# Multiphysics Modelling and Multilevel Optimization of Thermoelectric Generator for Waste Heat Recovery.

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## Abstract:-

Waste heat is inevitable in any heat engine while producing useful mechanical work. A lots of heat energy is often dissipated to surrounding environment as waste, which limits the system efficiency. In almost all of the industrial processes, half of the heat energy is turned into waste heat. Many innovation and investment is been happening to convert waste heat into useful work. The waste heat is been used in various way to get useful work in various industries. Producing electricity in a convenient way from the waste heat is a challenge, that every industry face. There are many known technologies to produce electrical energy from waste heat. One of the approach is using Thermoelectric Devices, where a temperature gradient across the semiconductor modules produces voltage that causes electric current to flow producing electric power. This phenomenon is referred as Seebeck effect. Developing a optimized TEG Device for maximum power output from waste heat is a challenging one, which need more attention in energy industry. In this work, the numerical modelling and simulation of a Thermoelectric Generator (TEG) is investigated. The studied model is consists of P-Type and N-Type Bismuth Telluride (Bi2Te3) semiconductor modules connected electrically in series and thermally in parallel. The produced electric voltage, current and power from temperature gradient is investigated. The Design Module, Thermoelectric Effect Module, Heat Transfer Module and AC/DC module of COMSOL Multiphysics software is used to simulate and predict Thermoelectric power output. The numerical simulation and investigation of TEG device in COMSOL Multiphysics shows more potentials for numerous research and application of TEG in several industries.

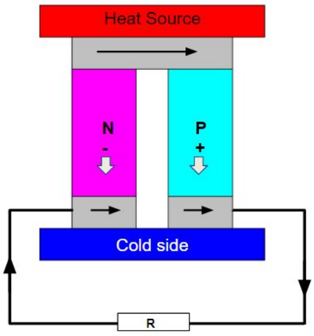
Keywords:- Thermoelectric, TEG, Seebeck effect, Generator.

## Introduction:-

Thermoelectric Generator (TEG) is a solid state device which converts temperature gradient into electric power, a phenomena called as Seebeck effect. The thermoelectric effect is the direct conversion of temperature gradient to electric voltage and vice versa via a thermocouple. A thermoelectric device creates voltage when there is a different temperatures on two opposite sides. Conversely, when a voltage is applied, it creates a temperature gradient. At the atomic scale, an applied temperature gradient causes charge carriers in the material to diffuse from the hot side to the cold side. This effect can be used to generate electricity, measure temperature or change the temperature of objects. The direction of heating and cooling is predicted by the polarity of the applied voltage. Thermoelectric devices can be used as temperature controllers.

## Thermoelectric Generator (TEG):-

A thermoelectric generator composed with materials of different Seebeck coefficients (p-doped and n-doped) semiconductors. A thermoelectric schematic circuit diagram is mentioned in fig 1.1. If the load resistor (R) is replaced with a voltmeter (V), the circuit then functions as a temperature-sensing thermocouple. The Seebeck effect is a classic example of an electromotive force (emf) and leads to measurable currents or voltages in the same way as any other emf.



( Figure 1.1 : Unitcouple TEG )

Electromotive forces modify Ohm's law by generating currents even in the absence of voltage differences (or vice versa); the local current density is given by

$$J = \sigma(-\nabla V + E_{emf})$$

Where V is the local voltage, and $\sigma$ is the local electrical conductivity. In general, the Seebeck effect is described locally by the creation of an electromotive field

$$E_{emf} = -S\nabla T$$

Where S is the Seebeck coefficient (also known as thermopower), a property of the local material, and ΔT is the temperature gradient. The Seebeck coefficients generally vary as function of temperature and depend strongly on the composition of the material. For ordinary materials at room temperature, the Seebeck coefficient may range from −100 μV/K to +1,000 μV/K. If the system reaches a steady state, where J = 0, then the voltage gradient is given simply by the emf: -V =

