

Multiphysics Modeling and Multilevel Optimization of Thermoelectric Generators for Waste Heat Recovery

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About ATOA

ATOA is a group of companies with a vision to proliferate engineering for all. ATOA stands for Atom to Application. ATOA currently offers, Multiphysics CAE services, Engineering Apps and 3D printing, through ATOA Scientific Technologies, ATOA Software Technologies and ATOA Smart Technologies, respectively. Our social mission is delivered through our ATOAST Jyothi Foundation.

Our Purpose

We want to be a Good, Great and Growth Company.

Good: Do Good for our Employees, Client and Humanity.

Great: Develop Great Technology.

Growth: Grow into a Billion Dollar Company by 2020.

Our Solution

Engineering Services, Specialty Multiphysics CAE for Innovation

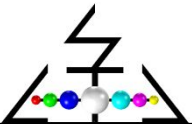
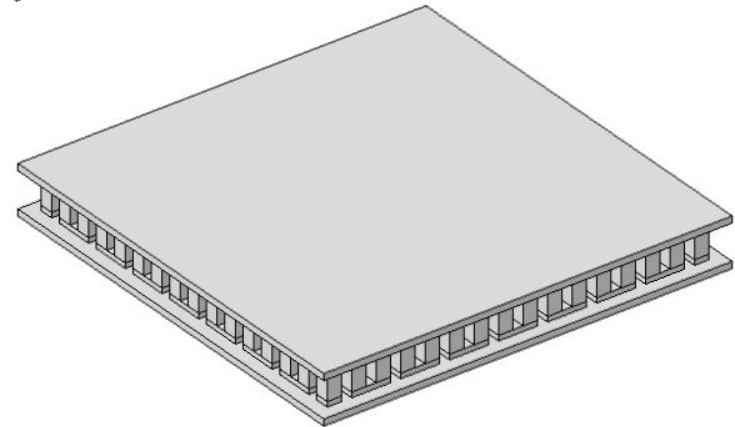
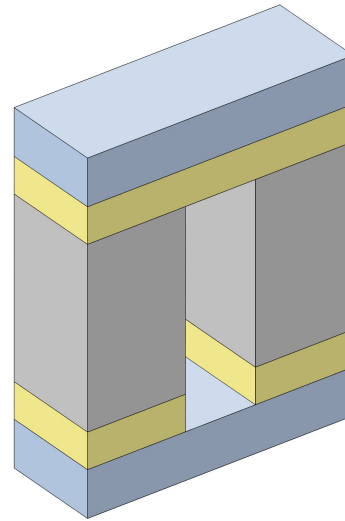
Engineering Apps for Design on the Go

3D Printing for Next-Gen Products



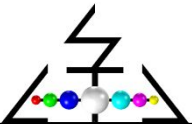
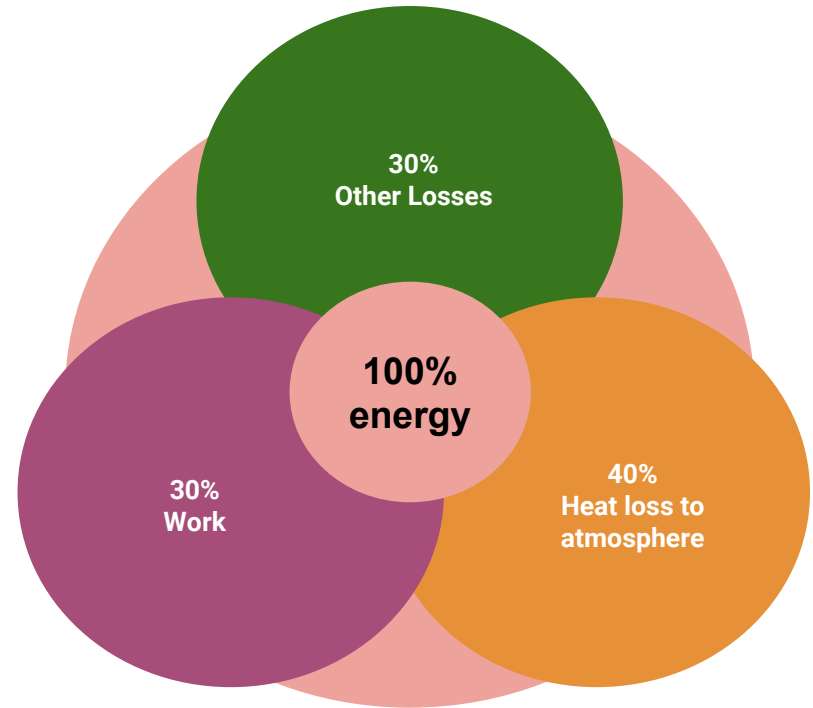
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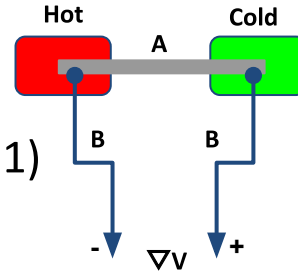
Introduction and Objective

- Waste heat is inevitable in any heat engine.
- Approximately 30% of heat energy is used for work while remaining 70% is lost to atmosphere.
- Waste heat energy reduces system efficiency and affect fuel economy.
- Thermoelectric Generation is a potential waste heat recovery technology.
- This paper explores the potential of Thermoelectric Generators for waste heat recovery.



