Numerical Study on Optimizing the Geometry of Segmented Asymmetrical Thermoelectric Generator

H C Luo\(^1\) and L S Cheng\(^1,2\)

\(^1\)College of Mechanical & Electrical Engineering, Shaanxi University of Science and Technology, Xi’an 710021, China

E-mail: lsheng.ch@sust.edu.cn

Abstract. Quite large amount of heat generated in various industrial processes was wasted. Recovering the waste heat can save cost and benefit the environment protection. The device that convert heat energy to electricity is called thermoelectric generator (TEG), and therefore it can be used for waste heat recovery. Improving the efficiency is the main direction of present study. The configuration and geometry of the thermoelectric legs are proved can influence the thermoelectric performance of the thermoelectric generator. Compared with the conventional TEG which is assembled with symmetrical (rectangular) legs, asymmetrical thermoelectric generator (ATEG) has a greater temperature gradient in a leg due to the convergent geometry which can reduce overall thermal conduction of the device and Thomson effect is also harnessed. In this study, three-dimensional finite element analysis (COMSOL) is employed to investigate the numerical simulations of a segmented pyramidal thermoelectric generator (SPTEG) and a segmented cone thermoelectric generator (SCTEG) to optimize the leg length ratio of two materials, and it’s effect on the electrical and mechanical performances of SPTEG and SCTEG was also studied. Results obtained shows that the height ratio of SATEG can influence electrical and mechanical performances and the optimum height ratio provided a better electrical performance while thermal stress developed in leg was less. In addition, the open-circuit voltage of two types SATEG is similar because they have the same cross sectional area and the same volume, however, SCTEG has a dispersive thermal stress distribution while the thermal stress of SPTEG concentrates in four corners. Compared to the maximum von Mises stress in SPTEG, the maximum von Mises stress in SCTEG reduced about 10%. Results obtained from this study would provide references in producing and design of segmented asymmetrical thermoelectric generators.

1. Introduction

Improving the energy efficiency is always the focal point since human-beings were able to control fire. Recycling the waste heat is one of the most valid way to improve energy utilization ratio and thermoelectric generator (TEG) is a device that can convert temperature difference to electricity straightly and shares the characteristics of non-selection to heat source, noiselessness, no-moving parts, long lifetime, and high reliability, has attracted more and more attention in last several years \[1\]. However, due to the low transfer efficiency it’s application is still limited in some fields. Therefore, enhancing thermoelectrical and mechanical performance of TEG is the main target. It can be achieved by optimizing thermoelectric generator geometry and employing thermoelectrical materials with higher thermoelectric material figure of merit \((Z = \frac{\alpha^2}{\kappa \cdot R})\) which is generally used to describe the performance
where $R$ is electrical resistivity, $\kappa$ is thermal conductivity and $\alpha$ is the Seebeck coefficient. Materials with low thermal conductivity, high electrical conductivity ($\sigma$) and high Seebeck coefficient are better to raise the thermoelectric figure of merit [2].

Optimizing geometry is another way to improve efficiency of thermoelectric generator [3]. Ferreira-Teixeira et al. [4] optimized the configuration of a thermoelectric generator using finite element method. They studied cylindrical and cubic thermoelectric legs using COMSOL software. Results obtained showed that two geometries have the same thermoelectrical performance for they have the same cross-sectional area and volume and there is an optimal width and height ratio of the thermoelectric legs that can improve the performance of thermoelectric generator. Fabián-Mijangos et al. [5] studied asymmetrical thermoelectric generator experimentally. They found that asymmetrical legs can reduce the thermal conductivity that enlarge the temperature difference. Results obtained showed the thermoelectric figure of merit of asymmetric leg is almost double compared to conventional symmetric one. Shittu et al. [6] also used finite element method, and they built a three-dimensional model to research the performance of segmented pyramid thermoelectric generator under pulse heat flux, they found under transient condition, thermal stress developed in the hot side of asymmetrical leg reduced by 7.45% compared to thermal stress developed in symmetrical leg. Optimized height ratio can enhance electrical performance and reduce thermal stress thereby increasing module’s reliability.