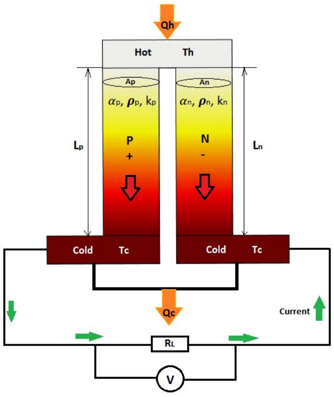
SΔT.Thermoelectric materials must have high electrical conductivity (σ) and low thermal conductivity (K) to be good thermoelectric material. Low thermal conductivity in these materials ensures that when one side made hot other side stays cool, which helps to generate high voltage while in a temperature difference. More will be the temperature gradient more will be the electric voltage. But the thermoelectric devices works efficiently within a certain temperature range. The Efficiency of thermoelectric material is governed by its “figure of merit” zT.

$$zT = \frac{S^2 \sigma T}{K}$$

Where S denotes the Seebeck Coefficient, which is the measure of magnitude of electrons flow in response to temperature gradients across the thermoelectric material, $\sigma$ is the material electrical conductivity, $T$ is the reference temperature, $K$ is the thermal conductivity. Thermoelectric materials like Bismuth Telluride ($Bi_2Te_3$), Lead Telluride (PbTe), and silicon germanium (SiGe) are the three main semiconductors have both high power factor and low thermal conductivity were mainly used for many years, are very rare elements which makes them expensive.

## Thermoelectric Generator (TEG) Analytical Derivation:-

A thermoelectric generator is a power generating device that directly converts thermal energy into electrical energy. When the connected junctions of two dissimilar materials (n-type and p-type) have a temperature difference, an electrical current is generated as shown in Figure 1.2. For a thermoelectric generator, subscript 1 is used for the hot side in equation 1.10 and 1.11 and subscript 2 is used for the cold side.



( Figure 1.2 : TEG Schematic Diagram )

$\alpha$ = total seebeck coefficient
$\alpha_p$ = P-leg seebeck coefficient
$\alpha_n$ = N-leg seebeck coefficient
$\varrho_p$ = P-leg electrical resistivity
$\varrho_n$ = N-leg electrical resistivity
$k_p$ = P-leg thermal conductivity
$k_n$ = N-leg thermal conductivity
R = total electrical resistance
K = total thermal conductance
$L_p$ = P-leg length
$L_n$ = N-leg length
$A_p$ = P-leg cross-sectional area
$A_n$ = N-leg cross-sectional area
$Q_h$ = Heat supplied
$Q_c$ = Heat rejected
$R_L$ = Load resistance

$$Q_h = \alpha T_h I - \frac{1}{2}(I^2 R) + K(T_h - T_c) \qquad 1.10$$

$$Q_c = \alpha T_c I - \frac{1}{2}(I^2 R) + K(T_h - T_c) \qquad 1.11$$

By applying the first law of thermodynamics, the electric power $W$ generated from the thermocouple is

$$W = Q_h - Q_c \qquad 1.12$$

Or,

$$W = \alpha I(T_h - T_c) - I^2 R \qquad 1.13$$

Also,

$$W = I^2 R_L \qquad 1.14$$

Where $R_L$ is the load resistance.

$$\alpha = \alpha_p - \alpha_n \qquad 1.15$$

$$R = \frac{\rho_p L_p}{A_p} + \frac{\rho_n L_n}{A_n} \qquad 1.16$$

$$K = \frac{k_p A_p}{L_p} + \frac{k_n A_n}{L_n} \qquad 1.17$$

Moreover, Ohm’s Law is defined as

$$V = IR_L = \alpha(T_h - T_c) - IR \qquad 1.18$$

Therefore, current $I$ can be written as

$$I = \frac{\alpha(T_h - T_c)}{R_L + R} \qquad 1.19$$

The thermal efficiency of the thermoelectric generator is defined as the ratio of power output to the heat input.

