig. 2 represents that the variation of the output voltage with the length ratio \(\theta_1\) and the changes of the temperature at the hot side and if using the ratio at the cold side to the total length, the chart will also get the same result but in opposite trend. From the Fig. 2 shown, it can be proved that the increase of the temperature difference, the output voltage of the SATEG are also increasing. It also showed that the thermoelectric performance of SATEG is higher than the single material of the annular thermoelectric generators even has the same parameters as shown in Fig. 3 and the Tab. 1 below.

**Table 1.** The comparison between the output voltages of the single thermoelectric materials annular thermoelectric generators in different temperature.

| Temperature of \(T_h, T_c = 25^\circ C\) | Output voltage of single Bi\(_2\)TE\(_3\) (mV) | Output voltage of single skutterudites (mV) |
|----------------------------------------|---------------------------------------------|---------------------------------------------|
| 200                                    | 1.006288585                                 | 1.237673502                                 |
| 300                                    | 1.36262853                                  | 1.95442832                                  |
| 400                                    | 1.56266366                                  | 2.67805565                                  |

**Figure 3.** Comparison between the temperature of the hot-segment and the output voltage

As the difference of the temperature increase, the Fig. 4 above has represented that there is an obvious trend of increasing and more curve of output voltage until the length ratio has reach in \(\theta_1 = 0.583\) and then decreasing gradually as the length ratio increase. Through this chart, there are always have an optimal value of the max output voltage in which the length ratio is from 0 to 1, the maximum output voltage at the temperature of \(T_h = 673.15\) K (400\(^\circ\)C) is at the length ratio of 0.583, which is 5.263 mV. The reason why the trend on the chart occurred is because of the material properties of the bismuth telluride is suitable and better in the low temperature compared to the skutterudites. Besides that, as the temperature difference is getting smaller, the SATEG module has a minor of advantage. When the temperature difference is large, the SATEG module has proved that there is an improvement for the traditional thermoelectric devices. The optimization of the SATEG parameter is around 0.4167 to 0.583. However, these cases and situations are also similar to the result of the output power varies with the length ratio shown in Fig. 4 and Tab. 2.
Table 2. The comparison between the length ratio and the output power of the SATEG in different temperature.

| The ratio of the hot side leg to total leg, $\theta_1$ | Output power, W. At $T_h = 200^\circ C$, $T_c = 25^\circ C$ | Output power, W. At $T_h = 300^\circ C$, $T_c = 25^\circ C$ | Output power, W. At $T_h = 400^\circ C$, $T_c = 25^\circ C$ |
|--------------------------------------------------|--------------------------------------------------|--------------------------------------------------|--------------------------------------------------|
| 0.083                                            | 1.59E-03                                         | 3.70E-03                                         | 6.44E-03                                         |
| 0.167                                            | 1.90E-03                                         | 4.56E-03                                         | 8.23E-03                                         |
| 0.250                                            | 2.15E-03                                         | 5.25E-03                                         | 9.65E-03                                         |
| 0.330                                            | 2.35E-03                                         | 5.78E-03                                         | 1.07E-02                                         |
| 0.417                                            | 2.46E-03                                         | 6.09E-03                                         | 1.13E-02                                         |
| 0.500                                            | 2.53E-03                                         | 6.27E-03                                         | 1.17E-02                                         |
| 0.583                                            | 2.50E-03                                         | 6.19E-03                                         | 1.15E-02                                         |
| 0.670                                            | 2.41E-03                                         | 5.98E-03                                         | 1.12E-02                                         |
| 0.750                                            | 2.20E-03                                         | 5.44E-03                                         | 1.02E-02                                         |
| 0.830                                            | 1.92E-03                                         | 4.76E-03                                         | 8.88E-03                                         |
| 0.917                                            | 1.49E-03                                         | 3.69E-03                                         | 6.86E-03                                         |

Figure 4. The comparison between the length ratio of the hot-segmented leg to the total length and the output power in different temperature difference.

3.2. Analysis of the bismuth telluride and skutterudites

Besides the performances of the output voltage and power of the SATEG, the research of the thermoelectric materials including bismuth telluride and skutterudites are also have been carry out to investigate the performances of the SATEG. The SATEG consist of two types of legs, which are p-leg and n-leg, each of the legs have embedded with the bismuth telluride and skutterudites, where it is known as p-Bi$_2$Te$_3$, n-Bi$_2$Te$_3$, p-sku and n-sku. In order to examined the thermoelectric performances, the variation between the length ratio and the output voltage for each leg has been simulated. The Fig. 5 shows the comparison between the length ratio of the p-leg thermoelectric material and the output power on the p-leg in different temperature environment.
Figure 5. The comparison between the length ratio of the hot-segmented leg to the total length and the output power with respect of different temperature difference in p-leg bismuth telluride.

Figure 6. The comparison between the length ratio of the hot-segmented leg to the total length and the output power with respect of different temperature difference in n-leg bismuth telluride.

Based on the Fig. 5, the chart had stated that the output voltage of the p-leg bismuth telluride decreases drastically from the ratio of 0.083 to 0.25 as the length ratio $\theta_1$ increase. This has shown that as the length of the bismuth telluride decrease, the output voltage at the p-leg is also decrease. The reason why the trend of the chart happens is because the bismuth telluride has a high electrical resistivity and low thermal conductivity as the length of the p-leg decrease and temperature increase. The Seebeck coefficient on p-leg bismuth telluride also decrease as the temperature increase. Besides the length ratio, the temperature difference on the Fig. 5 has showed that it affected the performance of the SATEG on p-leg as the temperature increase. Besides taking the numerical simulation on the p-leg, the n-leg on the SATEG is also recorded as shown in below Fig. 6. Based on the Fig.6, the chart has stated that at first the output voltage on the n-leg in both thermoelectric materials have increasing at the ratio from 0.083 to 0.583. The reason why the trend occurred on these charts is due to the n-leg thermoelectric materials have higher thermal conductivity compared to the specific p-leg thermoelectric materials. Besides that, the output voltage at the n-leg have been decrease gradually after the length ratio of 0.583. Throughout
this chart, it can be showed that the output voltage of n-leg is higher than the p-leg as the open circuit on the SATEG move from the positive direction to the negative direction.

