# Multiphysics Analysis of Thermoelectric Phenomena

S.P. Yushanov, L.T. Gritter, J.S. Crompton*and K.C Koppenhoefer
AltaSim Technologies, Columbus, OH

*Corresponding author: 130 East Wilson Bridge Road, Suite 140, Columbus, OH 43085, jeff@altasimtechnologies.com

**Abstract:** Thermoelectric phenomena provide the direct conversion of heat into electricity or electricity into heat, the phenomena is described by three related mechanisms: the Seebeck, Peltier and Thomson effects. The Seebeck effect describes the conversion of temperature differences directly into electricity; at the atomic scale, an applied temperature gradient causes charged carriers in the material to diffuse from the hot side to the cold side generating a current flow. The Peltier effect describes the production of heat at an electrified junction of two different materials, the forced flow of charged carriers creates a temperature difference, and the Thomson effect describes the heating or cooling of a current carrying conductor in the presence of a temperature gradient. To analyze these phenomena accurately the thermoelectric field equations have to be solved, here the Seebeck-Peltier effect is implemented using the weak form.

**Keywords:** Seebeck, Peltier, weak-form.

## 1. Introduction

Thermoelectric devices have found many applications that include temperature measurement, solid state heating or cooling and direct energy conversion from waste heat. The Seebeck coefficient, *S*, measures the magnitude of an induced thermoelectric voltage in response to a temperature difference across that material, and the entropy per charge carrier in the material. An applied temperature difference causes charged carriers in the material to diffuse from the hot side to the cold side. Mobile charged carriers migrating to the cold side leave behind their oppositely charged nuclei at the hot side thus giving rise to a thermoelectric voltage. Since a separation of charges creates an electric potential, the buildup of charged carriers on the cold side eventually ceases at some maximum value. The material's temperature and crystal structure influence *S*; typically metals have small Seebeck coefficients whereas semiconductors can be doped to tailor the behavior and increase the Seebeck coefficient.

The Peltier effect describes the presence of heat at an electrified junction of two different metals. The Peltier coefficients, P, represent how much heat current is carried per unit charge through a given material. Since charge current must be continuous across a junction, the associated heat flow will develop a discontinuity if the Peltier coefficients of the two materials are different. Depending on the magnitude of the current, heat must accumulate or dissipate at the junction due to a non-zero divergence there caused by the carriers attempting to return to the equilibrium that existed before the current was applied by transferring energy from one connector to another. Individual couples can be connected in series to enhance the effect.

For the Thomson effect an electric current flows along a single conductor while a temperature gradient exists in the conductor, an energy interaction takes place in which power is either absorbed or rejected, depending on the relative direction of the current and gradient. The Seebeck effect is therefore the result of both the Peltier and Thomson effects.

## 2. Use of COMSOL Multiphysics

The governing equations determining the analysis of the Seeback and Peltier effects are:

Electric current balance:

$$-\nabla \cdot \left(\sigma \nabla V\right) = 0 \qquad (1)$$

Heat energy balance:

$$\begin{cases} \rho C_p \dfrac{\partial T}{\partial t} + \nabla \cdot \mathbf{q} = Q \\ \mathbf{q} = -k\nabla T + \underline{\underline{P\mathbf{J}}} \end{cases} \quad (2)$$

where

$\sigma$ : electric conductivity $[S/m]$

$V$ : electric potential $[V]$

$\rho$ : density $[kg/m^2]$

$C_p$ : heat capacity $[J/(kg\cdot K)]$

$T$ : temperature $[K]$

$\mathbf{q}$ : heat flux $[W/m^2]$

$k$ : thermal conductivity $[W/(m\cdot K)]$

$P$ : Peltier coefficient $[V]$

$\mathbf{J}$ : current density $[A/m^2]$

$Q = \mathbf{J}\cdot(-\nabla V)$ : Joule heating $[W/m^3]$

Thomson's second relation between Seebeck $(S)$ and Peltier $(P)$ coefficients provides:

$$P = -ST \quad (3)$$

To transfer energy balance to a weak form, multiply each side of energy balance by a test function, $T_{test}$ and integrate over the computational domain $\Omega$:

$$\int_\Omega \rho C_p \frac{\partial T}{\partial t} T_{test} d\Omega + \int_\Omega (\nabla) T_{test} d\Omega = \int_\Omega Q T_{test} d\Omega \quad (4)$$

Using the vector identity:

$$\nabla\cdot(T_{test}\mathbf{q}) = \mathbf{q}\cdot\nabla T_{test} + T_{test}\nabla\cdot\mathbf{q} \quad (5)$$

Then equation (4) becomes,

$$\int_\Omega \rho C_p \frac{\partial T}{\partial t} T_{test} d\Omega + \int_\Omega [\nabla\cdot(T_{test}\mathbf{q}) - \mathbf{q}\cdot\nabla T_{test}] d\Omega = \int_\Omega Q T_{test} d\Omega \quad (6)$$

By using the Gauss theorem:

$$\int_\Omega \nabla(T_{test}\cdot\mathbf{q}) = \int_{\partial\Omega} T_{test}\mathbf{q}\cdot\mathbf{n}\partial\Omega \quad (7)$$

where $\mathbf{n}$ is unit normal to the boundary $\partial\Omega$ of domain $\Omega$, then equation (7) becomes:

$$\int_\Omega \rho C_p \frac{\partial T}{\partial t} T_{test} d\Omega + \int_{\partial\Omega} T_{test}\mathbf{q}\cdot\mathbf{n}\partial\Omega - \int_\Omega \mathbf{q}\cdot\nabla T_{test} d\Omega = \int_\Omega Q T_{test} d\Omega \quad (8)$$

