Numerical Analysis of Thermoelectric module for Power Generation

DISSERTATION

Submitted in partial fulfillment of the requirement for the award of the Degree of

MASTER OF TECHNOLOGY IN Mechanical Engineering

By

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Under the Guidance of

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DECLARATION

I, ANSHUL KUMAR, student of B.Tech - M.Tech (Dual Degree) under Department of Mechanical Engineering of Lovely Professional University, Punjab, hereby declare that all the information furnished in this thesis report is based on my own intensive research and is genuine.

This thesis does not, to the best of my knowledge, contain part of my work which has been submitted for the award of my degree either of this university or any other university without proper citation.

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CERTIFICATE

I hereby certify that the work which is being presented in the dissertation entitled **"Numerical Analysis of Thermoelectric module for Power Generation"** in partial fulfilment of the requirement for the award of degree of **Masters of Technology** and submitted in Department of Mechanical Engineering, Lovely Professional University, Punjab is an authentic record of my own work carried out during period of Dissertation under the supervision of **Ms. Garima (17916)**, Department of Mechanical Engineering, Lovely Professional University, Punjab.

The matter presented in this dissertation has not been submitted by me anywhere for the award of any other degree or to any other institute.

This is to certify that the above statement made by the candidate is correct to best of my knowledge.

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The M-Tech (ME), Dissertation-II Evaluation has been held by May, 2015

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ABSTRACT

This paper presents a mathematical model of temperature profile along Thermoelectric leg of a thermoelectric module in power generation mode when a temperature difference along the legs of p-n pair of semiconductor material produces an electric potential difference across leg. This model is developed solely because of the incapability of conventional models to handle large temperature difference. As high operating temperature is considered, it is of absolute obviousness that all the Thermoelectric properties are to be considered, i.e., Thomson effect, Seebeck effect and Peltier effect along with the Thermal and electrical property to be a quadratic function of temperature. Thomson effect is to be considered as a differential function of Seebeck coefficient, according to the lord Kelvin's relation. Constant Seebeck coefficient was not considered as it would result in zero Thomson effect. Hence, the inner effects including Seebeck effect, Fourier effect, Joule effect and Thomson effect, and external heat transfer are taken into account in the model. Energy balance across the legs of the module was done to determine the temperature profile analytically by considering all the aspects. The temperature profile so obtained was substituted in the energy equation and the Heat input and Heat output was noted. The results hence obtained can be used to determine the energy conversion efficiency. Numerical simulations based on Finite element method were then performed in ANSYS to determine the energy transfer. The Simulation result shows that the model developed in this paper is accurate even while working at high temperature difference. Hence giving a scope of improvement and proper development of Thermoelectric generators for high temperature applications.

TERMINOLOGY

Nomenclature

А	Area
Ι	Working electrical current (A)
K	Thermal Conductance (WK ⁻¹)
k	Thermal Conductivity (Wm ⁻¹ K ⁻¹)
1	Length
Po	Power output (W)
Q	Heat Flow Rate (W)
R	Resistance
Т	Temperature
V	Electric potential difference (Volts)
W	Power (Watts)

- dx Small elemental length (m)
- $d\bar{x}$ Non-dimensionalised small elemental length

Greek letters

- α Seebeck Coefficient (VK⁻¹)
- π Thomson Coefficient (VK⁻¹)
- ρ Electrical Resistivity (Ω m)
- σ Electrical Conductivity ($\Omega^{-1}m^{-1}$)
- $d\theta$ Non-dimensional elemental temperature difference
- η Conversion efficiency

Δ Difference

Subscripts

Н	Heat source
L	Heat sink
t	Thomson effect
j	Joule effect
K _{in}	Fourier heat input
Kout	Fourier heat output
e	Electrical
Т	Thermal
l	Electrical load
р	p-junction diode

n n-junction diode

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Introduction

In the wake of energy crisis, it is of absolute importance that whatever raw energy is available to us is converted to proper useful energy to the extent as possible. There are many modes of energy conversion, but the most used indirect modes of energy conversion includes a large amount of losses while conversion. The most practical method of energy conversion which came in last century is the direct mode of energy conversion, like Thermoelectric method of energy conversion. Thermoelectric generator uses the temperature gradient to produce electricity. The waste heat from industries and combustion of fuels can easily be used to generate electricity using thermoelectric modules. Thermoelectric effects were discovered during the first half of 19th century. The Seebeck effect, Peltier effect and finally the Thomson effect are the most prominent Thermoelectric effects on which the Thermoelectric modules work. Different studies highlight the importance of Thomson effect, but the interdependencies of other factors on it make it difficult to study.

In the past it has been more economical for the industries to use the conventional method for waste heat recovery, i.e., employing conventional heating and cooling systems rather than the non-conventional Thermoelectric conversion method as it offered very low conversion efficiency (as low as 4%-6%). But as the Thermoelectric technology is advancing and new thermoelectric materials are being synthesized which are much better than the past bulk material, thermoelectric conversion is being viewed as a viable alternative to the conventional conversion methods. More so, the conventional methods are heavy setups, require continuous maintenance, too much losses while conversion and also suffers a comparatively low life span as compared to the Thermoelectric method of energy conversion which once setup doesn't require any maintenance, work without any noise, is light and can keep working without fuss for pretty long time. The practicality of Thermoelectric generator is evident from the fact that NASA uses this method in their Thermionic converters for deep space mission that lasts for even more than 30-40 years.