$$\eta_{th} = \frac{W}{Q_h}$$

2.10

$$\eta_{th} = \frac{I^2 R_L}{\alpha T_h I - \frac{1}{2} I^2 R + K(T_h - T_c)}$$

2.11

The output power and thermal efficiency can also be rewritten in terms of $R_L / R$ as follows.

$$W = \frac{\alpha^2 T_c^2 \left[ \left( \frac{T_c}{T_h} \right)^{-1} - 1 \right]^2 \left( \frac{R_L}{R} \right)}{R\left(1+\frac{R_L}{R}\right)^2}$$

2.12

$$\eta_{th} = \frac{\left(1-\frac{T_c}{T_h}\right)\left(\frac{R_L}{R}\right)}{\left(1+\frac{R_L}{R}\right) - \frac{1}{2}\left(1-\frac{T_c}{T_h}\right) + \frac{\left(1+\frac{R_L}{R}\right)^2 \frac{T_c}{T_h}}{ZT_c}}$$

2.13

For maximum conversion efficiency

$$\frac{d\eta_{th}}{d\left(\frac{R_L}{R}\right)} = 0 \Rightarrow \frac{R_L}{R} = \sqrt{1 + z\overline{T}}$$

2.14

Where $T$ is the average temperature between the hot and cold junction and is equal to

$$\overline{T} = \frac{T_c + T_h}{2} = \frac{1}{2} T_c \left[ 1 + \left( \frac{T_c}{T_h} \right)^{-1} \right]$$

2.15

As a result, the maximum conversion efficiency, $\eta_{mc}$ , is

$$\eta_{mc} = \left( 1 - \frac{T_c}{T_h} \frac{\sqrt{1+Z\overline{T}}-1}{\sqrt{1+Z\overline{T}}+\frac{T_c}{T_h}} \right)$$

2.16

For maximum power efficiency

$$\frac{dW}{d\left(\frac{R_L}{R}\right)} = 0 \Rightarrow \frac{R_L}{R} = 1$$

2.17

As a result, the optimum current $I_{mp}$ maximum power $W_{max}$ and maximum power efficiency $\eta_{mp}$ are

$$I_{mp} = \frac{\alpha \Delta T}{2R}$$

2.18

$$W_{max} = \frac{\alpha^2 \Delta T^2}{4R}$$

2.19

$$\eta_{mp} = \frac{(1-\frac{T_c}{T_h})}{2-\frac{1}{2}(1-\frac{T_c}{T_h})+\frac{4\frac{T_c}{T_h}}{ZT_c}}$$

3.10

The above analysis explains the concepts of the thermoelectric generator of one thermocouple while multiple couples are being used in many of the TEG Modules. The thermoelectric parameters for multiple couples as shown in Figure 1.3 can be predicted by multiplying unitcouple parametres with number of couples, $n$, as follows.

$(W)_n = nW$

$(Qh)_n = nQh$

$(R)_n = nR$

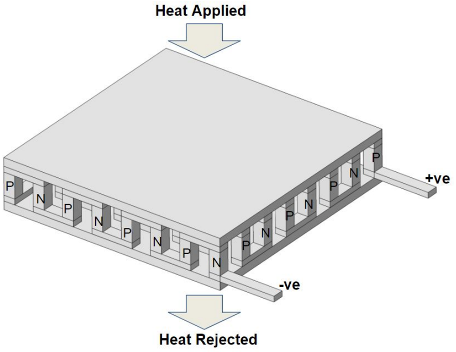
$(RL)_n = nRL$

$(V)_n = nV$

$(K)_n = nK$

$(I)_n = I$

$(\eta_{th})_n = \eta_{th}$

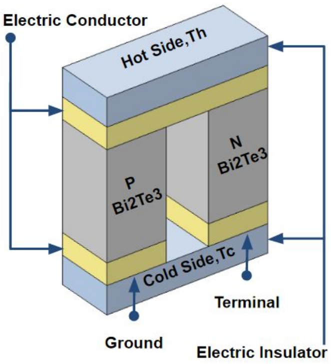


( Figure 1.3 : Conventional TEG Module )

