Two-Dimensional Modeling of Thermoelectric Cells

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Presentation outline

• Introduction
• Mathematical formulation
• Numerical scheme
• Model validation
• Sensitivity analysis
• Concluding remarks
The present paper is therefore aimed at advancing a two-dimensional model suitable to evaluating the sensitivity of the thermophysical properties and the cell geometry on its thermodynamic performance.
Formulation

Key Assumptions

- Steady-state two-dimensional model

- Thermophysical properties of the thermoelectrical material is function of the temperature only

- The internal contact resistances (both thermal and electric) are negligible

- n and p elements have the same Seebeck coefficient, but with different signs

- The heat transfer by advection and radiation are disregarded (\(Nu=1\))
A thermoelectric cell is comprised of several pairs of p and n semiconductors connected electrically in series and thermally in parallel, and separated from each other by a cavity filled with air. The physical model is restricted to a thermoelectric pair.

<table>
<thead>
<tr>
<th>Subdomain</th>
<th>Description</th>
<th>Material</th>
<th>Dimensions [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 &amp; 6</td>
<td>Bottom (1) and top (6) electric insulators</td>
<td>Al₂O₃</td>
<td>4.8 x 0.62</td>
</tr>
<tr>
<td>2 &amp; 9</td>
<td>Left (2) and right (9) electric conductors at the bottom</td>
<td>Cu</td>
<td>1.9 x 0.41</td>
</tr>
<tr>
<td>3 &amp; 7</td>
<td>n-type (3) and p-type (7) semiconductors</td>
<td>Bi₂Te₃</td>
<td>1.4 x 1.14</td>
</tr>
<tr>
<td>4</td>
<td>Electric conductor at the top</td>
<td>Cu</td>
<td>1.9 x 0.41</td>
</tr>
<tr>
<td>5 &amp; 10</td>
<td>Left (5) and right (10) side air cavities</td>
<td>Air</td>
<td>0.5 x 1.55</td>
</tr>
<tr>
<td>8</td>
<td>Central air cavity</td>
<td>Air</td>
<td>1.0 x 1.55</td>
</tr>
</tbody>
</table>
Formulation

Energy balances for thermoelectric materials

\[ \vec{\nabla} \cdot \vec{q} = \dot{q} \]

\[ \vec{q} = -k \vec{\nabla} T + \alpha \vec{E} \]

\[ \dot{q} = \vec{j} \cdot (-\vec{\nabla} V) = \rho \vec{j} \cdot \vec{j} + \alpha \vec{j} \cdot \vec{\nabla} T \]

heat generation

heat flux

2nd thermodynamics relation

\[ \tau dT = T d\alpha \]

\[ \vec{\nabla} \cdot (k \vec{\nabla} T) - \vec{j} \cdot \vec{\nabla} T + \rho \vec{j} \cdot \vec{j} = 0 \]

Potential distribution for thermoelectric materials

\[ -\vec{\nabla} V = \rho \vec{j} + \alpha \vec{\nabla} T \rightarrow \vec{j} = -\gamma \vec{\nabla} V - \gamma \alpha \vec{\nabla} T \]

\[ \vec{\nabla} \cdot \vec{j} = 0 \]

\[ \vec{\nabla} \cdot (\gamma \vec{\nabla} V) + \vec{\nabla} \cdot (\gamma \alpha \vec{\nabla} T) = 0 \]
Formulation

Boundary conditions

Prescribed Temperature

\[ V_{\text{out}} = V_{\text{in}} \left( 1 - \frac{1}{N} \right) \]

Prescribed voltage

\[ \frac{dV}{dy} = 0 \]

Non electron flux

\[ \frac{dT}{dy} = 0 \]

Symmetry

\[ \frac{dT}{dx} = 0 \]
Numerics

Features

- solved iteratively due to non-linearities $\Rightarrow T$ and $V$
- finite-volume method
- The properties $(T, V)$ are evaluated at the centroids
- the fluxes $(q, j)$ are evaluated at the control surfaces
- non-uniform Cartesian mesh
- set of linear equations have been solved iteratively through the TDMA algorithm

Grid

typical control volume

non-uniform grid with 3120 control volumes
(producing mesh independent solution)
Validation

Experimental data

The code predictions were validated against experimental data obtained from the manufacturer of a particular thermoelectric module.

