Geometry Design-Based Thermoelectric Optimization Module

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ABSTRACT - One alternative energy source is thermoelectric, which is able to convert waste heat into electricity. However, study on thermoelectric still needs a lot of development, particularly in module design because there is still not many thermoelectric development in terms of the module geometry design when compared to the development in material structure. Therefore, research on thermoelectric optimization based on the module design was carried out using computer simulation. One of the parameters that can be used for analysis is the maximum output power which is thought to be increased through the cross-sectional area, length, shape, and type of pairs of legs. The thermoelectric properties used in the simulation are the Seebeck effect, resistivity, thermal conductivity, finite element analysis (FEA), and power output to understand the processing of simulation results. The research begins by making a design for each variation, entering the specifications, then the running process and calculations to obtain the maximum output power. From the simulation results, it is known that the thermoelectric design will be optimal for small leg lengths, large cross-sectional areas, and using similar materials (Unileg) which have good specifications with a maximum output power value of 3.713x10^-8 W for blocks, 3.634x10^-8 W for cylinders, and 8.617x10^-8 W for Unileg N-N.

INTRODUCTION

The human need for energy is increasing. Therefore, many scientists are starting to develop alternative energy sources. Many alternative energy sources have been developed, some of which are steam, nuclear, solar cells, and so on. One alternative energy that has been widely studied is thermoelectric which is an alternative energy source which can convert waste heat into electrical energy. One of the related studies is optimization in terms of material improvement which has been carried out considerably. Other optimizations can be carried out by using a thermoelectric module geometry design which is easier and cheaper since this optimization can be done by simply forming a printed thermoelectric material. Thereof, a study will be carried out on thermoelectric optimization through the module geometry design.

A thermoelectric is a device which can convert energy between heat to electricity [1]. Thermoelectric requires materials which have high electrical conductivity and Seebeck coefficient, while the thermal conductivity is low [2]. Thermoelectric can convert a temperature difference to a potential difference thus it has a role as a generator (Thermoelectric Generator) as in Figure 1 or converts a potential difference into a temperature difference which can be used for cold temperatures thus it can act as a cooler (Thermoelectric Cooler).

![Figure 1. Energy conversion process in Unicouple thermoelectric module](image-url)

The core of the thermoelectric material is a semiconductor, which is a material with a very small band gap between the conduction band and the valence band so that semiconductors have electrical conductivity between conductors and insulators. Based on the impurity (doping), semiconductors are divided into two, namely pure intrinsic semiconductors without any impurities and extrinsic semiconductors which have impurities such as N-type with impurity atoms with more electrons than the basic structure atoms and P-type with atoms with fewer electrons than structural atoms, basically [3].

One of the parameters related to see effectiveness of a semiconductor material used in thermoelectric devices is the figure of merit (zt). the higher the zt value, the better the thermoelectric performance. zt value of thermoelectric is...
influenced by electrical conductivity (related to the ability of the material to flow electrons) [4], thermal conductivity (related to the ability of the material to conduct heat) [5], and seebeck coefficient (related to the ability to convert between heat and electricity) [6]. The relationship between these three factors can be seen in Equation (1).

\[
\varepsilon T = \frac{\sigma S^2 T}{\kappa}
\]

(1)

Where \( \sigma \) is the electrical conductivity, \( \kappa \) is the thermal conductivity, \( S \) is Seebeck coefficient, and \( T \) temperature [7]. Finite element analysis (FEA) is an analytical method based on the finite element method. The method describes a complex system into a simple one by dividing it into elements and solving them partially. To get the results of computational analysis using the FEA method, several stages are needed, starting from the description of the actual system and modelling it. Furthermore, comparison of real models with physical phenomena (Physical Modelling). From the obtained physical phenomena, modelling of all the required formulas and equations (Mathematical Modelling) is carried out. After obtaining formulas and equations, the system is divided into small elements, the formula is applied to each element using computer calculations (computation). Eventually, after being processed by a computer, the results are compiled and analyzed in order that they become systematic data such as the distribution of heat, electricity, and so on [8],[9].