## Thermoelectric Generator (TEG) Numerical Simulation:-

## Unit Couple TEG Simulation:-

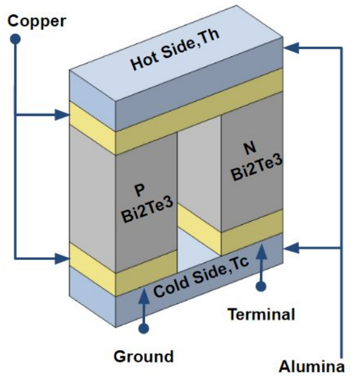
A multiphysics cae model for a unit couple TEG module is developed using finite element analysis. The unit couple TEG module consists of P-Type and N-Type bismuth telluride $Bi_2Te_3$ of leg dimension as 1.4mm x 1.4mm x 2.5mm. The TEG legs are connected electrically in series and thermally in parallel.



( Figure 1.4 : Unit Couple TEG Module )

## Material Properties:-

The material properties such as Density, Seebeck Coefficient, Electrical Conductivity, Thermal Conductivity, Relative Permittivity, Heat capacity for TEG material $Bi_2Te_3$ and conducting material Copper are given in the below tables. The arrangements for the material to the TEG module is shown in figure 1.5.



( Figure 1.5 : TEG Module Material Definition )

The Seebeck Coefficient, Electrical Conductivity and thermal conductivity of Bismuth Telluride (Bi2Te3) are a function of temperature, that is these values are temperature dependent. The temperature dependent material properties are represented graphically in table 1.

| T (K) | S (V/K) | K (W/mK) | $\sigma$ (S/m) |
|---|---|---|---|
| 200 | 168E-6 | 24E-1 | 1.4286E5 |
| 250 | 192E-6 | 19E-1 | 1.1111E5 |
| 300 | 210E-6 | 16E-1 | 0.86957E5 |
| 350 | 225E-6 | 16E-1 | 0.71429E5 |
| 400 | 237E-6 | 17.5E-1 | 0.58824E5 |

( Table 1 : Bi2Te3 Temperature Dependent Material Properties )

## Governing Equations:-

Multiphysics CAE Model of a Thermoelectric Generator is developed using COMSOL 5.2. The numerical problem is solved using Thermoelectric Effect Module in temperature gradients of $70^C$, $170^C$ and $270^C$. The governing equations are mentioned below.

### (1) Heat Transfer in Solids:-

The heat transfer in solid interface is used to model heat transfer in solids by conduction, convection and radiation. The temperature equation defined in solid domains corresponds to the differential form of the Fourier's law that may contain additional contributions like heat sources.

$$\rho C_p u.\nabla T + \nabla.q = Q + Q_{ted},\ q = -k\nabla T$$

### (2) Electric Currents:-

The physics interface solves a current conservation equation based on Ohm's law using the scalar electric potential as the dependent variable. The interface is used to compute electric field, current, and potential distributions in conducting media.

$$\nabla J = Q_j\ ,\ J = \sigma E + J_e\ ,\ E = -\nabla V$$

### (3) Thermoelectric Effects:-

The physics interface combines the Electric Currents and the Heat Transfer in Solids interfaces for modeling Peltier-Seebeck-Thomson effects.