Thermoelectric Generator (TEG)

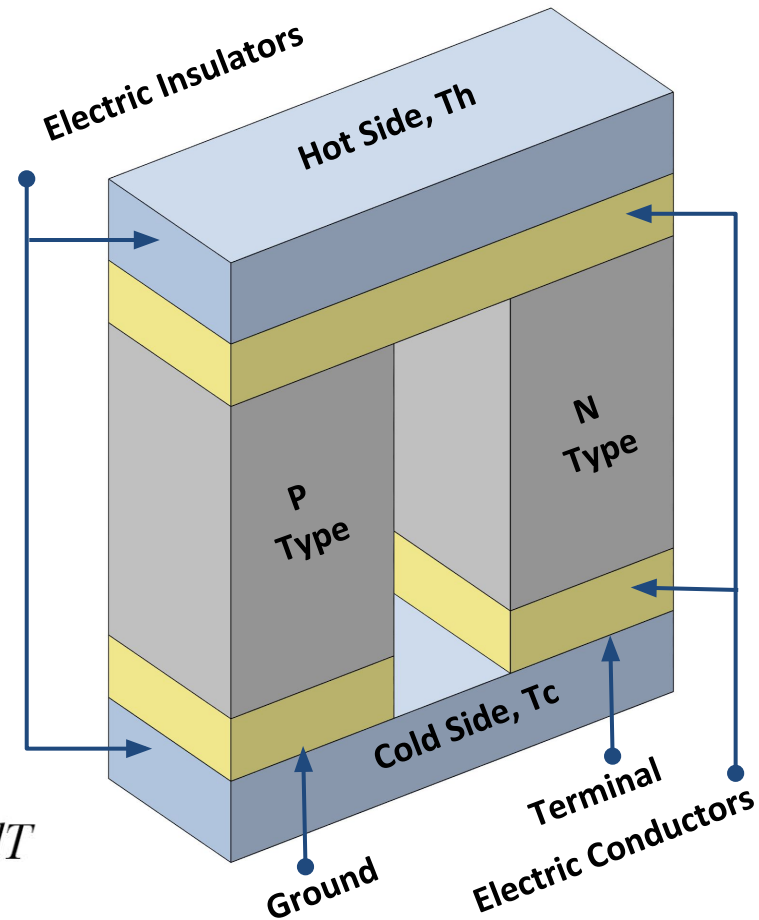
- Energy harvesting device.
- Converts temperature difference ($T_h - T_c$) into electrical energy (Voltage).
- Thermoelectricity.
 - Seebeck effect.
 - Alessandro Volta (1794)
 - Thomas Johann Seebeck (1821)
- Thermoelectric materials
 - Bismuth Telluride (Bi_2Te_3)
 - Lead telluride (PbTe)
 - Silicon Germanium (SiGe)
 - Skutterudite (CoAs_3)
- Seebeck Coefficient (α)
- Thermal Conductivity (k)
- Figure of Merit (ZT)



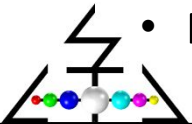
$$\alpha = \alpha_P - \alpha_N$$

$$V_{OC} = \int_{T_c}^{T_h} \alpha(T) dT$$

$$\nabla V \text{ or } V_{OC} = \alpha(T_h - T_c)$$



(Seebeck Effect, TEG)



Thermal System

- The thermal system of an Unit Couple TEG is represented.
- All domains are considered as thermal domains.
- As shown in the picture the thermal resistances are connected in series and parallel.
- The total thermal resistance of the unit couple is R.

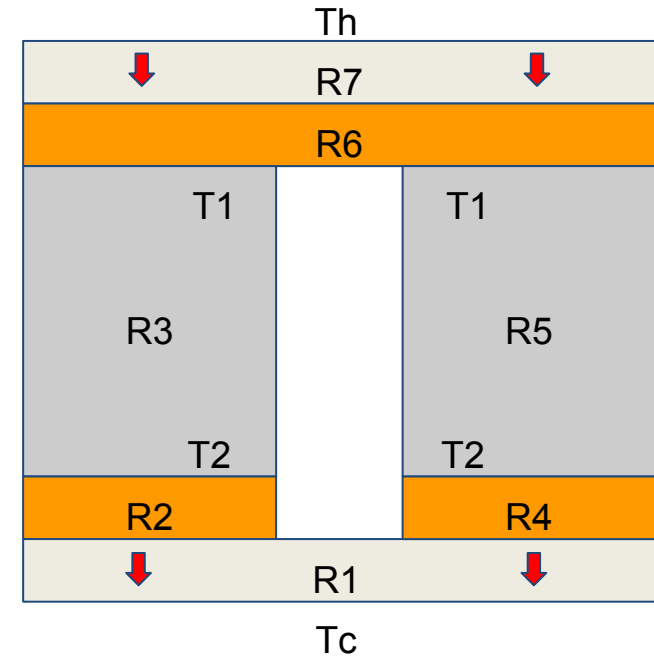
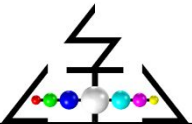
$$R = R1 + \frac{R2 R4}{R2} + R4 + \frac{R3 R5}{R3} + R5 + R6 + R7$$

$$Q = \frac{Th - Tc}{R}$$

$$T1 = Th - Q(R1 + R2)$$

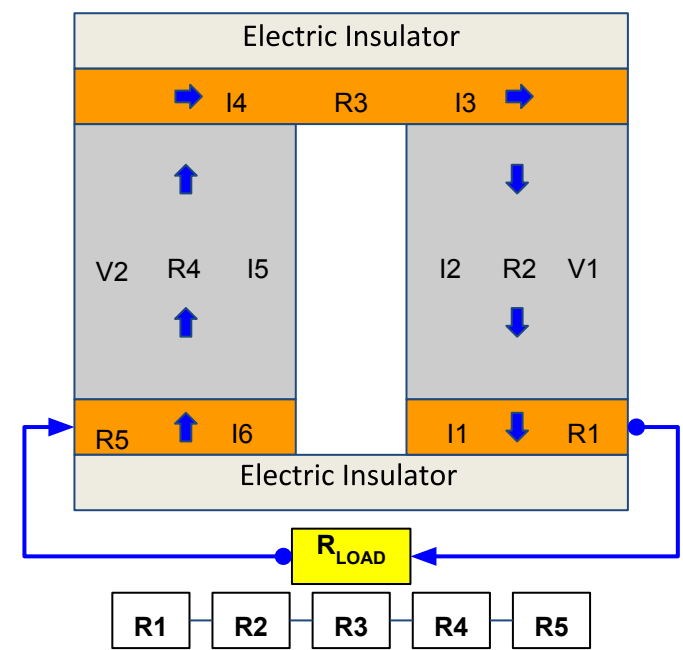
$$T2 = Th - Q\left(R1 + \frac{R2 R4}{R2} + R4 + \frac{R3 R5}{R3} + R5\right)$$

$$\nabla T = T1 - T2$$



Electrical System

- The electrical system of unit couple TEG is represented.
- The Copper and P-Type, N-Type legs are only consider as electrical domain.
- The ceramics on the top and bottom are considered as electrical insulators.
- As shown in the picture the electrical resistances are connected in series.
- The total electrical resistance of the unit couple will be sum of all resistances.
- Total produced voltage $V = V1+V2$.
- Current in the system remain same since the circuit is in series.

