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Investigation on Thermoelectric Model of Antimony Telluride and Bismuth Telluride Using MATLAB

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ABSTRACT

Thermoelectric energy conversion offers a solid state method for directly converting heat into electrical energy by using the Seebeck effect, and it is being useful for waste heat recovery and low power generation applications. This work investigates the thermoelectric modeling of antimony telluride (Sb_2Te_3) and bismuth telluride (Bi_2Te_3) using a MATLAB based computational framework. Material transport properties are parameterized, and simulations are performed under representative engine exhaust conditions with hot side temperature of 250°C and cold side temperature of 40°C . Engine parameters such as power, volumetric efficiency, density, and specific heat are included to estimate available thermal input. Simulation results demonstrate stable and physically consistent voltage, current, power characteristics for both materials across the selected temperature range. Bi_2Te_3 shows strong n-type electrical response with favourable conductivity behaviour, while Sb_2Te_3 demonstrates reliable p-type Seebeck performance. The MATLAB model successfully predicts load-matching conditions, output trends, and efficiency behaviour, confirming its suitability for a design and optimization tool and for low power thermoelectric generator systems prior to experimental implementation.

Keywords: Thermoelectric model, p-type of Antimony Telluride (Sb_2Te_3), n-type of Bismuth Telluride (Bi_2Te_3).

1. INTRODUCTION

Thermoelectric energy conversion has attracted significant attention due to its capability to directly convert heat into electrical energy and vice versa through solid state mechanisms [1]. This conversion is primarily governed by Seebeck and Peltier effects, where a temperature gradient across a material generates an electrical potential, and an applied current produces a temperature difference, respectively. Thermoelectric modules are widely used in cooling, power generation from waste heat, and precision temperature control because they are compact, noiseless, and reliable, with no moving mechanical parts [2]. Despite of their relatively low conversion efficiency, advances in material science and modelling techniques have improved their applicability in modern energy systems [3]. Mathematical modelling and simulation of thermoelectric devices play a crucial role in performance analysis, design optimization, and control strategy development [4]. Block based and equation based models implemented in MATLAB/Simulink enable researchers to represent thermoelectric behaviour by using coupled electrical and thermal equations, including Seebeck voltage generation, Joule heating, and thermal conduction [4, 5, 27]. Such models allow parameter extraction, dynamic analysis, and verification of thermoelectric generator and thermoelectric cooler performance under different operating conditions, which reduces experimental cost and development time.

Among available thermoelectric materials, bismuth telluride (Bi_2Te_3) and antimony telluride (Sb_2Te_3) are considered as benchmark compounds for near room temperature applications due to their high Seebeck coefficient, favourable electrical conductivity, and relatively low thermal conductivity [6-8]. These materials are commonly used as n-type and p-type elements in practical thermoelectric modules. The performance of such materials is typically evaluated by using figure of merit parameters and temperature dependent transport properties, which can be incorporated into simulation models for accurate prediction of voltage, current, and power characteristics. MATLAB based thermoelectric models built from governing equations and datasheet parameters have been successfully used to simulate generator behaviour, load matching, and efficiency trends [9, 10].

In this article, a detailed MATLAB based thermoelectric model of Sb_2Te_3 and Bi_2Te_3 materials is investigated. The model is developed from fundamental thermoelectric relations and implemented by using equation blocks to represent Seebeck effect, internal resistance, and thermal conduction mechanisms. Through simulation, the electrical and thermal responses of the materials are analyzed under varying temperature gradients and load conditions, and this analysis provides a systematic framework for performance evaluation and further optimization of thermoelectric systems.

2. MATERIALS

Antimony telluride (Sb_2Te_3) and bismuth telluride (Bi_2Te_3) are two of the most widely used chalcogenide thermoelectric materials for near room temperature applications. Both belong to the tetradyte crystal family and exhibit layered rhombohedral structures, which support strong anisotropic transport behaviour [6, 10]. Their layered bonding and narrow band gaps make them highly suitable for thermoelectric energy conversion, especially in low and medium temperature ranges. Here, Bi_2Te_3 is used as an n-type thermoelectric material, while Sb_2Te_3 is widely used as a p-type thermoelectric material in MATLAB based thermoelectric module. Their complementary carrier types allow them to be paired in p–n couples for thermoelectric generators and coolers. The Seebeck coefficient, electrical resistivity, and thermal conductivity of both materials fall within favourable ranges for achieving high thermoelectric figure of merit (ZT).

