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

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About ATOA
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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 (Th-Tc) into electrical energy (Voltage).
- Thermoelectricity.
  - Seebeck effect.
  - Alessandro Volta (1794)
  - Thomas Johann Seebeck (1821)
- Thermoelectric materials
  - Bismuth Telluride (Bi$_2$Te$_3$)
  - Lead telluride (PbTe)
  - Silicon Germanium (SiGe)
  - Skutterudite (CoAs$_3$)
- Seebeck Coefficient ($\alpha$)
- Thermal Conductivity ($k$)
- Figure of Merit (ZT)

\[ \alpha = \alpha_P - \alpha_N \]

\[ V_{OC} = \int_{T_c}^{Th} \alpha(T) dT \]

\[ \nabla V \text{ or } V_{OC} = \alpha(Th - Tc) \]
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 \( R \).

\[
R = R_1 + \frac{R_2 R_4}{R_2} + R_4 + \frac{R_3 R_5}{R_3} + R_5 + R_6 + R_7
\]

\[
Q = \frac{Th - Tc}{R}
\]

\[
T_1 = Th - Q(R_1 + R_2)
\]

\[
T_2 = Th - Q(R_1 + \frac{R_2 R_4}{R_2} + R_4 + \frac{R_3 R_5}{R_3} + R_5
\]

\[
\nabla T = T_1 - T_2
\]
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 \( V = V_1 + V_2 \).
- Current in the system remain same since the circuit is in series.

\[
R = R_1 + R_2 + R_3 + R_4 + R_5 = R_{LOAD}
\]

\[
V = V_1 + V_2 = \alpha(Th - Tc)
\]

\[
I = I_1 = I_2 = I_3 = I_4 = I_5 = I_6 = \frac{V}{R + R_{LOAD}}
\]

\[
Power (P) = VI = I^2R_{LOAD}
\]
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.

\[ \alpha = \text{Total Seebeck Coefficient} \]
\[ \alpha_p = \text{P-leg Seebeck Coefficient} \]
\[ \alpha_n = \text{N-leg Seebeck Coefficient} \]
\[ \rho_p = \text{P-leg Electrical Resistivity} \]
\[ \rho_n = \text{N-leg Electrical Resistivity} \]
\[ k_p = \text{P-leg Thermal Conductivity} \]
\[ k_n = \text{N-Leg Thermal Conductivity} \]
\[ R = \text{Internal Electrical Resistance} \]
\[ K = \text{Total Thermal Conductance} \]
\[ L_p = \text{P-Leg Length} \]
\[ L_n = \text{N-Leg Length} \]
\[ A_p = \text{P-Leg Cross-Sectional Area} \]
\[ A_n = \text{N-Leg Cross-Sectional Area} \]
\[ Q_h = \text{Heat Supplied at Hot Side} \]
\[ Q_c = \text{Heat Rejected at Cold Side} \]
\[ R_L = \text{Load Resistance} \]
**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

\[ \eta_{th} = \frac{W}{Q_h} \]

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

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

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

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

For maximum conversion efficiency

\[ \frac{d\eta_{th}}{d\left( \frac{R_L}{R} \right)} = 0 \Rightarrow \frac{R_L}{R} = \sqrt{1 + zT} \]

Average Temperature

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

Figure of Merit

\[ zT = \frac{\alpha^2 \sigma T}{k} \]

Maximum Conversion Efficiency

\[ \eta_{mc} = \left( 1 - \frac{T_c}{T_h} \right) \left( \frac{1}{\sqrt{1 + zT - 1}} \right) \]
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 $\eta_{mp}$ 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
\[
\eta_{mp} = \frac{(1 - \frac{T_c}{T_h})}{2 - \frac{1}{2}(1 - \frac{T_c}{T_h}) + \frac{4T_c}{ZT_c}}
\]
Comsol Simulation
Governing Equations

Heat Transfer in Solid

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

Electric Current

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

Thermoelectric Effect

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

\( \rho \) = Density
\( u \) = Velocity field
\( C_p \) = Specific heat
\( Q \) = Heat source
\( Q_{\text{ted}} \) = 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
\( \sigma \) = 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.

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

$$Z = \frac{\alpha^2 \sigma T}{k} = 1$$
Simulation in Comsol

Steps

New
Model Wizard

3D

Heat Transfer
- Heat Transfer in Solids (ht)
- Heat Transfer in Fluids (ht)
- Local Thermal Non-Equilibrium
- Heat Transfer in Porous Media (ht)
- Bioheat Transfer (ht)
- Heat Transfer in Thin Shells (htsh)
- Conjugate Heat Transfer
- Radiation
- Electromagnetic Heating
- Thermoelectric Effect

Preset Studies for Selected Physics Interfaces
- Boundary Mode, Frequency-Stationary
- Boundary Mode, Frequency-Transient
- Frequency-Stationary
- Frequency-Transient
- Small-Signal Analysis, Frequency Domain
  - Stationary
  - Time Dependent

Component
- Definitions
- Geometry
- Materials

Heat Transfer in Solids
- Electric Currents
- Electrical Circuit
- Multiphysics
- Mesh

Study
- Parametric Sweep
  - Step 1: Stationary 1
  - Step 2: Stationary 2
- Solver Configurations
- Job Configurations

Results
- Data Sets
- Views
- Derived Values
- Tables
Unit Couple TEG

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

Effects of Temperature gradient (\(\nabla T\)) on Voltage (\(\nabla V\)), 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 mm\(^2\)
- 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\(\Omega\)
- Cold side temperature Tc = 20°C
- Hot side temperature Th = 100°C to 300°C
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.
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 ($\nabla V$), Current ($I$) and Power ($W$) from Temperature gradient ($\nabla T$)

Effects of Temperature gradient ($\nabla T$) on Voltage ($\nabla V$), 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 mm$^2$
- 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 $Tc = 20^\circ C$
Hot side temperature $Th = 100^\circ C$ to $300^\circ C$
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 $300^\circ C$ and minimum of $20^\circ C$.
- The match load voltage or optimal voltage obtained is $8.14V$ when internal resistance and load resistance are equal at $5.28\Omega$. 
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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