Segmented thermoelectric generator has attracted much attention in research in last few years. This is because that all the thermoelectric materials are unstable within the whole temperature region, and combining two different thermoelectric materials which have high figure of merit in different temperature range [7]. In ideal condition, both of two materials enable to operate in their most efficiency temperature region and the performance of the module can be enhanced. A numerical analysis of an annular segmented thermoelectric generator was performed by Shittu et al. [8] Results obtained showed reducing the length of leg can improve the electrical performance while the mechanical reliability decline. And the edge of leg is the most vulnerable position. The optimization of segmented cone thermoelectric generator is presented in this paper. Many studies merely focus on electric performance and neglect thermal stress produced by thermal expansion of the materials. It has been proved asymmetrical geometry can improve electric performance and reduce thermal stress simultaneously by Shittu et al [6]. In this study, thermal and electric performance of two kinds of asymmetrical thermoelectric generators with the same heat source is compared. COMSOL 5.4 Multiphysics software is used. To ensure the accuracy some thermoelectric material properties which are temperature dependent are taken into consideration. Section 2 provides a detail description of the geometry model and material properties. Section 3 describes numerical model including boundary conditions, and the thermal stress and thermoelectric analyses. The results obtained from simulation are presented in section 4. Finally conclusion is drawn in section 5.

2. Geometric model description

![Figure 1. geometry model (a)SPTEG model (b)SCTEG model](image-url)
A segmented pyramidal thermoelectric (SPTEG) geometry is showed in Figure. 1a while that segmented cone thermoelectric (SCTEG) geometry is showed in Figure. 1b. There are four parts in TEG including alumina ceramic which is heat conductor and electric insulation, copper conductor connects two semiconductor legs promotes the electric conductivity in the generator, solder layer is used to reduce the thermal stress produced by thermal expansion of thermoelectric materials, and a pair of p-type and n-type legs are the core parts in the whole device which convert temperature difference into electric. Two different thermoelectric materials are applied as shown in Figure. 1b. The dimensions are kept totally same for the accuracy of performance comparison. The height of two kinds of thermoelectric legs is same therefor,

\[ H = H_1 + H_2 \]  

where \( H_1 \) is the height of hot/section while \( H_2 \) is the height of cold/section.

Changing the cross-section area along the z-axis is way to get asymmetric leg, to simplify the simulation, the radius and width of cold side are twice that of hot side therefor,

\[ R_{leg} = R_c = 2 \times R_h \]  
\[ W_{leg} = W_c = 2 \times W_h \]

where \( R_{leg} \) is the radius of the cone leg, \( R_c \) is the radius of cold side cone thermoelectric leg, \( R_h \) is that in hot side, \( W_{leg} \) is width of pyramidal leg, \( W_c \) is the width of cold side pyramidal leg and \( W_h \) is that of hot side. Area ratio is kept constant in this study. However, it is reported that optimized segmented height ratio can improve the performance [6], this ratio is also varying to find optimum value, so

\[ H_m = \frac{H_1}{H_2} \]

where \( H_m \) is the height ratio of two different thermoelectric materials.

The geometry dimensions of SCTEG and SPTEG are shown in Table 1. In this study, temperature in hot side varied from 650K to 750K, thermoelectric materials Skutterudite (CoSb3) and Bismuth telluride (Bi2Te3) are selected for the hot segment/side and cold segment/side respectively to make two materials operate at the optimum temperature range. Bi2Te3 is thought as the best thermoelectric material at present for it has high figure of merit for low temperature range (<500K) while Skutterudite’s thermoelectric performance improves when the temperature increases. In addition, both of them have strong mechanical performance so these two materials are selected in this study. thermoelectric materials’ properties which are temperature dependent are shown in Figure 2 and Table 2. shows other parameters used in this study. Ceramic and thermoelectric materials are set as brittle materials and the strength of CoSb3 is 14.1GPa [9] while the yield stress of Bi2Te3 is 112MPa [11]. Solder and copper are elastoplastic materials, tangential modulus and the yield stress of solder are 8.9GPa and 26MPa respectively while those of copper are 24GPa and 70MPa respectively [12].