Figures 1a and 1b show a transport perspective. Bi_2Te_3 typically exhibits higher electron mobility and stable electrical conductivity, which supports strong n-type performance. Sb_2Te_3 , on the other hand, generally shows higher hole concentration and good p-type Seebeck behaviour, making it effective for the hot side leg in thermoelectric modules. Modeling studies show that both materials can be effectively parameterized in MATLAB by using temperature dependent Seebeck coefficient, electrical resistance, and thermal conductance inputs for accurate device simulation (Table 1). Thermal conductivity in both materials is relatively low when they are compared with conventional conductors, which is beneficial for thermoelectric efficiency. Their figure of merit depends strongly on doping level, microstructure, and temperature [11-14]. MATLAB based thermoelectric models frequently use assumed parameter sets for Bi_2Te_3 p-type legs and related telluride compounds to simulate module behaviour and optimize performance before fabrication. Additional details about programming and output are given in Supplementary Details section.

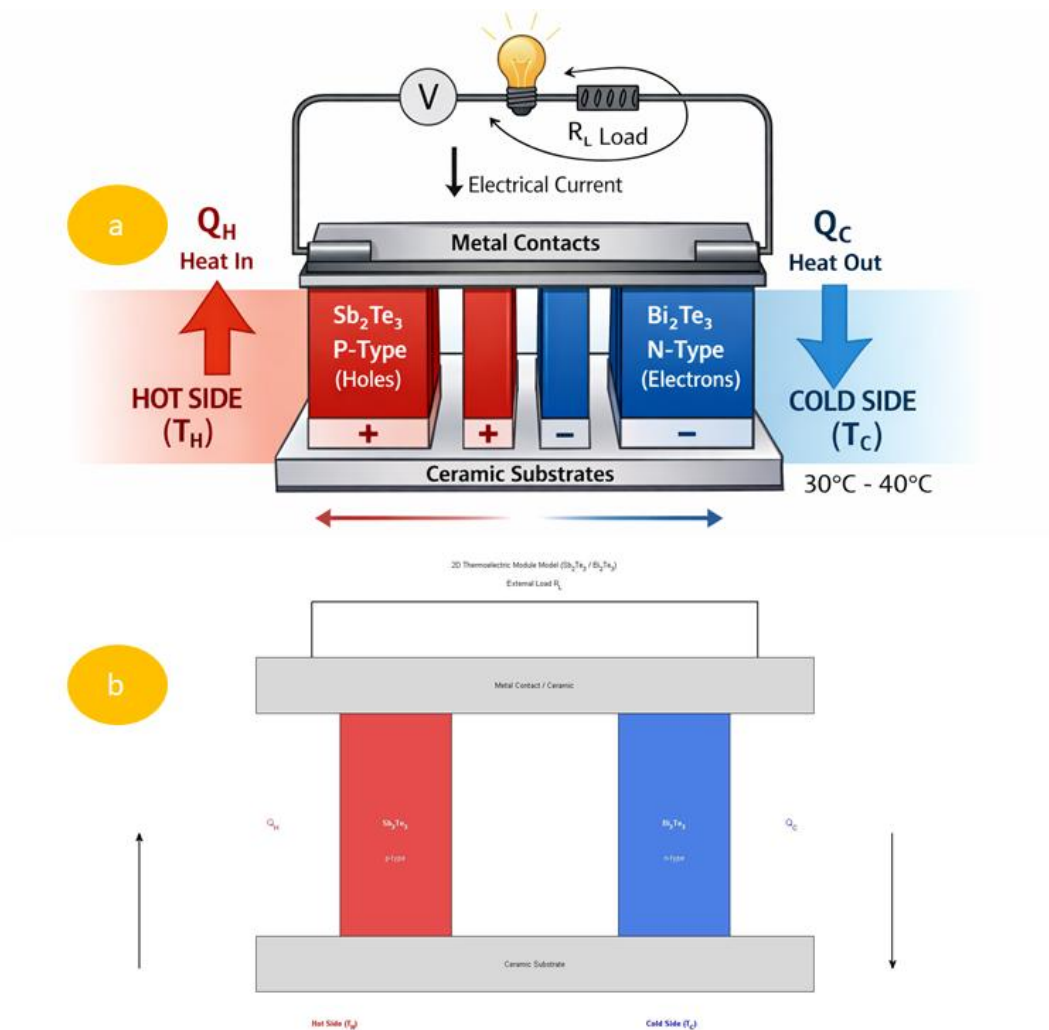


Figure 1. a) Schematic Diagram of Thermoelectric Model; b) MATLAB Model.