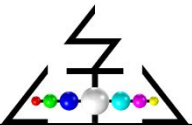


$$R = R1 + R2 + R3 + R4 + R5 = R_{LOAD}$$

$$V = V1 + V2 = \alpha(T_h - T_c)$$

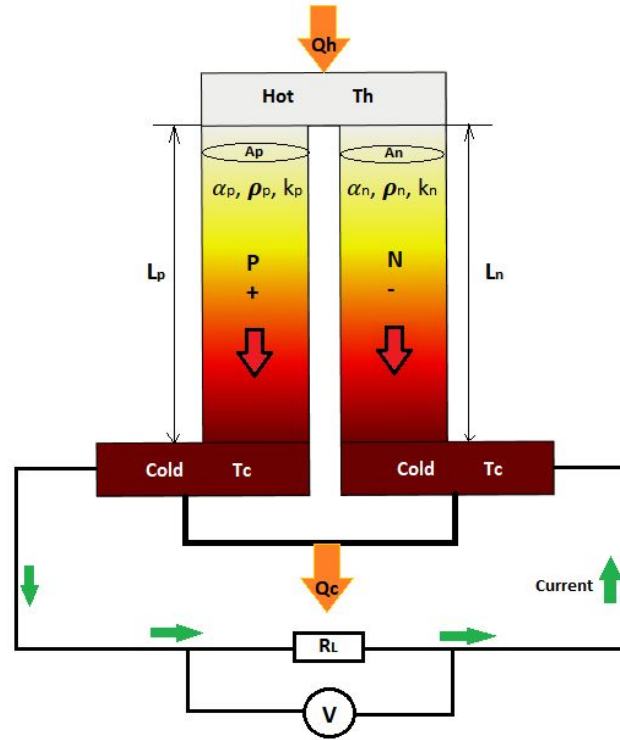
$$I = I1 = I2 = I3 = I4 = I5 = I6 = \frac{V}{R + R_{LOAD}}$$

$$Power (P) = VI = I^2 R_{LOAD}$$



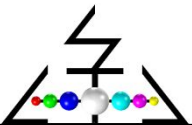
Analytical Derivation

- The analytical model for thermoelectric generator is presented.
- A schematic diagram of thermoelectric generator model is represented.
- Temperature difference is maintained at the connected junction of P-Type and N-Type thermoelectric legs.
- The produced voltage, current and power is derived analytically.



(TEG Schematic Diagram)

α = Total Seebeck Coefficient
 α_p = P-leg Seebeck Coefficient
 α_n = N-leg Seebeck Coefficient
 Q_p = P-leg Electrical Resistivity
 Q_n = N-leg Electrical Resistivity
 k_p = P-leg Thermal Conductivity
 k_n = N-Leg Thermal Conductivity
 R = Internal 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 at Hot Side
 Q_c = Heat Rejected at Cold Side
 R_L = Load Resistance



Analytical Derivation

Total Seebeck Coefficient

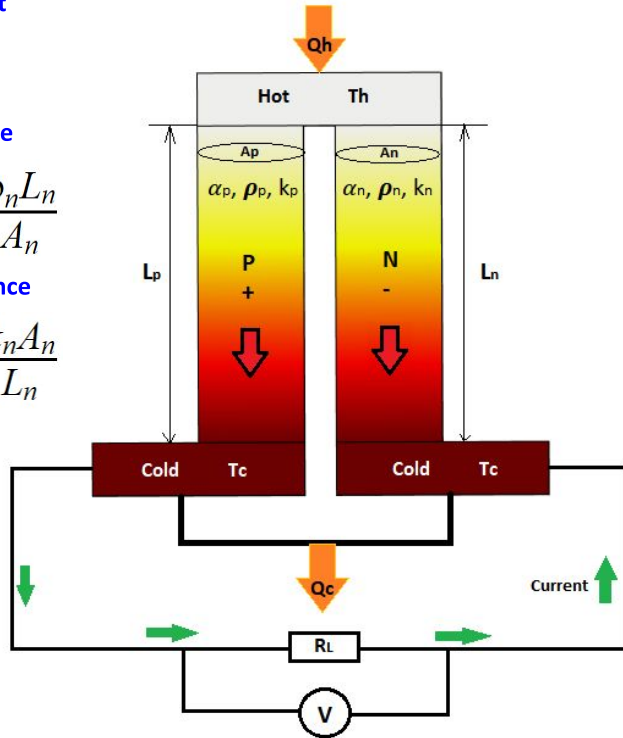
$$\alpha = \alpha_p - \alpha_n$$

Total Electrical Resistance

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

Total Thermal Conductance

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



Heat Absorbed at Hot Side

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

Heat Rejected from Cold Side

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

Power Generated

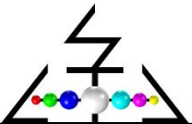
$$W = Q_h - Q_c, \quad W = \alpha I (T_h - T_c) - I^2 R$$

Voltage

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

Current

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



Analytical Derivation

Thermal Efficiency

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

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

Thermal Efficiency and Power can be written in terms of R_L/R

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

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

For maximum conversion efficiency

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

Average Temperature

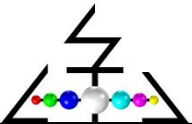
$$\bar{T} = \frac{T_c + T_h}{2} = \frac{1}{2} T_c \left[1 + \left(\frac{T_c}{T_h}\right)^{-1} \right]$$