The Seebeck effect, discovered in 1821, expresses that a voltage difference is created in the presence of a temperature difference between two different metals or semiconductors. This phenomenon dictates in the production of an electric power between two semiconductors when applied to a temperature gradient. Heat is accepted into one side of the couples and is

rejected from the opposite side. An electrical current is produced, proportional to the temperature gradient between the hot and cold sides. The temperature difference across the legs of diode produces direct current to a load producing a terminal voltage and a terminal current. On the other hand, a complementary effect, called the Peltier effect (1834), results in a heat source or heat sink driven by an electrical current flowing through the junction between two different materials. It leads to the Thermoelectric cooling phenomenon. When an electric current passes through a junction of two semiconductor materials with different properties, the heat is rejected and absorbed from the two sides of its leg. At last, the Thomson effect (1854) reflects the heat released or absorbed when a single material is crossed by an electrical current and submitted to a thermal gradient.

A thermoelectric module consists of an array of p-type and n-type semiconductor elements that are adequately doped with electrical carriers. Usually the doping is kept on a higher side to keep the electrical conductivity high. The elements are so arranged that they are electrically connected in series but thermally connected in parallel. This array is then sandwiched between two ceramic plates, to keep the thermal conductive but prohibiting any kind of electrical conductivity.

The most unique feature of a thermoelectric device is it's reversibility. The same device can be used for generator mode (TEG) when it is exposed between temperature difference and also as a cooling device (TEC) for refrigeration purpose when the electric junction is supplied with suitable potential difference in DC mode. This reversible nature of thermoelectric energy converters brings the difference from many other conversion systems. Electrical input power can be directly converted to pumped thermal power for heating or cooling/refrigerating, or heat input power can be converted directly to electrical power for any work. Any thermoelectric device can be used in either mode of operation, although the design of a particular device is usually optimized for its specific purpose.

In order to improve the modelling of thermoelectric devices, my work focuses on the key part which is the thermoelectric leg. Different studies highlight the importance of the Thomson effect when considering a TEG or TEC mode. Although the physical phenomena are well known, the literature shows that they are sometimes not properly considered.

Chapter 2

Literature Review

A research work is termed as a good research only if the earlier works are studied thoroughly and a comprehensive review has been done on the research papers published earlier. In this work the study was carried out for increasing the knowledge on non-linear dependencies of the thermoelectric phenomenological effects and differences encountered while considering them as a constant or neglecting them and assuming them as zero. The thermoelectric effects were studied exhaustively to know the behaviour of the module.

2.1. Review of the Papers

It is reported from the beginning that considering the Thermoelectric properties to be constant is not very accurate. Jon Henderson/Analysis of a heat exchanger Thermoelectric Generator System/ Intersociety Energy Conversion Engineering Conference/ Boston, Massachusetts (1979), has also considered the thermoelectric properties of his analysis to be constant for his work on Ocean Thermal Energy Conversion. In his work he assumed that the operating temperature difference is small, hence has neglected the Thomson coefficient and other Thermoelectric properties are constant. At the end he concluded that conventional fixed temperature TEG analysis techniques are inadequate for investigation purposes. For applications, where maximum power generation is desired, detailed and simplified numerical techniques have to be considered.

Considering the above facts, Jincan Chen et al, in their work Non-equilibrium analysis of a Thermoelectric device/ Pergamon/ Energy Vol. 22 (1997), had considered the effects of Thomson heat and derived the expressions for the COP and the rate of heat pumping on a Heat Pump. Further he also analysed the effect of Thomson effect on the COP and the rate of heat pump on design model. He had observed and noted the difference when he had considered the Thomson effect and when he had not. The difference was noted when the Thomson effect was considered as a constant and not as a linear function or a non-linear function of the Seebeck effect, where even the Seebeck effect was a constant and not a nonlinear function of temperature.

S.B. Riffat et al. / Applied Thermal Engineering 26 (2006), have developed a computer model to simulate the performance of a novel heat pump system considering a non-linear

Seebeck effect and considering Seebeck coefficient to be a quadratic function of temperature as against assumed a constant in the above works. But, in conclusion it was noted and summarised that there still were discrepancies in the results when the theoretical model was compared with the experimental model. It was noted that there were very significant differences between the results and these were duly noted after comparison and correction factors were determined, but that was valid only for that model and not for a general model.

Later, A. Chakraborty et al. / Thermodynamic modelling of a solid state thermoelectric cooling device: Temperature–entropy analysis/ International Journal of Heat and Mass Transfer 49 (2006) coined the concept that Thomson effect bridges the Joule heat and the Fourier heat across the Thermoelectric elements of a Thermoelectric cooling cycle. They developed a temperature-entropy flux diagram and demonstrated it in tha analysis of cooling cycle of a Thermoelectric element. They successfully revealed the temperature dependency of Seebeck coefficient by considering a non-linear dependency. The presence of Thomson heat was however incorporated in performance estimation as a constant value and not as a function of Seebeck coefficient.