| Parameter                | Symbol | Value   |
|--------------------------|--------|---------|
| Ceramic height           | Hce    | 0.75mm  |
| Solder height            | Hs     | 0.175mm |
| Cooper height            | Hc     | 0.3mm   |
| Leg height               | Hleg   | 2.15mm  |
| Cooper width in hot side | Wch    | 3.52mm  |
| Ceramic width            | Wce    | 3.94mm  |
| Leg radius in cold side  | Rc     | 0.79mm  |
| Leg depth in cold side   | Dleg   | 1.4mm   |
| Ceramic depth            | Dce    | 1.77mm  |
Figure 2. temperature dependent properties of materials (a)Seebeck coefficient (b)thermal conductivity (c)electric resistance [10]

| Material   | Thermal conductivity, $\kappa (\text{W/m} \cdot \text{K})$ | Electrical conductivity, $\sigma (\text{S/m})$ | special heat capacity, $C_p (\text{J/kg} \cdot \text{K})$ | Density, $\rho (\text{kg/m}^3)$ | coefficent of thermal expansio, $n_s (1/K)$ | Young’s Modulus, E (GPa) | Seebeck coefficient, $\alpha (V/K)$ | Poisson’s ratio |
|------------|-----------------------------------------------------------|-------------------|---------------------|-------------------|------------------------------------------|-------------------|----------------------------------|---------------|
| Ceramic    | 25                                                        | 1e-12             | 800                 | 3970              | 0.68e-5                                  | 340               | 0                               | 0.22          |
| Copper     | 385                                                       | 5.9e7             | 386                 | 8930              | 1.7e-5                                   | 120               | 6.5e-6                          | 0.3           |
| Solder     | 55                                                        | 2e7               | 210                 | 7240              | 2.7e-7                                   | 44.5              | 0                               | 0.33          |
| Bi2Te3     | -                                                         | -                 | 154.4               | 7740              | 0.8e-5~1.32e-5                           | 65                | -                               | 0.23          |
| CoSb3      | -                                                         | -                 | 238.7               | 7582              | 6.36e-6                                  | 145.38            | -                               | 0.223         |
3. Numerical model
Analysis including thermoelectric and thermal stress are carried out on SCTEG and SPTEG.

3.1. Governing equation of thermal stress analysis
Materials’ thermal conductivity are temperature dependent and the model established in this study is three-dimensional. Therefore, mechanical and thermodynamic characteristics are nonlinear in the z-axis direction. Thermal stress field can be calculated by temperature field for temperature influence the model deformation.

The heat conduction equation can be expressed as [13]

\[
\frac{\partial}{\partial x} \left[ k \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[ k \frac{\partial T}{\partial y} \right] + \frac{\partial}{\partial z} \left[ k \frac{\partial T}{\partial z} \right] = 0
\]

(1)

where \( T = f(x, y, z) \) and \( k = f(T) \) obtained temperature filed is used in thermal stress analysis.

The expansion of the material leads to thermal stress develop in the device. the displacement-strain relation governing equation can be expressed as [14]

\[
-\varepsilon_{xx} = \frac{\partial w}{\partial x} - \varepsilon_{yy} = \frac{\partial v}{\partial y} - \varepsilon_{zz} = \frac{\partial w}{\partial z}
\]

\[
-\varepsilon_{xy} = 0.5 \left( \frac{\partial w}{\partial y} + \frac{\partial v}{\partial x} \right), \varepsilon_{xz} = 0.5 \left( \frac{\partial w}{\partial z} + \frac{\partial v}{\partial x} \right), \varepsilon_{yz} = 0.5 \left( \frac{\partial w}{\partial z} + \frac{\partial v}{\partial y} \right)
\]

(2)

(3)