Table 1. Input parameters.

Property	Bi_2Te_3	Sb_2Te_3
Typical conduction used in present modules	n-type	p-type
Seebeck coefficient	Moderate to high (negative, n-type)	Moderate to high (positive, p-type)
Electrical resistivity	Low and moderate	Moderate
Thermal conductivity	Low	Low
Carrier type	Electrons	Holes
Best operating range	~300 to 800 K	~300 to 800 K

3. METHOD

The thermoelectric model was developed under the following simplified assumptions to enable tractable numerical analysis, while available thermoelectric material data were compiled from research articles [5, 15]. Governing equations implemented in the computational code were adopted from established thermoelectric theory reported in literature [2, 10, 16-20]. As shown in Figure 1a, cold side temperature was fixed between 30°C and 40°C to represent typical ambient conditions. The graphical user interface and baseline calculations were configured for a 2 W output target. For parametric plots, a temperature range was selected and evaluated by using a fixed incremental step size [16, 26]. The engine operating specifications were provided as model inputs. They include exhaust temperature, estimated heat availability, and other relevant thermal parameters. When exact values were unavailable, validated default values were retained to maintain continuity of simulation. Then, thermoelectric material was selected from a predefined database. Each material entry contains Seebeck coefficient, electrical resistivity, and thermal conductivity values [11, 17]. These parameters were treated as constants throughout each simulation run.

The physical dimensions of the module area and length were used to compute internal electrical resistance and thermal conductance. Electrical load conditions were defined by selecting the intended accessory set to be powered by the generator. Load selection determines the external resistance used in the output power calculations [16, 17, 21]. After parameter entry, the computational routine was executed. The numerical model calculates temperature difference across the module, open circuit voltage, internal resistance, output current, power output, and conversion efficiency by using standard thermoelectric governing equations implemented in the M-code environment [10, 20]. Parametric analysis was performed across a defined temperature range by using fixed step increments. Output characteristics such as temperature, power, and efficiency were plotted to evaluate thermoelectric module under varying thermal conditions.

4. RESULTS AND DISCUSSION

MATLAB based thermoelectric generator model was developed to evaluate the performance of a bismuth telluride (Bi_2Te_3) module operating under engine exhaust heat recovery conditions [6]. The simulation used engine and thermo physical input parameters including engine capacity of 123.7 cc, air density of 1.170 kg/m³, specific fuel consumption of 230 g/kWh, rated power of 6.72 kW, volumetric efficiency of 98%, specific heat capacity of exhaust gas of 1.17 kJ/kg·K, and operating temperature limits of 250°C (hot side) and 40°C (cold side). The imposed hot side and cold side temperatures produce a temperature difference of 210°C approximately across the thermoelectric module.

This temperature gradient is the primary driving force for Seebeck voltage generation in the Bi_2Te_3 based model [7]. Simulation results show that the available temperature span lies within the effective operating window for near room temperature thermoelectric materials, ensuring stable transport behaviour and predictable parameter response. Because the cold side temperature was fixed near ambient conditions, the model demonstrates that performance is strongly governed by exhaust side temperature stability and heat exchanger effectiveness.

The specified engine power and specific fuel consumption, the MATLAB model estimates the recoverable exhaust heat fraction and corresponding heat flux into the thermoelectric hot plate. With high volumetric efficiency (98%), the exhaust flow is nearly proportional to displacement based theoretical intake, resulting in consistent thermal input to the module. The selected exhaust gas specific heat value ($1.17 \text{ kJ/kg}\cdot\text{K}$) yields moderate thermal storage capacity, which reduces transient fluctuations in calculated heat rate during parametric sweeps. The results (Figure 2a, Figure 2b) indicate that increasing exhaust temperature produces a near linear rise in heat input to the module, but the useful converted electrical output grows sub linearly due to simultaneous increases in conductive heat leakage through the thermoelectric legs. This confirms the expected relation between thermal conductance and electrical generation in Bi_2Te_3 modules.