Figure of Merit

$$ZT = \frac{\alpha^2 \sigma T}{k}$$

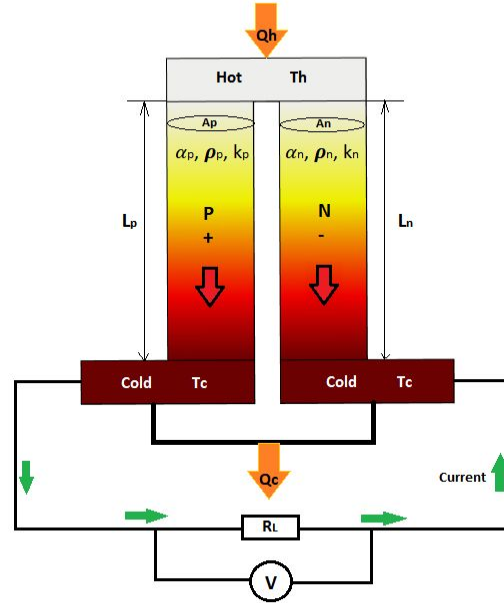
Maximum Conversion Efficiency

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



Analytical Derivation

- For maximum power efficiency the ratio of R_L / R is 1.
- As a result, the optimum current I_{mp} , maximum power W_{max} and maximum power efficiency η_{mp} can be derived as shown in the given equations.



For maximum power efficiency

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

Optimum Current

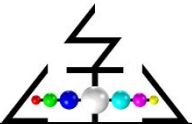
$$I_{mp} = \frac{\alpha \nabla T}{2R}$$

Maximum Power

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

Maximum Power Efficiency

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



Comsol Simulation

Governing Equations

Heat Transfer in Solid

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

Electric Current

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

Thermoelectric Effect

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

ρ = Density

u = Velocity field

C_p = Specific heat

Q = Heat source

Q_{ted} = Thermoelastic effects

Q_j = Current source

q = Heat flux in conduction

K = Thermal conductivity

T = Temperature

P = Peltier Coefficient

J = Induced Electric Current

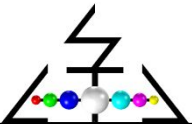
J_e = External Current Source

E = Electric field

V = Electric Potential

S = Seebeck Coefficient

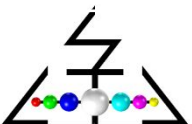
σ = Electrical Conductivity



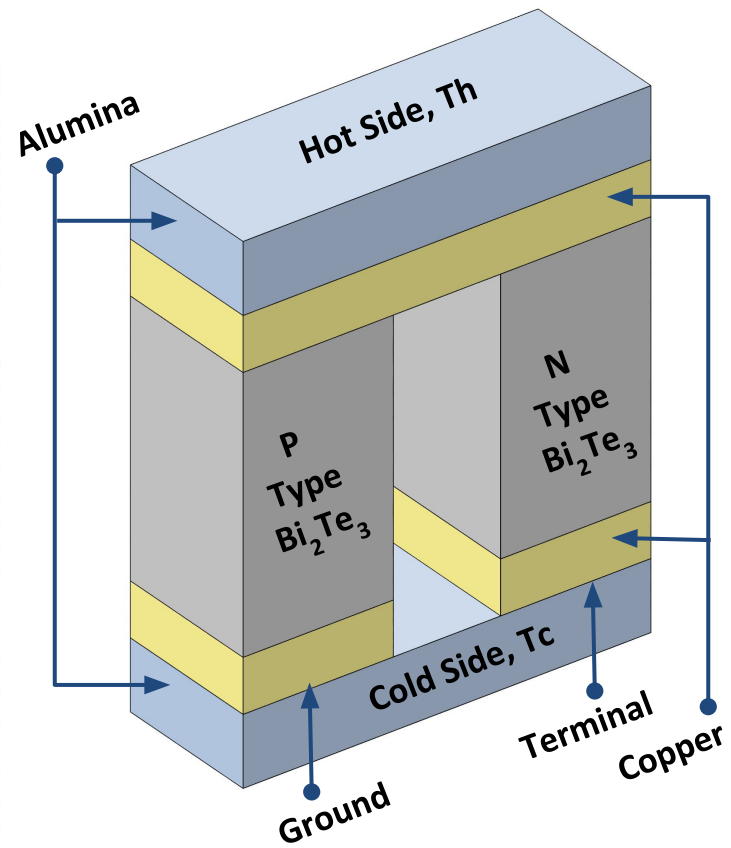
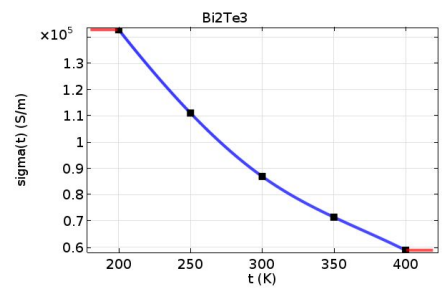
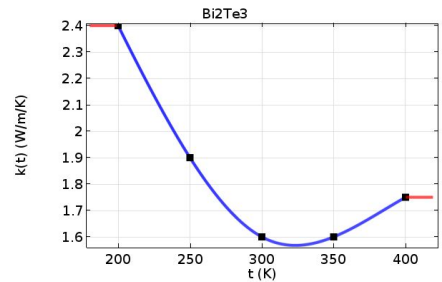
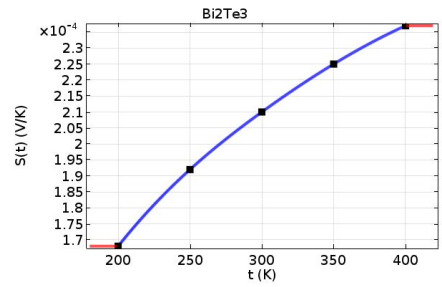
Material Properties

- The thermoelectric material properties such as Seebeck Coefficient, Electrical Conductivity, Thermal Conductivity are given in the below table.
- The temperature dependent material properties are represented graphically.
- The Seebeck Coefficient of Bi2Te3 is positive for P-Type while negative for N-Type.
- Thermal conductivity and electrical conductivity of Bi2Te3 is decreases with increase in temperature.