Using Jacobian the displacement-strain relation is expressed in a dimensionless form gives,

\[
\begin{bmatrix}
\sigma_{xx} \\
\sigma_{yy} \\
\sigma_{zz} \\
\sigma_{xy} \\
\sigma_{yz} \\
\sigma_{xz}
\end{bmatrix} = \frac{-E}{(1+\nu)(1-2\nu)} \begin{bmatrix}
1-\nu & \nu & 0 & 0 & 0 \\
\nu & 1-\nu & 0 & 0 & 0 \\
\nu & \nu & 1-\nu & 0 & 0 \\
0 & 0 & 0 & 1-2\nu & 0 \\
0 & 0 & 0 & 0 & 1-2\nu \\
0 & 0 & 0 & 0 & 0
\end{bmatrix} \begin{bmatrix}
\varepsilon_{xx} \\
\varepsilon_{yy} \\
\varepsilon_{zz} \\
\varepsilon_{xy} \\
\varepsilon_{yz} \\
\varepsilon_{xz}
\end{bmatrix} \times \begin{bmatrix}
1 \\
1 \\
1 \\
0 \\
0 \\
0
\end{bmatrix}
\]

(4)

\( \sigma_1, \sigma_2, \sigma_3 \) represent the three-principle stress in device respectively and von Mises equivalent stress can be obtained from the fourth strength theory of mechanics of materials which is expressed as,

\[
\sigma = \sqrt{\frac{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2}{2}}
\]

(5)

3.2. Governing equation of thermoelectric analysis
thermoelectric governing equations were coupled by Shittu et al. [8],
\[
\n\nabla \cdot \left( T \alpha J \right) - \nabla \cdot \left( \lambda \nabla T \right) = q
\]

(6)

\[
\nabla \cdot \left( \sigma \alpha \nabla \phi \right) + \nabla \cdot \left( \sigma \nabla \phi \right) = 0
\]

(7)

where \( \alpha \) is the Seebeck coefficient, \( T \) is the temperature, \( J \) is the current density vector, \( \lambda \) is coefficient of heat transfer, \( \phi \) electric scalar potential, \( q \) is the heat generation rate per unit volume.

3.3 Boundary conditions
To simplify simulation some assumptions are made in this study without huge deviation from real conditions. The assumptions are:

(a) all surfaces are adiabatic except heat source and heat sink.
(b) ignoring the electric contact resistance and thermal contact resistance.
(c) temperature in cold side is fixed while hot side varying.
(d) during the thermal stress analysis only hot surface is fixed
(e) heat loss caused by radiation and convection on all surface are neglected.

the device is assumed to be cooled by heat sink which is connect to cold side. Temperature in cold surface is 300K.

4. Results and discussion

4.1 Effect of hot side temperature
Since the temperature in cold surface is constant through the study, the effect of hot side temperature on mechanic and electric performance is shown in Figure 3 Increasing temperature can enlarge the temperature difference which will facilitate thermal expansion in the devise therefore, the max von Mises stress in thermoelectric leg increases. The open-circuit voltage can evaluate the conversion efficiency which is one of the most vital performance. Due to the highest temperature in this study is 750K within CoSb3’s working temperature range, it's can be seen from Figure 3b open-circuit voltage increases significantly when temperature in hot side gets higher.

4.2 Effect of segment ratio
There is no doubt that using two different materials can improve performance and enlarge the operating temperature range of the device. In the thermal stress analysis, it can be seen from Figure 3a that optimum height ratio varies while working conditions changing. When the height ratio gets higher the temperature in hot side of Bi2Te3 approach the limitation of the material and there is a point of intersection of two materials’ Seebeck coefficient curves with temperature increasing that's why the function curves in Figure 3b verge to gentle. It can be seen from Figure 4 the temperature in bismuth telluride section beyond the operating temperature range of the material when height ratio \( H_m=3:1 \) and temperature of heat source is 750K.