The simulated open circuit voltage increases proportionally with temperature difference across the module, which is consistent with Seebeck based generation [8]. Under load conditions, the MATLAB model shows that output current is strongly dependent on the ratio between internal module resistance and selected load resistance. Maximum power transfer occurs when load resistance approximately matches the modelled internal resistance of the Bi_2Te_3 leg configuration. For the defined 2 W design target, the modelled module geometry (Figure 1b) and material parameters successfully achieve the required output within the specified temperature range. Figure 2a and Figure 2b reveal that the conversion efficiency remains modest, as expected for single stage Bi_2Te_3 thermoelectric systems operating in the low to medium temperature range. The MATLAB results show that efficiency increases with temperature difference but begins to saturate at higher hot side temperatures due to increased thermal backflow and resistive losses. This behaviour aligns with thermoelectric efficiency limits governed by the material figure of merit (Figure 2c) and confirms that simply increasing hot side temperature does not proportionally increase efficiency.

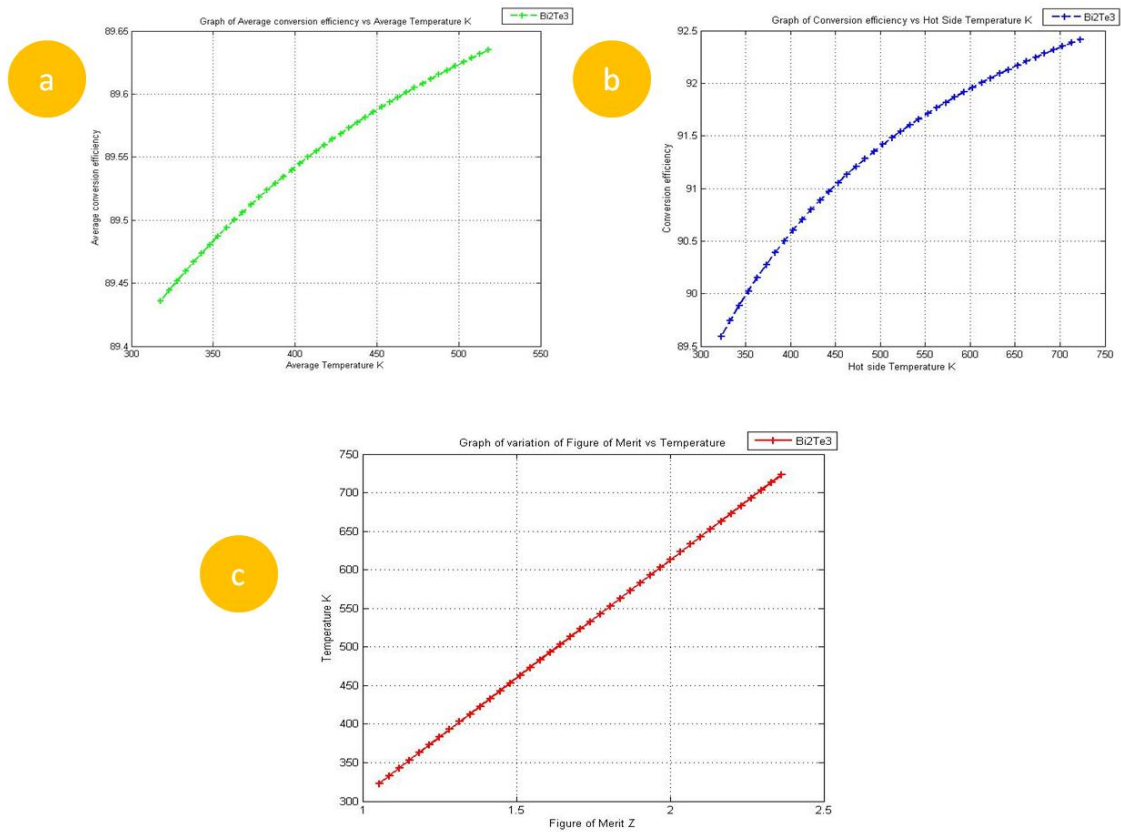


Figure 2. a) Average temperature output, b) conversion efficiency output, c) figure of merit for Bi₂Te₃