$$q = PJ\ ,\ P = ST\ ,\ J_e = -\sigma S \nabla T$$

Where

$\rho$ = Density

Cp = Specific heat

Q = Heat source

Qted = Thermoelastic effects

$Q_j$ = Current Source

q = Heat flux in conduction

K = Thermal conductivity

T = Temperature

P = Peltier Coefficient

J = Induced Electric Current

$J_e$ = External Current Source

E = Electric field

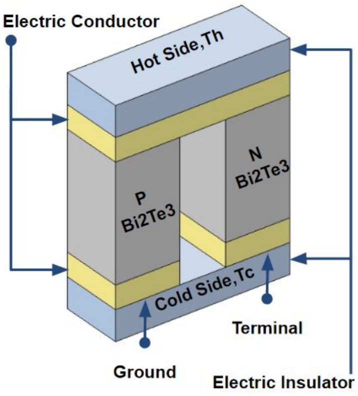
V = Electric Potential

S = Seebeck Coefficient

$\sigma$ = Electrical Conductivity

### Boundary Definition:-

The boundary definitions for the TEG module in COMSOL Multiphysics are mentioned in below figure. Top planar surface is defined as the TEG heat source or hot side temperature as $100^C$, $200^C$, $300^C$. Bottom planar surface are defined as cold surfaces, temperature as $30^C$. The TEG Modules P-Type and N-Type are arranged electrically in series and thermally in parallel. One end of the TEG is defined as Terminal and other as Ground. The convective and radiative heat transfer and the contact resistance of the unitcouple is neglected in the experiment. The heat is considered to flow from the hot side and rejected from the cold side with no other means than the ceramics, thermoelements and connecting conductors.



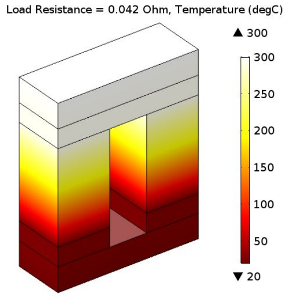
( Figure 1.6 : TEG Boundary Definition )

## COMSOL Solver:-

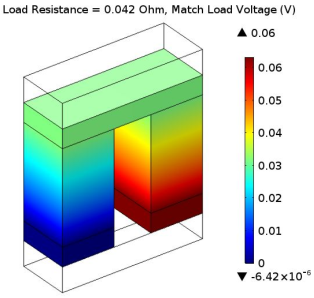
A fully coupled, direct, stationery study is implemented to the TEG model to predict the electrical power production from temperature gradient.

## Result Evaluation:-

The temperature distribution and electric potential contour plots are plotted graphically as shown in below figures.

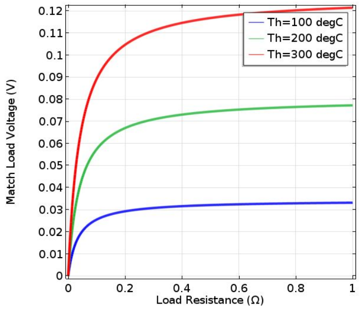


( Figure 1.7 : TEG Temperature Distribution )

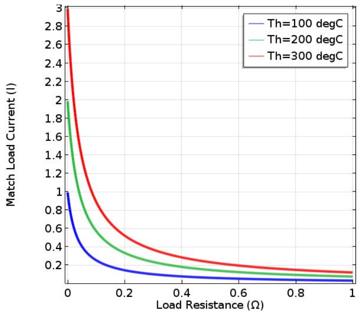


( Figure 1.8 : TEG Electric Potential )

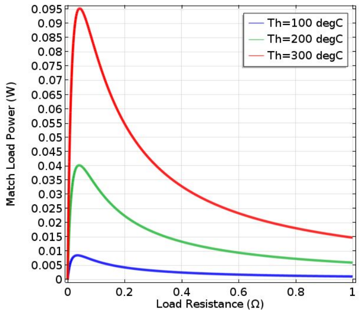
The voltage, current and power relationship produced in unit couple TEG module with the temperature gradients are plotted graphically in below figures. The optimal power produced 0.095W from unit couple TEG is possible when TEG internal resistance (R) equals to load resistance ($R_L$) at 0.042Ω and a maximum temperature of $300^C$. The optimal voltage (Vopt) of 0.06V and optimal current (Iopt) 1.5A is produced at 0.042Ω and $300^C$ respectively.