Materials	ρ (kg/m3)	k (W/mK)	σ (S/m)	Cp (J/kg.K)	S (V/K)
Bi2Te3(P)	7700	k(T)	sigma(T)	154	S(T)
Bi2Te3(N)	7700	k(T)	sigma(T)	154	-S(T)
Copper	8700	400	5.998E7	385	0.0
Alumina	3900	27	0.0	900	0.0



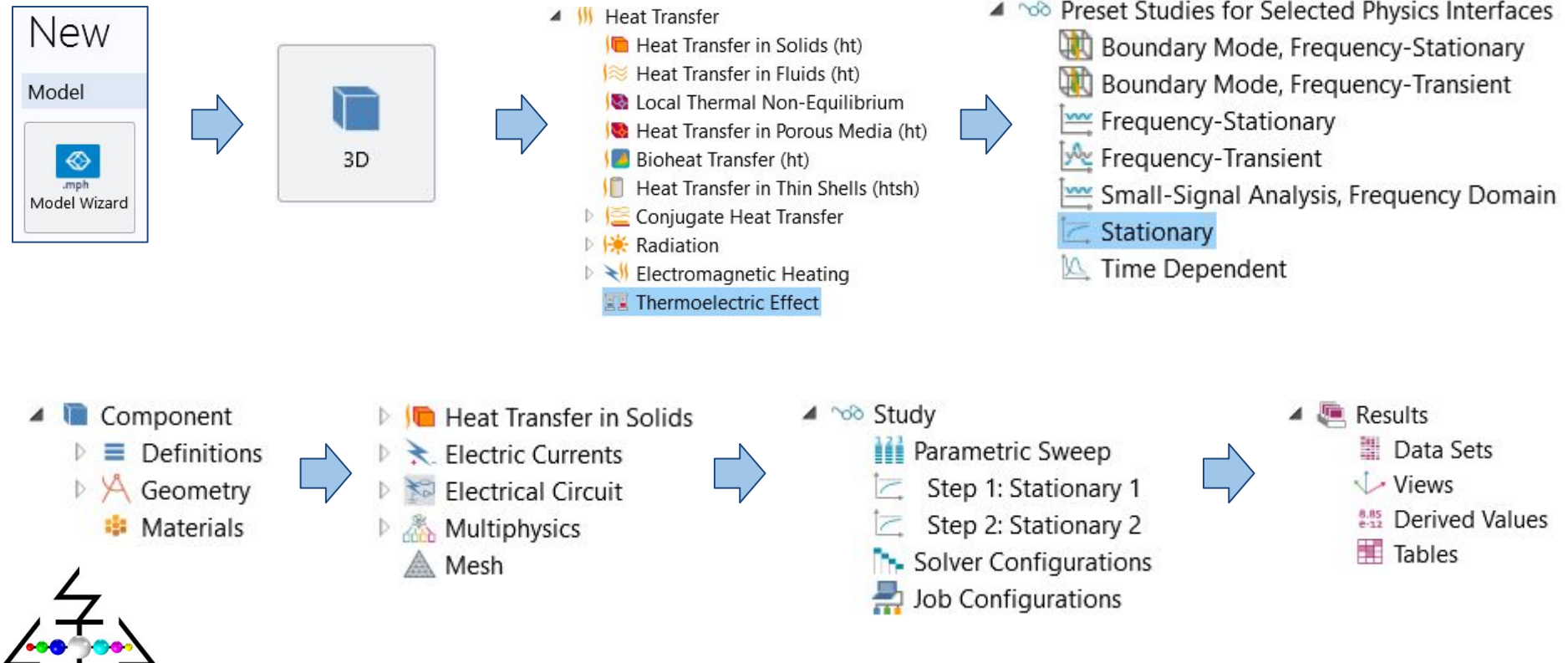
$$zT = \frac{\alpha^2 \sigma T}{k} = 1$$



(Material Definition)

Simulation in Comsol

Steps



Unit Couple TEG

Voltage (∇V), Current (I) and Power (W) from Temperature gradient (∇T)

Effects of Temperature gradient (∇T) on Voltage (∇V), Current (I) and Power (W) is calculated for the Unit Couple TEG, thermally in parallel and electrically in series.