Similarly, MATLAB based thermoelectric generator simulation was carried out for a p-type antimony telluride (Sb₂Te₃) module under engine exhaust heat recovery conditions. The model incorporated engine and thermo physical inputs, including engine capacity of 127.4 cc, exhaust gas density of 1.167 kg/m³, specific fuel consumption of 226 g/kWh, rated power of 6.81 kW, volumetric efficiency of 94%, specific heat capacity of exhaust gas of 1.16 kJ/kg·K, and operating temperatures of 250°C at the hot side and 40°C at the cold side. The MATLAB results (Figure 3a and Figure 3b) show a proportional rise in Seebeck voltage with temperature difference, confirming correct implementation of the Seebeck relation in the numerical model. Because Sb₂Te₃ is modelled as a p-type material with a positive Seebeck coefficient, the simulated polarity and voltage direction are consistent with theoretical expectations [22-24, 28]. The results further indicate that maintaining the cold side temperature near 40°C is critical, since any modelled increase on the cold side directly reduces the effective temperature gradient and lowers predicted voltage output [9]. With engine power of 6.81 kW and specific fuel consumption of 226 g/kWh, the MATLAB heat availability submodel estimates a steady exhaust heat source suitable for low power thermoelectric recovery. Compared with higher SFC cases [10, 25], the lower SFC here implies improved fuel to power conversion and slightly more favourable recoverable heat per unit fuel input. The modelled exhaust specific heat capacity (1.16 kJ/kg·K) produces moderate heat carrying capability. Simulation sweeps show that heat input to the thermoelectric hot plate increases with exhaust temperature but also increases conductive heat leakage through the thermoelectric leg [6-8]. As a result, net converted electrical power rises with temperature but at a reduced slope compared with raw thermal input, matching expected thermoelectric behaviour [11-17]. The MATLAB output curves for the Sb₂Te₃ module show linear open circuit voltage growth with temperature difference and load dependent current variation. Because Sb₂Te₃ is modelled with moderate electrical resistivity relative to n-type counterparts, the simulated internal resistance is slightly higher, which influences the current level under load.

Maximum power output occurs when the external load resistance matches the modelled internal resistance of the thermoelectric leg. Under this matched condition, the simulation meets the low watt design objective used in the graphical user interface framework (Figure 3a and Figure 3b). Temperature, power, and efficiency curves follow the expected parabolic power profile, confirming correct coupling of thermal and electrical sub models. The computed conversion efficiency remains within the typical low single digit percentage range for single stage thermoelectric systems operating in this temperature band. MATLAB parametric plots show that efficiency increases with temperature difference but gradually approaches saturation at higher hot side temperatures due to increased conductive heat backflow, joule heating inside the leg and fixed material parameter to volumetric efficiency as 94%. The figure of merit results are gotten as 2.4 (no unit) for Bi_2Te_3 , 1.38 (no unit) for Sb_2Te_3 , which are provided in Figure 2c and Figure 3c. The Sb_2Te_3 MATLAB thermoelectric model produces physically consistent electrical and thermal trends under the specified operating conditions. The p-type leg model demonstrates stable voltage generation across the defined temperature range and predictable load matching behaviour. While constant property assumptions simplify computation, they likely lead to slight overestimation of performance compared with temperature dependent real material behaviour [21].