First, to describe a thermal electrical system, two main equations are needed, namely Equation (2) and Equation (3) (heat transfer and continuity of current density phenomena) for thermoelectric [9].

\[
\rho c \frac{\partial T}{\partial t} + \vec{v} \cdot \vec{q} = Q
\]

(2)

\[
\vec{v} \left( \vec{E} \right) + \vec{v} \cdot \vec{J} = Q
\]

(3)

\( T \) is temperature, \( \vec{E} \) is electric field, \( \vec{q} \) is heat flux, \( \vec{J} \) is electrical current density, \( Q \) is internal heat generator, \( \rho \) is density, \( c \) is heat capacity, and \( \varepsilon \) is electric permittivity. Then, all the variables are described as in Equation (4) (Joule Heat), Equation (5) (Peltier Effect), and Equation (6) (Electric Field Relationship and Potential).

\[
\vec{J} = \sigma \vec{E} - \sigma S \vec{V} \nabla T
\]

(4)

\[
\vec{q} = \Pi \vec{J} - \kappa \vec{V} \nabla T
\]

(5)

\[
\vec{E} = -\vec{V} \phi
\]

(6)

\( \phi \) is electric potential. Next, the main variables (temperature T and Potential) are described into the interpolation function in Equation (7) to Equation (8).

\[
T = [N][T_e]
\]

(7)

\[
\phi = [N][\phi_e]
\]

(8)

\( T_e \) is vector of nodal temperature, \( \phi_e \) is vector of nodal electrical potential, and \( N \) is element shape functions. Then, all the variables in Equation (2) and Equation (3) are replaced with all the described variables (Equation (4) to Equation (8)) and the FEA matrix equation like Equation (9) is made.

\[
\begin{bmatrix}
C_T & 0 \\
0 & C_E
\end{bmatrix}
\begin{bmatrix}
\frac{\partial^2 T}{\partial t^2} \\
\frac{\partial^2 \phi}{\partial t^2}
\end{bmatrix}
+ \begin{bmatrix} K_T & 0 \\ K_{TE} & K_E \end{bmatrix}
\begin{bmatrix}
[T_e] \\
[\phi_e]
\end{bmatrix}
= \begin{bmatrix} Q \\ \Pi \end{bmatrix}
\]

(9)

\( C \) and \( K \) are element of matrix which describe coefficient in finite element equation. Equation (9) is what will be converted into computational form and used to process input data [9]. Every electronic device has a load (resistance/impedance) in it, therefore the device will always consume power when operated. Power itself is a measure of energy per unit of time thus power is related to the movement of energy. The energy in question can be anything such as chemical, heat, or electricity. One method to see the thermoelectric performance is to look at the output power of an electronic device (load). With the same temperature difference, it can be seen which thermoelectric module is better by comparing the maximum output power of the module. At the same temperature, the output power is also indirectly related to the thermoelectric conversion efficiency. The thermoelectric output power is related to the yield potential \( (V = \alpha \Delta T = \alpha(T_T - T_e)) \), the internal resistance of the material (foot resistance = R), and the load resistance \( (R_L) \). Mathematically shown by Equation (10).
Po is the output power, $\alpha$ is Seebeck coefficient, $T_H$ is the hot side temperature, $T_C$ is the cold temperature, $R_L$ is the load resistance, and $R$ is the internal resistance \[10\]. The output power will be maximum when \[11\]. Another parameter which can be used for thermoelectric analysis is its efficiency ($\eta$, conversion efficiency) which is the ratio of the input heat power ($Q_h$) to the output power ($P_o$). Mathematically the value can be written as in Equation (11).

$$\eta = \frac{P_o}{K\Delta T + ([\alpha_P] + [\alpha_N])T_H I + \frac{1}{2} I^2 R}$$