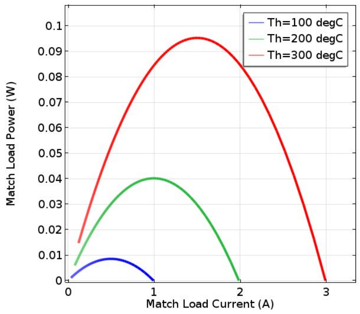
( Figure 1.9 : Resistance vs Voltage )



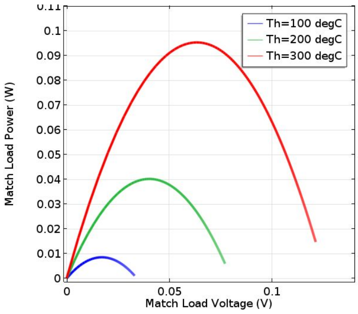
( Figure 2.1 : Resistance vs Current )



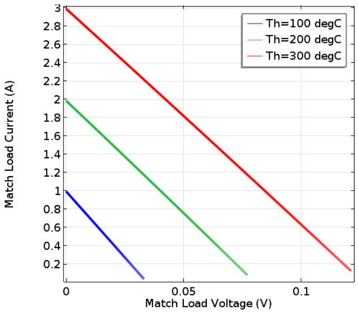
( Figure 2.2 : Resistance vs Power )



( Figure 2.3 : Current vs Power )



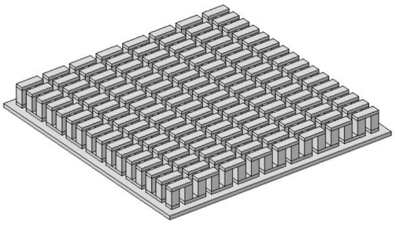
( Figure 2.4 : Voltage vs Power )



( Figure 2.5 : Voltage vs Current )

## TEG Module Multiphysics Simulation:-

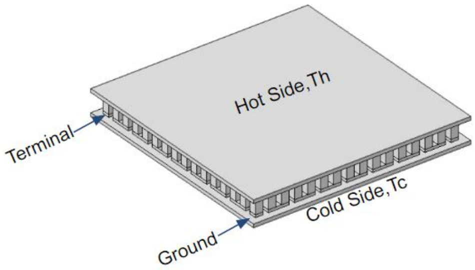
The multiphysics cae model for 128 thermocouple TEG consisting of 256 legs connected electrically in series and thermally in parallel is developed using finite element methods. The leg dimension and module dimension is taken as 1.4mm x 1.4mm x 2.5mm and 40mm x 40mm x 4.8mm respectively.



( Figure 2.6 : TEG Module )

## Boundary Definition-

The boundary definitions for the TEG module in COMSOL Multiphysics are mentioned in below figure. Top planar surface is defined as the TEG heat source or hot side temperature as $300^C$. Bottom planar surface are defined as cold surfaces, temperature as $30^C$. The TEG Modules P-Type and N-Type are arranged electrically in series. One end of the TEG is defined as Terminal and other as Ground. The convective and radiative heat transfer and the contact resistance of the module is neglected in the experiment. The heat is considered to flow from the hot side and rejected from the cold side with no other means than the ceramics, thermoelements and connecting conductors.



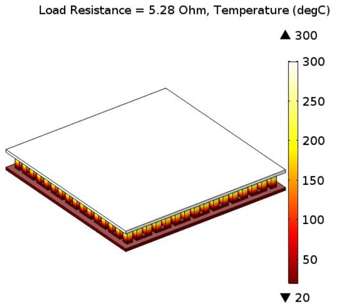
( Figure 2.7 : TEG Device Boundary Definition )

## COMSOL Solver:-

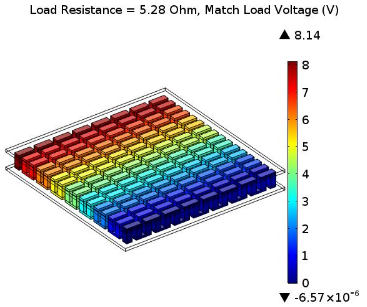
A fully coupled, direct, stationery study is implemented to the TEG model to predict the electrical power production from temperature gradient.

## Result Evaluation:-

The temperature distribution and electric potential contour plots are plotted graphically as shown in below figures.