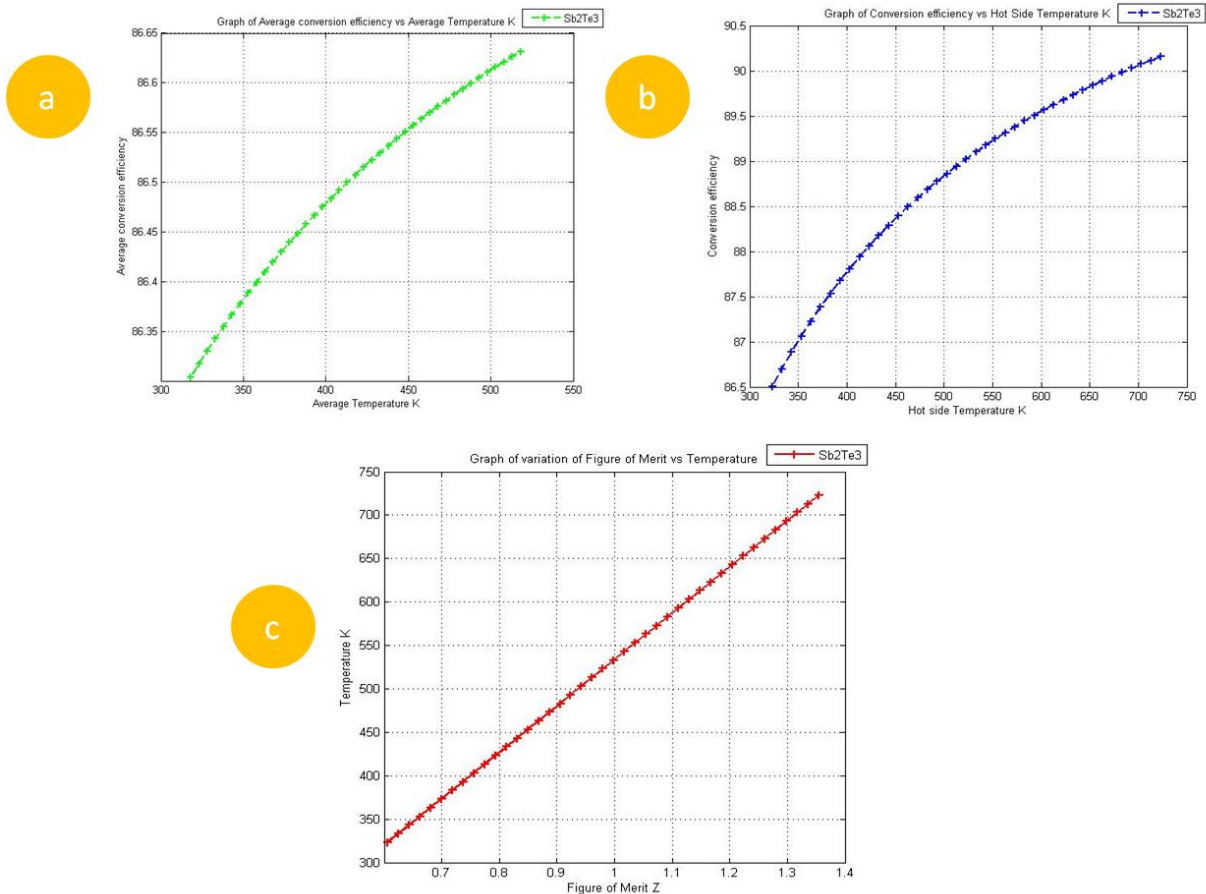


Figure 3.a) Average temperature output, b) conversion efficiency output, c) figure of merit for Sb_2Te_3

5. CONCLUSION

A detailed MATLAB based thermoelectric model for Sb_2Te_3 and Bi_2Te_3 materials was successfully developed and evaluated under engine exhaust heat recovery conditions. The modeling approach, based on fundamental thermoelectric relations and simplified constant property assumptions at 300 K to 800 K, enabled effective simulation of coupled thermal and electrical behaviour. The results confirmed that both materials operate reliably within the selected temperature window and produce predictable Seebeck driven voltage and power output trends. The Bi_2Te_3 model demonstrated stable n-type behaviour with favourable electrical conductivity and consistent output under varying load conditions, making it well suited for the n-leg of near room temperature thermoelectric modules. The Sb_2Te_3 model showed strong p-type response and dependable Seebeck characteristics, validating its role as a complementary p-leg material. For both materials, maximum power output was achieved under load matching conditions, and efficiency increased with temperature difference but showed saturation at higher gradients due to conductive and resistive losses. Sensitivity analysis indicated that exhaust temperature, cold side cooling level, volumetric efficiency, and specific fuel consumption significantly influence predicted thermoelectric performance. The model provides a strong foundation for further refinement and supports the feasibility of watt level power generation from small engine waste heat using telluride based thermoelectric materials.