P/N Leg Width = 1.4 mm

P/N Leg Depth = 1.4 mm

P/N Leg Height = 2.5 mm

P/N Leg cross-sectional area = 1.96 mm²

Unit Couple Total Height = 4.8 mm

Pitch = 1 mm

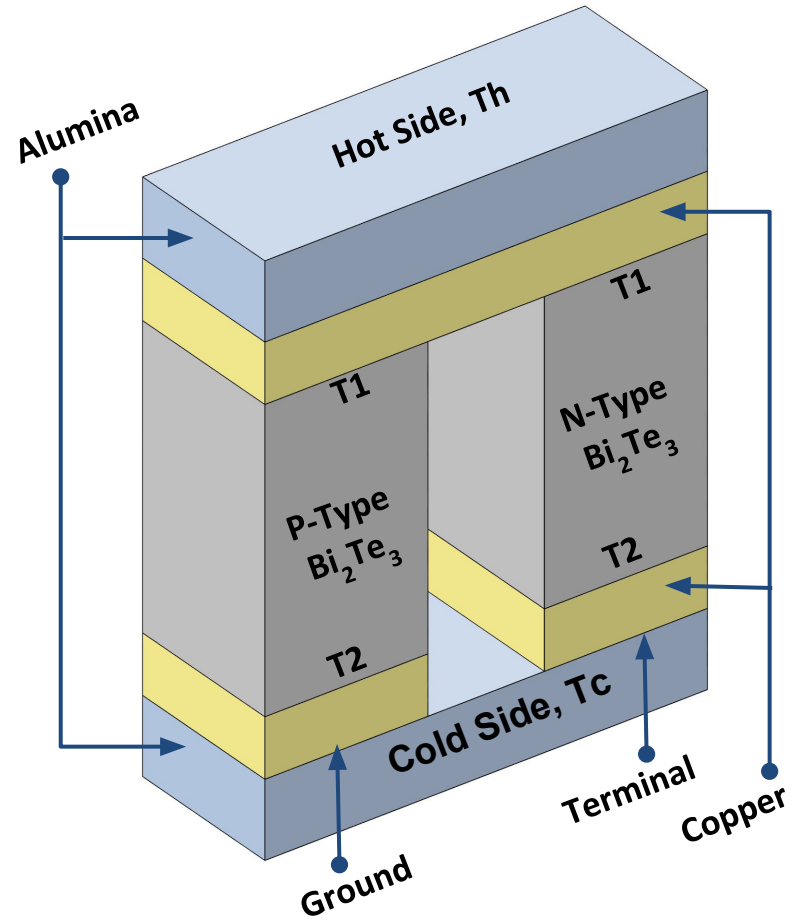
Copper Thickness = 0.5 mm

Alumina Thickness = 0.65 mm

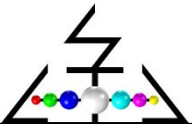
Load resistance = 0 to 1 Ω

Cold side temperature $T_c = 20^{\circ}\text{C}$

Hot side temperature $T_h = 100^{\circ}\text{C}$ to 300°C



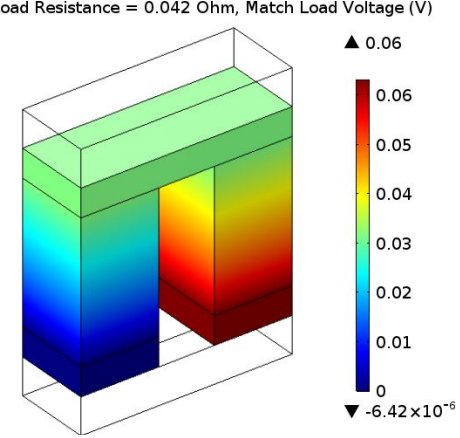
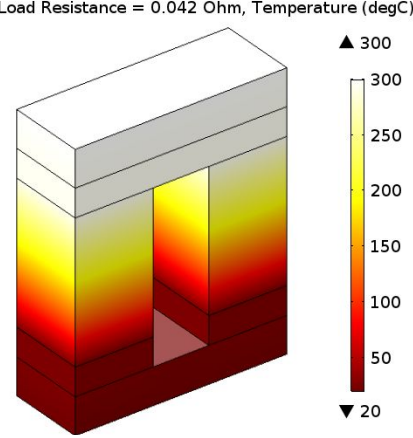
(Unit Couple TEG)



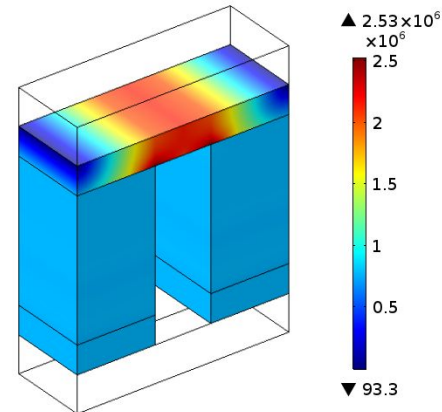
Unit Couple TEG Simulation Results:-

Close Circuit, Contour Plots:-

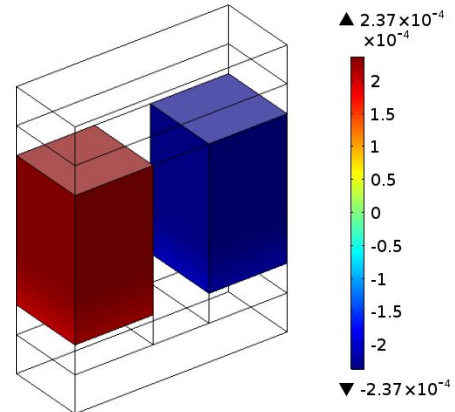
- A stationary study is assigned for the computational model.
- A fully coupled direct solver is implemented.
- The Temperature (C), Voltage (V), Current Density(A/m²) and Seebeck Coefficient (V/K) of Unit Couple TEG are plotted respectively at maximum temperature difference.
- The maximum temperature **300^C** and minimum of **20^C**.
- The match load voltage or optimal voltage obtained is **0.06V** when internal resistance and load resistance are equal at **0.042Ω**.



Load Resistance = 0.042 Ohm, Current Density Norm (A/m2)



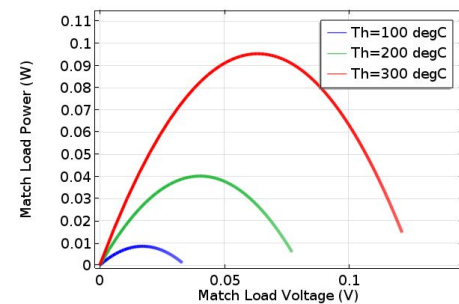
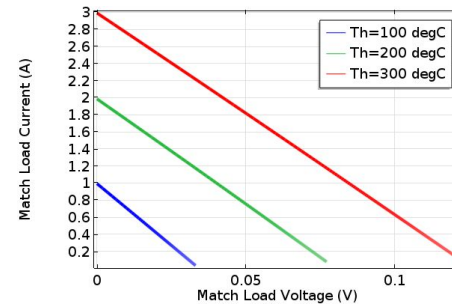
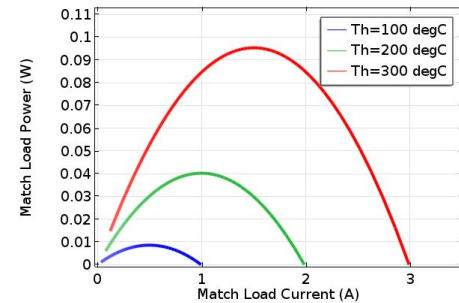
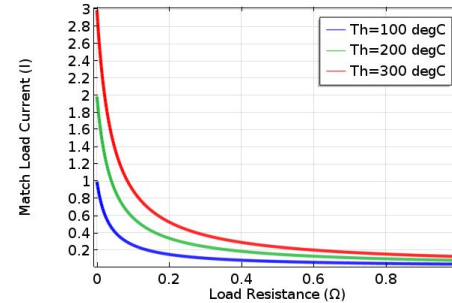
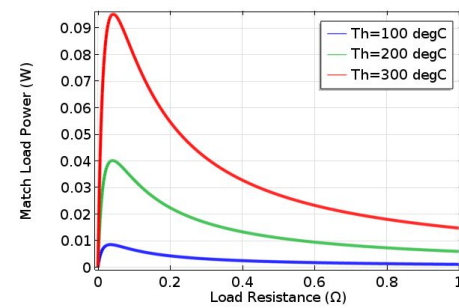
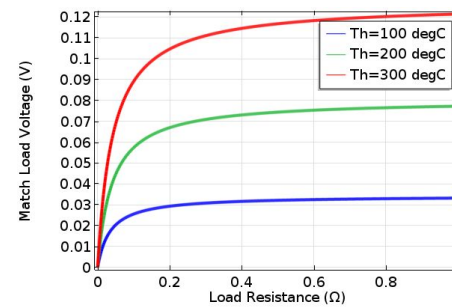
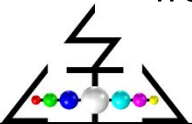
Load Resistance = 0.042 Ohm, Seebeck Coefficient (V/K)