4.3 Effect of geometry
The thermoelectric performance of SCTEG and SPTEG is totally similar for cone leg and pyramid leg have the same cross-section area and volume. However, thermal stress developed in SCTEG is less than that in SPTEG which is shown in Figure 3a. The imagery line represents the max von Mises in pyramid leg and the full line represents the von Mises in cone leg. The von Mises stress nephogram is shown in Figure 5 Obviously, thermal stress developed in SPTEG concentrates on the corners while the thermal stress distributes more dispersive in SCTEG so that cone legs contribute to reduce thermal stress compared with pyramid legs.
Figure 3. Variation of height ratio with SATEG (a) maximum von Mises stress (b) open-circuit voltage
5. Conclusion
In this study, finite element analysis is used to investigate the influence of geometry to mechanical and thermoelectric performance of segment asymmetric thermoelectric generator. COMSOL software is employed to perform numerical simulations and temperature dependent properties of the material are
considered. Six different height ratios are performed to investigate the optimum ratio for performance of SATEG. Following conclusions have been found from this study:

1. Geometry can influence thermal stress produced by thermal expansion, the maximum von Mises stress in segment cone thermoelectric generator reduced by 10% generally compared to that in segment pyramid thermoelectric generator.

2. \(H_m=3:1\) is the optimum height ratio which can enhance the electrical performance and reduce thermal stress when heat source temperature lower than 700K.

3. Geometry has no influence on electrical performance.

References

[1] Elghool A, Basrawi F, Ibrahim T K, Habib K, Ibrahim H and Idris DMND 2017 A review on heat sink for thermo-electric power generation: classifications and parameters affecting performance. *Energy. Convers. Manag.* **134** 260–77.

[2] Elsheikh M H, Shnawah D A, Sabri M F M, Said S B M, Hassan H M, Bashir A M B and Mohamad M 2014 A review on thermoelectric renewable energy: principle parameters that affect their performance, *Renew. Sustain. Energy Rev.* **30** 337–55.

[3] Li G Q, Samson Shittu, Ma X L and Zhao X D 2019 Comparative analysis of thermoelectric elements optimum geometry between photovoltaic-thermoelectric and solar thermoelectric, *Energy* **171** 599-610.

[4] Ferreira-Teixeira S and Pereira A M 2018 Geometrical optimization of a thermoelectric device: numerical simulations, *Energy Convers. Manag.* **169** 217–227.

[5] Fabián-Mijangos A, Min G and Alvarez-Quintana J 2017 Enhanced performance thermoelectric module having asymmetrical legs, *Energy Convers. Manag.* **148** 1372-81.

[6] Samson Shittu, Li G Q, Zhao X D, Ma X L, Akhlaghi Y G and Ayodele E 2019 Optimized high performance thermoelectric generator with combined segmented and asymmetrical legs under pulsed heat input power *Journal of Power Sources* **428** 53-66.

[7] Hadjistassou C, Kyriakides E and Georgiou J 2013 Designing high efficiency segmented thermoelectric generators, *Energy Convers. Manag.* **66** 165–72.

[8] Samson S, Li G Q, Zhao X D, Ma X L, Akhlaghi Y G and Ayodele E 2019 High performance and thermal stress analysis of a segmented annular thermoelectric generator *Energy Convers. Manag.* **184** 180-93.

[9] Li G, An Q, Li W, Goddard W A, Zhai P, Zhang Q and Snyder G J 2015 Brittle failure mechanism in thermoelectric skutterudite CoSb3, *Chem. Mater.* **27** 6329–36.

[10] Shen Z G, Liu X, Chen S, Wu S Y, Xiao L and Chen Z X 2018 Theoretical analysis on a segmented annular thermoelectric generator, *Energy* **157** 297–313.

[11] Al-Merbati A S, Yilbas B S and Sahin A Z 2013 Thermodynamics and thermal stress analysis of thermoelectric power generator: influence of pin geometry on device performance, *Appl. Therm. Eng.* **50** 683–92.

[12] Fan S and Gao Y 2018 Numerical simulation on thermoelectric and mechanical performance of annular thermoelectric generator *Energy* **150** 38-48.

[13] Wu Y, Ming T, Li X, Pan T, Peng K and Luo X 2014 Numerical simulations on the temperature gradient and thermal stress of a thermoelectric power generator. *Energy Convers. Manag.* **88** 915–27.

[14] Ming T et al. 2017 Numerical analysis on the thermal behavior of a segmented thermoelectric generator, *Int. J. Hydrogen Energy* **42**(5) 3521-35.