Material properties

\[ \rho = 2.3935 \cdot 10^{-11} T^2 + 2.9771 \cdot 10^{-8} T - 8.959 \cdot 10^7 \quad [\text{V m A}^{-1}] \]
\[ k = 3.682 \cdot 10^{-5} T^2 - 2.372 \cdot 10^{-2} T + 5.388 \quad [\text{W m}^{-1} \text{K}^{-1}] \]
\[ \alpha = -8.5952 \cdot 10^{-10} T^2 + 8.0546 \cdot 10^{-7} T + 4.329 \cdot 10^{-5} \quad [\text{V K}^{-1}] \]

<table>
<thead>
<tr>
<th>Material</th>
<th>( k ) [W m(^{-1}) K(^{-1})]</th>
<th>( \gamma ) [A m(^{-1}) V(^{-1})]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu</td>
<td>400</td>
<td>5.96 \times 10^7</td>
</tr>
<tr>
<td>Al(_2)O(_3)</td>
<td>30</td>
<td>-</td>
</tr>
<tr>
<td>Air</td>
<td>0.026</td>
<td>-</td>
</tr>
</tbody>
</table>

thermoelectric material
Fitted from data provided by Rowe (1995)

All simulations were carried out for \( T_h = 323 \text{ K} \) and different \( \Delta T \) and \( \Delta V \).
Validation

Electrical current

The maximum difference achieved (for ΔT=0 K and ΔV=16 V) was below the 10% threshold.

In all cases, one can see the model is able to follow the experimental trends closely.
Validation

Cooling capacity

\[ \dot{Q}_c = N L_z \sum_{i=1}^{n} \left( \frac{T_m - T_c}{k} \frac{\Delta x}{\delta y_m} \right)_i \]

The higher difference is observed for low voltages and \( \Delta T=0 \) K

Again, the experimental trends are well reproduced by the model...
Validation

Coefficient of Performance

...a similar behavior is observed for the COP!

\[
\text{COP} = \frac{\dot{Q}_c}{\dot{Q}_h - \dot{Q}_c}
\]
Joule + Fourier
$\Delta V=16V$
$\Delta T=0 K$

All effects
$\Delta V=16V$
$\Delta T=0 K$

The thermoelectric effect induces the inversion of the heat flux in the cold end.
As the $\Delta T$ becomes higher the cooling capacity is reduced and the maximum temperature inside the thermoelectric material approaches the hot end.
A 2-level (±5%), 3-factor factorial design was then planned totalizing $2^3=8$ runs for $\Delta T=0K$ and $\Delta V=16V$

- The cooling capacity is mainly affected by the electric conductivity and the Seebeck coefficient, and marginally affected by the thermal conductivity.
- The Seebeck coefficient plays a dominant role on the COP, followed by the thermal and electric conductivities, which played a marginal role.
- These trends are confirmed by the definition of the figure-of-merit of the thermoelectric material, $Z = \frac{\alpha^2 \gamma}{\kappa}$, which is straightforwardly related to the COP.
Sensitivity analysis

Sensitivity to Aspect Ratio

Increasing height \( (L_y) \) - constrained base area \( (L_x) \)

Increasing height \( (L_y) \) - constrained volume
Sensitivity analysis

Sensitivity to Aspect Ratio

COP is weakly affected by $L_y$ as the cooling capacity depletes inasmuch the electric current decreases, which diminishes the power consumption at the same rate.

As the COP is the ratio between the cooling capacity and the power consumption, one can expect the COP is not significantly changed from one case to the other.

Solid bullets $\Rightarrow$ constrained base area study
Open bullets $\Rightarrow$ constrained volume study
Concluding remarks

- The tailor-made model was coded in-house and its predictions for electric current, cooling capacity and COP were compared against experimental data obtained from the manufacturer of a particular thermoelectric cell. It was observed the numerical predictions and experimental data agreed to within 10% thresholds.

- The model was able to follow the experimental trends very closely.

- The influence of the thermophysical properties on the cooling capacity and COP study pointed out that the Seebeck coefficient and the thermal conductivity play major roles on the cooling capacity, whereas the COP is more sensible to the Seebeck coefficient.

- The study of the cell aspect ratio variation for constrained base area and constrained volume pointed out that both the cooling capacity and the power consumption vary at the same rates, in such a way the COP has showed a similar behavior for both studied cases.