$K$ is thermal conductance (W/K), $\alpha_P$ is P-type Seebeck coefficient (V/K), $\alpha_N$ is N-Type Seebeck coefficient (V/K), $T_h$ is temperature at hotspot (K), $I$ is current (A) \[11\]. Many factors can hinder thermoelectric efficiency. Therefore, there are also many methods which can increase thermoelectric performance. Among the many methods are reducing the thickness of the thermoelectric leg, like Al-Fath reported \[12\], simulation results in this study show that the smallest thickness can reduce internal resistance but cannot explain the anomalies in some fabricated thicknesses where the internal resistance value is even greater, other is increase cross-section of the leg, like Ge did which result can increase induced EMF \[13\], changing the shape of the leg like Liu did can reduce thermal stress to increase performance of thermoelectric \[10\], and can also change modules into a single type (Unileg) like Aljaghtam did, which result can increase more efficiency if use single type semiconductor since that can reduce the risk due to the use of two different types \[13\]–\[15\].

Resistance ($R$) is related to the level of the material's ability to flow electrons (create current) with a certain voltage. Resistance is also related to the dimensions of the material. The basic property of resistance is related to resistivity ($\rho$). Resistivity is a basic property of materials related to the material's ability to generate electric current regardless of dimensions. Therefore, if a material has a certain resistivity $\rho$ and volume dimensions $V$ ($V=1 \times A$), then the relationship between resistivity can be seen in Equation (12).

$$R = \frac{\rho l}{A}$$

$R$ is resistance (\(\Omega\)), $\rho$ is resistivity (\(\Omega\) m), $l$ is length of the material in the direction of the field from the potential difference (m), and $A$ is the cross-sectional area of the material perpendicular to the direction of the field from the potential difference. From Equation (12), it is known that the resistance will increase if the material is long and will decrease if the material is wide \[4\].

**EXPERIMENTAL METHODS**

**Materials and Instruments for Simulation**

The physical materials and equipment used for the simulation are a PC (personal computer) with ANSYS 2021 R2 Software, Microsoft Excel 2019 installed in it, and MATLAB Online for making graphs. While the virtual materials and equipment needed were material models, such as CaTiO$_3$ with oxygen void (CTO +VO) as a model material for P-type feet \[16\], SiC with a mixture of 30% AlN (SiC/AlN) as a model material for N-Type feet \[17\], alumina with a purity of 96% as a model material for insulators (electrically isolating the thermoelectric module), copper alloy as a model material for thermoelectric conductive parts (conducting output electricity), and a model material as a load test (Load) to determine the output power. Further specifications are as in Table 1 and Table 2.

**Table 1. Materials specification**

<table>
<thead>
<tr>
<th>Materials Name</th>
<th>Thermal Conductivity (W/m°C)</th>
<th>Seebeck Coefficient (V/C)</th>
<th>Resistivity ($\Omega$m)</th>
<th>Source of Data</th>
</tr>
</thead>
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<td>Alumina 96%</td>
<td>25</td>
<td>-</td>
<td>-</td>
<td>ANSYS Database (suhu 22-27)</td>
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<tr>
<td>Copper Alloy</td>
<td>401</td>
<td>-</td>
<td>1,69E-08</td>
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<td>Load</td>
<td>1</td>
<td>-</td>
<td>Depend on total internal resistance of leg</td>
<td>-</td>
</tr>
<tr>
<td>CTO(Tipe-N Leg)</td>
<td>4.806</td>
<td>-2.062E-04</td>
<td>2.049E-04</td>
<td>Li, 2021</td>
</tr>
<tr>
<td>SiC (Tipe-P Leg)</td>
<td>13.348</td>
<td>1.169E-04</td>
<td>0.099</td>
<td>Besisa, 2018</td>
</tr>
</tbody>
</table>
Simulation Conditions

The study started with the search for literature related to thermoelectrics, specifically in the module design section or the geometry of the thermoelectric. Next, several journals and books related to thermoelectricity were obtained, including two journals related to thermoelectric materials which use to model, CTO and SiC/AlN was chosen because journals which describe those materials are complete with the specification needed. After finding a journal which describes how to optimize thermoelectrically (like optimizing figure of merit, power output, etc), obtained four journals that focused on discussing variations which can optimize thermoelectric (cross-sectional area [13], leg length [12], shape [10], and types of pairs of legs [14]).