The energy flux is given by:

$$\mathbf{q} = -k\nabla T + P\mathbf{J} \quad (9)$$

Hence equation (8) becomes:

$$0 = \int_\Omega \left[ -\rho C_p \frac{\partial T}{\partial t} T_{test} + (-k\nabla T)\cdot\nabla T_{test} + (P\mathbf{J})\cdot\nabla T_{test} + Q T_{test} \right] d\Omega - \int_{\partial\Omega} (\mathbf{q}\cdot\mathbf{n}) T_{test}\partial\Omega \quad (10)$$

The Peltier weak contribution is then given by:

$$\begin{aligned}(P\mathbf{J})\nabla T_{test} &= PJ_x \frac{\partial T_{test}}{\partial x} + PJ_y \frac{\partial T_{test}}{\partial y} + PJ_z \frac{\partial T_{test}}{\partial z} = \\ &= P*ec.Jx*test(Tx) + P*ec.Jy*test(Ty) \\ &\quad + P*ec.Jz*test(Tz) \end{aligned} \quad (11)$$

where COMSOL notations for test function $T_{test} = test(T)$ and partial derivatives $\frac{\partial T}{\partial x} = Tx$, $\frac{\partial T}{\partial y} = Ty$, $\frac{\partial T}{\partial z} = Tz$ are used.

This can then be implemented in COMSOL V 4.2 in the heat transfer module.

## 3. Results

Implementation of the Seebeck –Peltier effect was examined for a number of idealized cases and for more realistic applications of Bismuth Telluride p-n junctions using standard material properties for typical thermoelectric materials found in the open literature. A summary of the relevant properties is provided in Table 1.

| | Bismuth Telluride | Copper electrode |
|---|---|---|
| **Seebeck coefficient, V/K** | p: $200 \times 10^{-6}$<br>n: $-200 \times 10^{-6}$ | $3.8 \times 10^{-6}$ |
| **Electrical conductivity, S/m** | $1.1 \times 10^{-5}$ | $6 \times 10^{7}$ |
| **Thermal conductivity, W/m.K** | 1.7 | 400 |
| **Heat capacity, J/kg.K** | 554 | 385 |
| **Density, kg/m3** | 7700 | 8800 |

Table 1: Summary of typical material properties for thermoelectric applications

An example of the analysis of Bismuth Telluride p-n junctions subject to an applied voltage is shown below, with the generation of focused heating and cooling due to the Peltier effect.

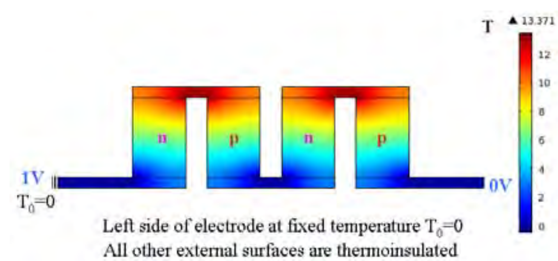


Figure 1: Temperature distribution resulting from imposition of voltage to Bismuth Telluride pellets: Peltier effect

Similarly, imposing a thermal gradient on an array of Bismuth Telluride pellets results in the generation of a potential across the surface of the module as shown in Figure 2 due to the Seebeck effect.

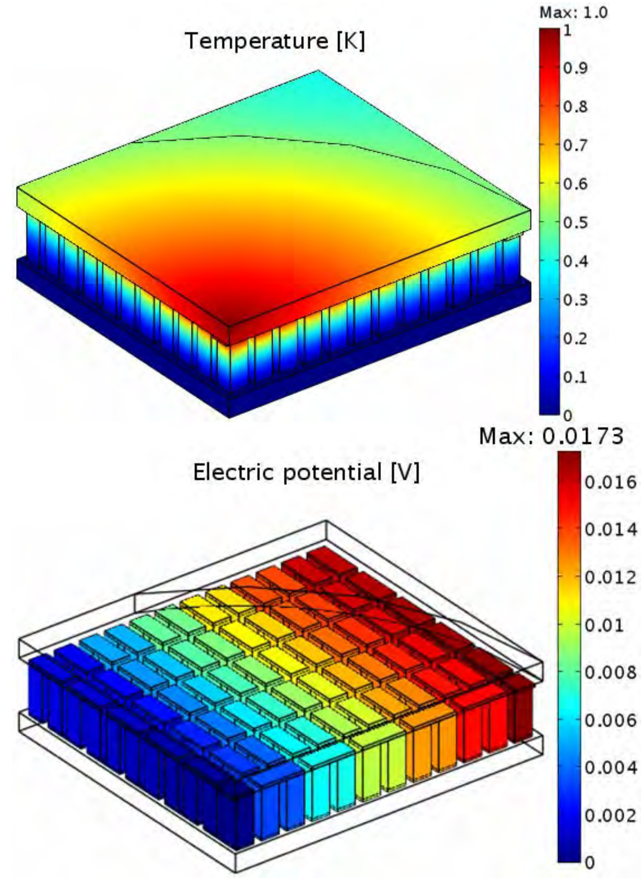


Figure 2: Electric potential for a thermoelectric module made up of an array of Bismuth Telluride pellets due to imposition of a non uniform temperature distribution: Seebeck effect.

## 4. Summary

This paper has demonstrated the implementation of the thermoelectric field equations for the Peltier-Seebeck effects in COMSOL Multiphysics V4.2. Examples of the application of the implantation have been provided for both the conversion of temperature differences directly into electricity and the generation of heat due to the imposition of an electric potential. Additional effects associated with temperature dependent material properties and transient effects can be readily added within the existing analytical framework of COMSOL Multiphysics