3.3. Analysis of optimization design of SATEG

From the above discussion, it can be said that the length ratio, $\theta_1$ has affected the thermoelectric performance. However, the length ratio has also affect the performances of the thermoelectric materials such as the bismuth telluride and skutterudites on the SATEG. In order to acquire the optimization of the SATEG for the improvement of the waste heat recovery, the length ratio of 0.5 (hot-segment leg 3 mm, cold-segment leg 3 mm) has been chosen for optimization structure of the SATEG as it has high thermoelectric performances. To analyse the optimized SATEG, the comparison between the single thermoelectric materials is needed to make a discussion.

**Figure 7.** The comparison between the maximum output voltage of the optimized design and the single thermoelectric material SATEG.

**Figure 8.** The comparison between the maximum output power of the optimized design and the single thermoelectric material SATEG

Fig. 7 demonstrates the trend of the maximum output voltage of the annular thermoelectric generator with the manipulated variable of the temperature, $T_h$. It can be stated that the thermoelectric performance
of the single bismuth telluride annular thermoelectric module is lower than the single skutterudites annular thermoelectric module. In fact, if compared with the optimized SATEG, the thermoelectric performance is better than the two single thermoelectric materials module. Besides the analysis of the maximum output voltage, the comparison of the maximum output power and the three types of annular thermoelectric devices with respect of the temperature. This comparison has been taken as the Fig. 8. Based on the Fig. 8, it can be seen that the maximum output power of the single bismuth telluride annular thermoelectric device is better than the single skutterudites annular thermoelectric generator in the temperature of 200°C, but lower as the temperature increase. In addition, if the optimized SATEG is compared with the other two single materials annular thermoelectric generators, the optimized SATEG would be better than the other two annular thermoelectric generators. Furthermore, in the temperature of 400°C, the maximum power of the optimized SATEG is 1.17E-02 W, which is almost twice of the other two annular thermoelectric generators.

3.4. Analysis for conversion efficiency for waste heat recovery
In the practical applications, the environment for the thermoelectric devices is always considering about the conversion efficiency of the thermoelectric device where it is providing for the improvement of the waste heat recovery system. In this section the effect of the efficiency on the thermoelectric performance of the SATEG with the optimized length ratio of 0.5 is studied.

![Figure 9](image-url)

**Figure 9.** The comparison between the length ratio of the hot-segmented leg to the total length and the conversion efficiency in different temperature difference

The Fig. 9 shows the trend of the conversion efficiency of the length ratio of hot-segment leg with respect of the temperature difference. It shows that the efficiency increased when the length ratio of the hot-segment to total length increase until 0.5, which means the efficiency of the SATEG is the highest when the bismuth telluride and skutterudites legs are 3 mm. As the efficiency of the SATEG has reach the peak, the trend will going down as the length ratio is more than 0.5, which means if the skutterudites legs have increase, the heat absorbed on the SATEG will also increase. Above all the efficiency analysis, the temperature surroundings are also affected by the efficiency of the annular thermoelectric generators as well as the length ratio. The optimized length of the SATEG is analysed with comparing the other two single materials annular thermoelectric generators just as the Fig. 10.
Figure 10. The comparison between the conversion efficiency of the optimized design and the single thermoelectric material SATEG

Based on the Fig. 12, it can be showed that the efficiency of the single bismuth telluride annular thermoelectric generator is higher than single skutterudites annular thermoelectric generator in low temperature region, but in high temperature region, it has been seen that the efficiency of the bismuth telluride is lower than the skutterudites of the annular thermoelectric generators. As for the optimized annular thermoelectric generator, it showed that the efficiency is always higher than the other annular thermoelectric generator even in low and high temperature region. At the temperature of 400°C, the efficiency of the optimized thermoelectric generator is 25.71% in which twice of the efficiency for the respective annular thermoelectric generators.

4. Conclusion

In a nutshell, the three-dimensional design of the SATEG is analyzed, and the optimal design with the high thermoelectric performance is acquired through the optimization of the parameter of the SATEG. Besides that, the thermoelectric performance of the respective bismuth telluride and skutterudites on the SATEG is studied. In a consequence, some of the cases can be concluded in this research. One of the conclusions can be made of is the length ratio of the hot segment to total thermoelectric length, $\theta_1$ is around 0.4167 to 0.583. When the length ratio parameter is around this range, the thermoelectric performance of the SATEG is mostly higher than the other two single material thermoelectric generators when the hot-segment temperature was from the range of 200°C to 400°C. The SATEG that has high thermoelectric performance can be acquired through the optimizing the parameter on the ANSYS software and Solidworks. In this research paper, the structural parameter $\theta_1$ of 0.5 is selected as the optimization design of SATEG. When the hot-segment temperature has achieved 400°C, the maximum output voltage and output power are 5.183278524 mV and 1.17E-02 W respectively, which is almost twice of the single bismuth telluride and single skutterudites annular thermoelectric generators in terms of output voltage and output power. In the conversion efficiency analysis, the efficiency of the SATEG is affected by the output voltage, output power and the temperature. It also has showed that the optimization design of the SATEG has higher efficiency than the other two single material annular thermoelectric materials.

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