Unit Couple TEG Simulation Results:-

Close Circuit, Graphical Plots:-

- The derived values from Unit Couple TEG simulation are plotted graphically.
- A Maximum Power of **0.095W** is produced from the Unit Couple TEG at **0.042Ω** and **280°C** temperature difference.
- The Optimum Voltage, Current and Power of **0.06V * 1.59A = 0.095W** is produced from Unit Couple TEG at **0.042Ω** and **280°C** temperature difference.
- A Maximum Voltage of **0.12V** is produced from Unit Couple TEG at **1Ω** and **280°C** temperature difference while the power is **0.0147W**.
- Maximum efficiency of **10%** is achieved from the Unit Couple TEG .



TEG Module

Voltage (∇V), Current (I) and Power (W) from Temperature gradient (∇T)

Effects of Temperature gradient (∇T) on Voltage (∇V), Current (I) and Power (W) is calculated for the TEG Module, thermally in parallel and electrically in series.

P/N Leg Width = 1.4 mm

P/N Leg Depth = 1.4 mm

P/N Leg Height = 2.5 mm

P/N Leg cross-sectional area = 1.96 mm²

Unit Couple Total Height = 4.8 mm

Number of Thermocouple = 128

Pitch = 1 mm

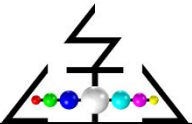
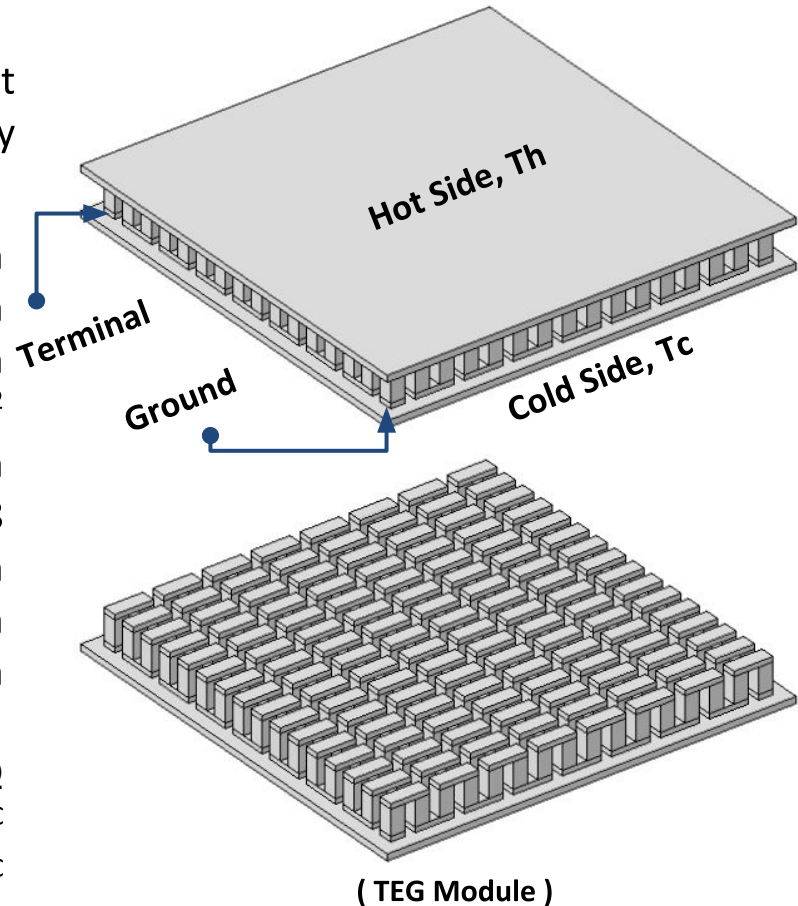
Copper Thickness = 0.5 mm

Alumina Thickness = 0.65 mm

Load resistance = 0 to 80Ω

Cold side temperature $T_c = 20^{\circ}\text{C}$

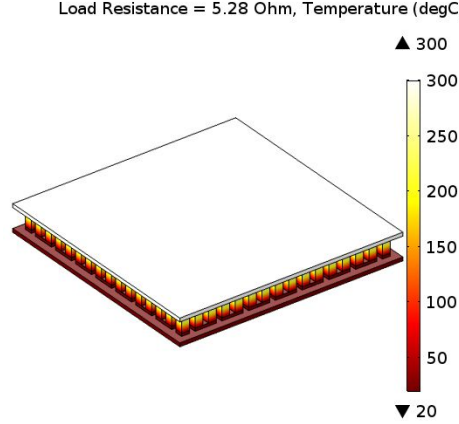
Hot side temperature $T_h = 100^{\circ}\text{C}$ to 300°C