Table 2. Other specification

<table>
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<th>Unit</th>
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<tr>
<td>Mesh Size</td>
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<td>m</td>
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<tr>
<td>Hot Temperature</td>
<td>27</td>
<td>°C</td>
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<tr>
<td>Cold Temperature</td>
<td>22</td>
<td>°C</td>
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Table 3. Variation used

<table>
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<th>Variation Type</th>
<th>Variation</th>
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<tr>
<td>Leg length/thickness</td>
<td>1 mm</td>
</tr>
<tr>
<td>Cross-section of leg</td>
<td>1X1 = 1 mm²</td>
</tr>
<tr>
<td>Shape of leg</td>
<td>Block</td>
</tr>
<tr>
<td>Type of pair of legs</td>
<td>UniLeg P-P</td>
</tr>
</tbody>
</table>

Sum of variation = 21 (Unicouple and Block 3x3x3 use the same design) (Unileg PP and NN use the same design)

Figure 2. Process of making thermoelectric module design: (a) bottom insulator plate; (b) bottom conductor plate (c) load; (d) thermoelectric leg; (e) top conductor plate; (f) top insulator plate; (g) size scale for block, and (h) size scale for cylinder
The next step is a simulation using Workbench Software (Includes Input Specifications and Running). The software used is ANSYS Workbench (ANSYS 2021 R2 Software Clump). The first step starts with the inclusion of specifications in the Engineering Data. Second, adjust the design parts with suitable materials and Mesh on the Model. Third, enter each probe used such as the temperature difference used and the Ground in Setup. Fourth, it is continued by entering the various desired results in the Solution menu and Fifth Running so that the results are obtained which will be recalculated to find the maximum output power and efficiency. Sixth, the maximum output power value graph is made using MATLAB and Excel.

### RESULTS AND DISCUSSION

After the simulation, the results of the potential output are obtained in Table 4. Then the calculations are carried out. After all the data has been calculated, the next step is to graph the maximum output power value in Table 4. Using MATLAB and Microsoft Excel, the data is processed to obtain results such as the color graphs in Figure 3, Figure 4, and Figure 5.

<table>
<thead>
<tr>
<th>Block</th>
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<tr>
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<td>7.135</td>
<td>22.99</td>
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<tr>
<td>3</td>
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<td>33.211</td>
<td>7.423</td>
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<table>
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<td>16.45</td>
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<table>
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<tr>
<th>Type of pair</th>
<th>Unicouple N-P (3x3x3)</th>
<th>Unileg P-P (3x3x3)</th>
<th>Unileg N-N (3x3x3)</th>
</tr>
</thead>
<tbody>
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<td></td>
<td>33.211</td>
<td>33.211</td>
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<td>548.3</td>
<td>87.47</td>
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</table>

**Table 4.** Experimental data

**Figure 3.** Color grid graph Maximum output power: (a) block leg and (b) cylinder leg
Dimension-related variables are the length/thickness of the foot and also the cross-sectional area related to its internal resistance. The shape of the foot is related to the distribution of thermal stress, as well as the deformation of the material. In addition, there are also variations in the types of pairs (Unileg and Unicouple) related to whether or not each material is used together or separately.

In this process, many design variations are made, the number of which corresponds to the product of the basic variables and form variables ($3 \times 3 \times 2 = 18$ variables) to ensure that each type of variable intersects with each other so that it can be analyzed thoroughly (Global, analyze just in one graphic). Especially for the Leg pairs variable, a special self-simulation was carried out to see the basic behavior (one stacked type) of the pair type.