6. SUPPLEMENTARY DETAILS

```
%MATLAB code for thermoelectricmodel
```

```
figure('Color','w');  
axis equal  
axis off  
hold on
```

```
% --- Base ceramic plate ---
```

```
rectangle('Position',[0 0 10 1],'FaceColor',[0.85 0.85 0.85],'EdgeColor','k')  
text(5,0.5,'Ceramic Substrate','HorizontalAlignment','center')
```

```
% --- Top ceramic plate ---
```

```
rectangle('Position',[0 5 10 1],'FaceColor',[0.85 0.85 0.85],'EdgeColor','k')  
text(5,5.5,'Metal Contact / Ceramic','HorizontalAlignment','center')
```

```
% --- P-type leg (Sb2Te3) ---
```

```
rectangle('Position',[1.5 1 2 4],'FaceColor',[0.9 0.3 0.3],'EdgeColor','k')  
text(2.5,3,'Sb_2Te_3','HorizontalAlignment','center','Color','w','FontWeight','bold')  
text(2.5,2.4,'p-type','HorizontalAlignment','center','Color','w')
```

```
% --- N-type leg (Bi2Te3) ---
```

```
rectangle('Position',[6.5 1 2 4],'FaceColor',[0.3 0.5 0.9],'EdgeColor','k')  
text(7.5,3,'Bi_2Te_3','HorizontalAlignment','center','Color','w','FontWeight','bold')  
text(7.5,2.4,'n-type','HorizontalAlignment','center','Color','w')
```

```
% --- Electrical connection line ---
```

```
plot([1 1 9 9],[6 7 7 6],'k','LineWidth',2)  
text(5,7.3,'External Load R_L','HorizontalAlignment','center')
```

```
% --- Heat arrows ---
annotation('arrow',[0.15 0.15],[0.2 0.45],'LineWidth',2)
annotation('arrow',[0.85 0.85],[0.45 0.2],'LineWidth',2)

text(1,-0.6,'Hot Side (TH)','Color','r','FontWeight','bold')
text(7,-0.6,'Cold Side (TC)','Color','b','FontWeight','bold')

% --- Labels ---
text(0.2,3,'QH','Color','r','FontSize',12)
text(9.5,3,'QC','Color','b','FontSize',12)

title('2D Thermoelectric Module Model (Sb2Te3 / Bi2Te3)')
```

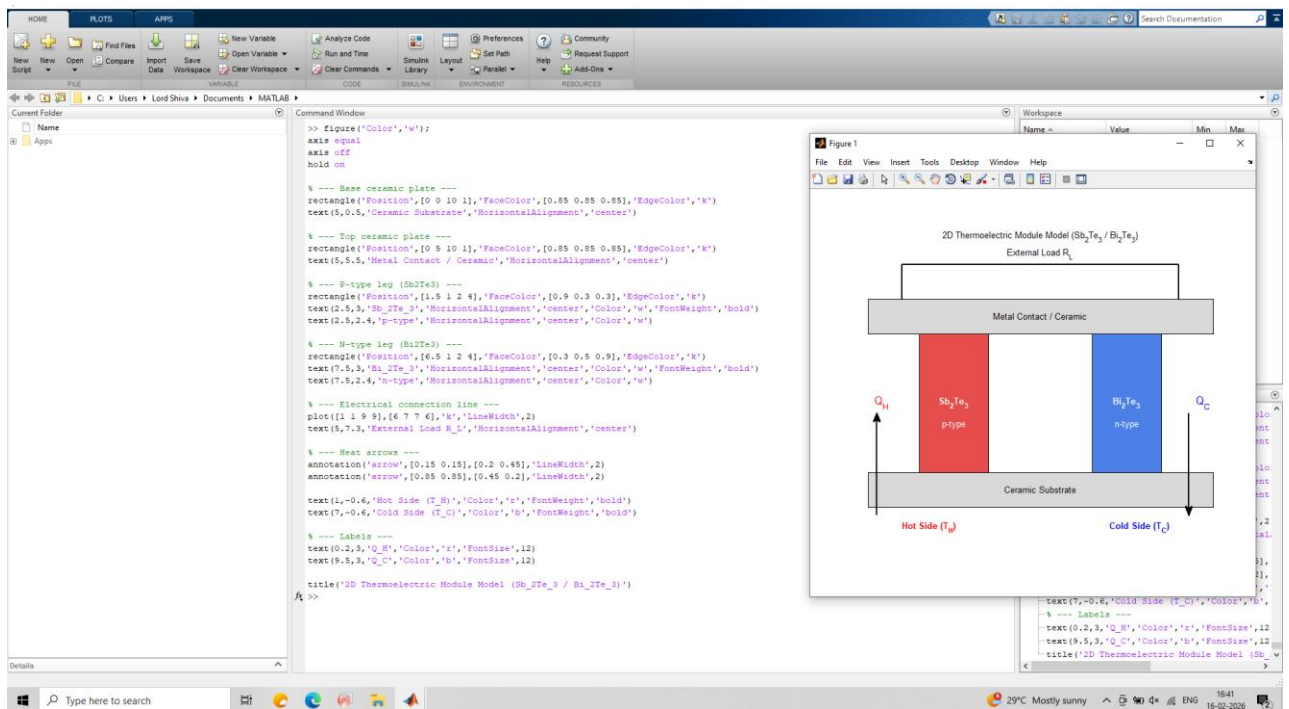


Figure 4. Thermoelectric MATLAB Model

Conflict of Interest

No conflict of interest is declared by the authors.

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