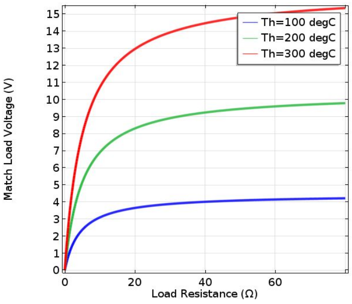


(Figure 2.8 : TEG Device temperature Distribution)

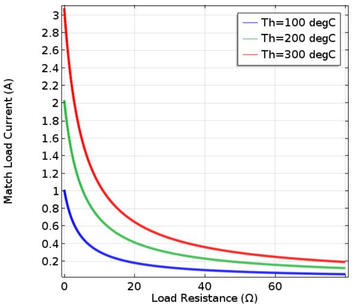


( Figure 2.9 : TEG Device Electric Potential )

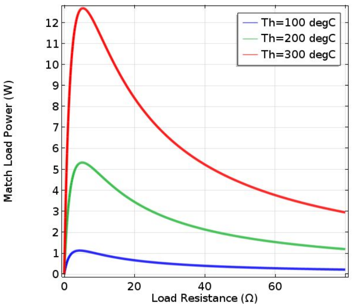
The voltage, current and power relationship produced in unit couple TEG module with constant temperature gradient are plotted graphically in below figures. The maximum power produced 12.54W TEG module is possible when TEG internal resistance (R) equals to load resistance ($R_L$) at 5.28Ω and a maximum temperature of $300^C$. The optimal voltage (Vopt) of 8.13V and optimal current (Iopt) 1.54A is produced at 5.28Ω and $300^C$ respectively.



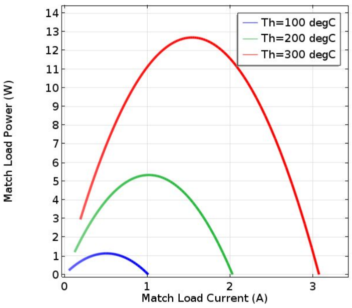
( Figure 3.1 : Resistance vs Voltage )



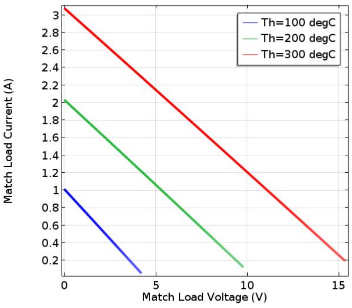
( Figure 3.2  : Resistance vs Current )



( Figure 3.3 : Resistance vs Power )



( Figure 3.4 : Current vs Power )



( Figure 3.5: Voltage vs Current )

## Conclusion:-

Thermoelectric Generators are environment friendly, maintenance free and cost effective in power production from waste heat. In this paper the working principle of thermoelectricity is explained both theoretically and numerically. A TEG module consisting arrays of thermoelectric elements is designed and simulated in COMSOL Multiphysics. The performance of TEG is investigated numerically. The multilevel optimization of TEG shows potential in maximum conversion of waste heat into useful electric power.

## References:-

[1]Introduction to Thermoelectricity, H.Julian Goldsmid, Springer Series in Material science.

[2]Thermoelectrics Design and Materials, HoSung Lee, Western Michigan University, USA, Wiley Publication.

[3]Analytical Modeling and Simulation of Thermoelectric Devices; Jordan Chase, Dr. Jean-Pierre Fleurial, Dr. Thierry Calliat, Samad Firdosy, Dr. Vilapanur Ravi, Bill Nesmith; JET PROPULSION LABORATORY PASADENA, CA.

[4]Analytical Modeling and Numerical Simulation of a Thermoelectric Generator Including Contact Resistances; Shripad Dhoopagunta; Western Michigan University.

[5]Modelling of thermoelectric devices for electric power generation, Doctoral Thesis, Bitschi, Andreas, Swiss Federal Institute of Technology, Zurich, 2009.

## Acknowledgement:-

This research was supported by Research & Innovation Department of ATOA Scientific Technologies, Bengaluru, India. The author would like to thank the technical team, who provided insight and expertise that greatly assisted the research.