In the temperature selection, a lower temperature equal to the base temperature/room temperature/default ambient temperature of ANSYS is selected. The temperature difference is kept small ($5\,^\circ\text{C}$) to avoid changes in material characteristics due to temperature changes. The mesh used is $0.0005\,\text{m}$. This is the minimum Mesh size that the personal PC can do with minimal crashes on the simulation. After creating the mesh, the next step is running (Solve) Software and the results are obtained.

The cross-sectional area and length of the thermoelectric leg are the basic variables of the shape of the thermoelectric leg. The basic variable is related to the basic properties it has. In the color Grid Graph in Figure 3, it can be seen that both cylinders and blocks have a high maximum output power value with a large cross-sectional area. One of the properties, which affect it, is resistance like in Table 4. Resistance and Maximum Power Output has inversely
relation like describe in Equation (10) if $R_L=R$. Resistance is inversely proportional to the cross-sectional area. The wider the cross-sectional area, the easier it is for electrons to pass through the material, so that the resistance is getting smaller and also the output power is getting bigger. This is because the reduced power wasted due to the internal resistance of the thermoelectric material [4]. It can also be seen in the color Grid Graph that the shorter leg length has the greater Maximum Power Output. Seen in This shows that there is an inverse relationship between power and the length or thickness of the foot. Likewise in the case of cross-sectional area. The length of the leg is also related to the maximum output power through resistance, where the resistance is directly proportional to the length of the leg like in Equation (12). Because the maximum output power also has a direct effect on efficiency, the graph form is not much different from the maximum output power, as shown in Figure 4. Thus, it is known the relationship between maximum output power and efficiency with the cross-sectional area and leg length, when the cross-sectional area is 9 mm$^2$ and the Leg length 1 mm. The maximum output power for the block is $3.713 \times 10^8$ W and the efficiency is $3.682 \times 10^{-9}$. For the cylinder, the maximum output power is $3.634 \times 10^{-8}$ W and the efficiency is $3.603 \times 10^{-9}$.

For the shape of the legs analysis, in previous study about shape [10], it was stated that the shape of the cylindrical foot can reduce the deformation due to stress which occurs at the corners of the copper alloy plate on the thermoelectric block. However, it is not directly related to the output power. In this study, the relationship is seen through simulation. From Figure 3, both shapes (blocks and cylinders) have the maximum side ($3.713 \times 10^8$ W for blocks and $3.634 \times 10^8$ W for cylinders), and minimum side ($2.121 \times 10^9$ W for blocks and $1.984 \times 10^9$ W for the cylinder). The maximum Power Output value is dominating with Block, as well as for efficiency. It can be concluded that the reduction in deformation is not related to the maximum output power or it may be related to the less-than-optimal meshing process (either in terms of square meshing shape or mesh size).

For the type of pair of legs analysis, in previous studies about pair of leg [14], it was proven that Unileg had a better performance than Unicouple. However, this research shows that Unileg is not always better than Unicouple, depending on the type of material itself. In this study, it can be seen that the maximum output power or efficiency of the P-N Unicouple is lower than the Unileg N-N but still higher than the Unileg P-P, as shown in Figure 5. This can happen because the thermoelectric performance of N is superior to the P-type so that if it paired, the P-type hinders the performance of the N-type legs. Therefore, the function of Unileg’s design is to make maximum use of single thermoelectric material (N only or P only) without using a partner which can actually hinder its performance.

CONCLUSION

Research on design-based thermoelectric optimization is carried out with several methods, including modifying the thickness of the legs, cross-sectional area, shape, and types of pairs of thermoelectric legs. Experiments were carried out using ANSYS software to obtain optimal results from these variables. From the simulation experiment, it is found that the Thermoelectric Module Design will be optimal when the leg length is small, the cross-sectional area is wide, the block shape, and also pairs of Unileg legs using good single material.

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