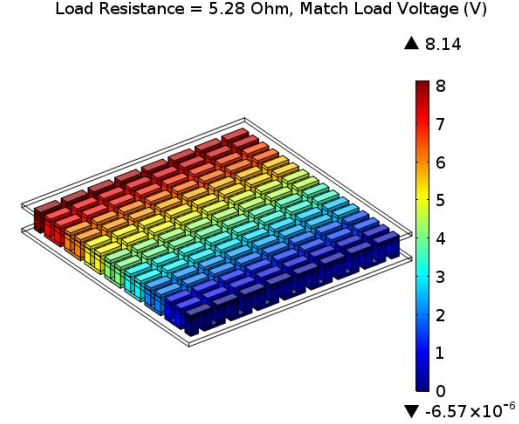
TEG Module Simulation Results:-

Close Circuit, Contour Plots:-

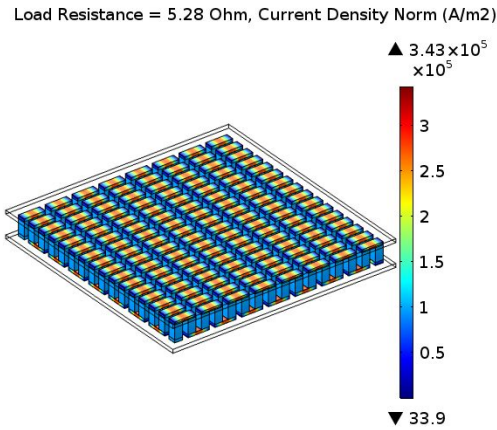
- A stationary study is assigned for the computational model.
- A fully coupled direct solver is implemented.
- The Temperature(C), Voltage (V), Current Density(A/m²) and Seebeck Coefficient (V/K) of Unit Couple TEG are plotted respectively at maximum temperature difference.
- The maximum temperature **300^c** and minimum of **20^c**.
- The match load voltage or optimal voltage obtained is **8.14V** when internal resistance and load resistance are equal at **5.28Ω**.



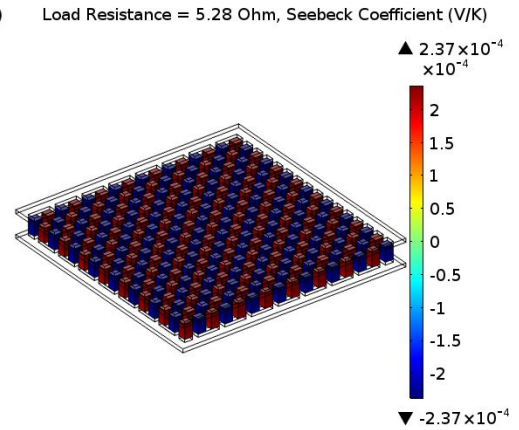
Temperature



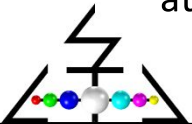
Match Load Voltage, Vopt



Match Load Current Density



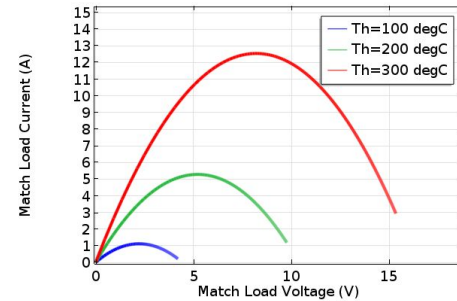
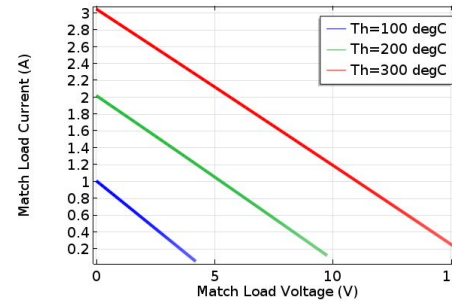
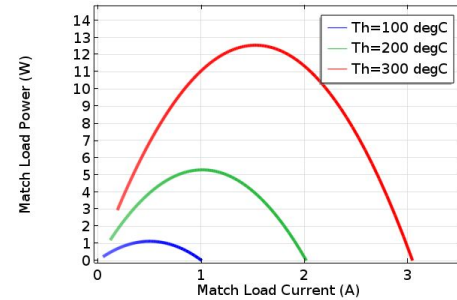
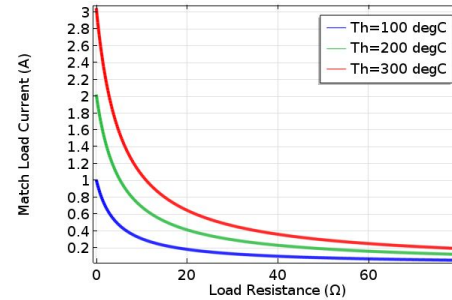
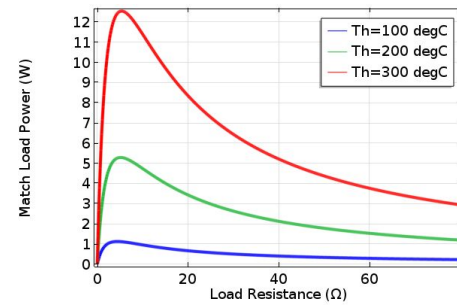
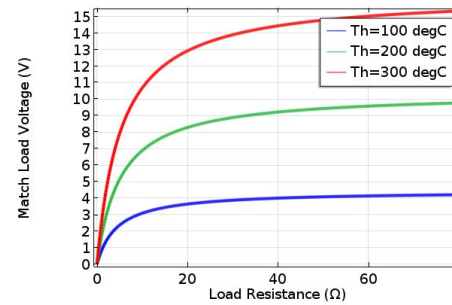
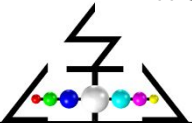
Seebeck Coefficient



TEG Module Simulation Results:-

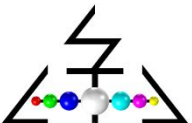
Close Circuit, Graphical Plots:-

- The derived values from TEG Module simulation are plotted graphically.
- A Maximum Power of **12.59W** is produced from the TEG Module at **5.28Ω** and **280°C** temperature difference.
- The Optimum Voltage, Current and Power of **8.14V * 1.5A = 12.59W** is produced from TEG Module at **5.28Ω** and **280°C** temperature difference.
- A Maximum Voltage of **15.33V** is produced from TEG Module at **80Ω** and **280°C** temperature difference while the Power is **2.94W**.
- Maximum efficiency of **10%** is achieved from the TEG Module.



Conclusion and Future Work

- In this paper the working principle and simulation of thermoelectric generator are explained both theoretically and numerically.
- An Unit Couple TEG and Optimized Multilevel TEG Module consisting arrays of thermocouples is designed and simulated in COMSOL
- The performance of Unit Couple TEG and TEG Module are investigated numerically.
- The optimized multilevel modeling of thermoelectric generators shows potential in maximum conversion of waste heat into useful electric power.



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