Y.Y. Hsiao et al. / Energy 35 (2010) in their study **A mathematic model of thermoelectric module with applications on waste heat recovery from automobile engine** have considered the Seebeck effect as constant and used iterative method to solve their mathematical model. They used a one dimensional thermal resistance model to predict the behaviour of the Thermoelectric module also, they verified the results with experiments. They were not able to note any significant improvement as they have ignored the Thomson effect and taken Seebeck effect as a constant for solving their Mathematical model and it can lose the accuracy as it has been solved iteratively and not an exact solution was developed.

X. Gou et al. / Applied Energy 87 (2010) in their work Modelling, experimental study and optimization on low-temperature waste heat thermoelectric generator system has established a thermoelectric generator system model based on the basic principles of thermoelectric generation technology and finite time thermodynamics. To investigate viability and further performance of a thermoelectric generator for waste heat recovery a practical setup was constructed. They also ignored the Thomson effect and neglected it also, the also ignored the non-linear Seebeck effect and assumed it to be a constant and hence the result that they obtained and compared it with their practical setup, they reported a significant deviation in both the observation. Hence in their work it's validated that not considering the Thomson effect and taking a constant Seebeck coefficient will result a variation in the result.

H. Lee/ The Thomson effect and the ideal equation on thermoelectric coolers/ Energy 56 (2013) has formulated the classical basic equations for a thermoelectric cooler from the Thomson relations to the non-linear differential equation with Onsager's reciprocal relations to basically study the Thomson effect in conjunction with the ideal equation in which the Thomson coefficient is assumed to be zero. In order to realistically study the Thomson effect on the temperature distributions with the temperature dependent Seebeck coefficient the author referred to a commercially available Thermoelectric module and the temperature dependent parameters and geometric dimensions were taken from it. Graphs were plotted for Seebeck coefficient v/s Temperature and the resulting data was implemented in the equation to study the Thomson coefficient. They concluded that a positive Thomson coefficient reduces the performance of a thermoelectric cooler while a negative Thomson coefficient the Thomson effect was in excellent agreement with numerical simulation against the iterative method which was not very accurate. Hence it can be noted that for small temperature difference in cooling mode also the Thomson effect plays a vital role.

L. I. Anatychuk et al. in their work on Theoretical and Experimental Study of Thermoelectric Generators for Vehicles / Journal of ELECTRONIC MATERIALS, (2011), have studied the general physical laws for reaching the maximum efficiency of generator using vehicular exhaust heat. The lumped and distributed parameters were basis of the physical model of the generator. They concluded that with the use of identical thermal converters of equal thermal conductivity, the temperature distribution between the hot plates of the modules must be exponential. If such a module is used where exponential temperature distribution is noted along the modules, it is not reasonable to use low-temperature modules. Hence for considering high-temperature application it is better to consider that the temperature profile is exponential.

G. Fraisse et al. / Energy Conversion and Management 65 (2013) in their comparative work Comparison of different modeling approaches for thermoelectric elements have attempted to analyse the simplified models' accuracy, with regards to the performance (COP, efficiency), the voltage–current characteristics and the thermal/electrical power. These models were compared to more accurate models, such as models based on an electrical

analogy and on the finite element method. Thermoelectric phenomena in a thermoelectric leg were simulated for different kinds of models and hence compared. No significant differences were noted in the simplified and improved simplified models where a constant Seebeck effect and zero Thomson effect were considered, but the improved simplified model showed a marked improvement as the Seebeck effect was considered as a varying parameter from hot to cold side of the leg. They concluded that in any case the introduction of Thomson effect contributed as an additive term which was valid only if a thermal dependence of the value of Seebeck coefficient is considered.

L. Chen et al. / Scientia Iranica, Transactions B: Mechanical Engineering 19 (2012) in their Research note on Maximum power and efficiency of an irreversible thermoelectric generator with a generalized heat transfer law has established an advanced model of irreversible thermoelectric generator with a generalized heat transfer law based on finite time thermodynamics. The inner effects including Seebeck effect, Fourier effect, Joule effect and Thomson effect, and external heat transfer were taken into account in the model. The nonlinear quadratic relation of Seebeck coefficient, Electrical resistivity and thermal conductivity were considered and the differential form of Thomson coefficient was taken by the second Kelvin relationship. At the end it was concluded that because of not taking the effect of heat transfer coefficient into account, not all the results hold true. However an advanced model of irreversible thermoelectric generator with a generalized heat transfer law is established which reduces the incomprehensiveness of conventional model.

J. Yu, H. Zhao, presented "A numerical model to predict the performance of thermoelectric generator with the parallel-plate heat exchanger". He based his paper for application on waste heat recovery. The model was based on an elemental approach to analyse the temperature change in thermoelectric generator. This elemental differential approach gave a much more detailed prediction for the temperature difference through thermoelectric modules. The effective temperature difference between the hot and cold side junction was estimated based on this model, which proved that the effective temperature difference between the junctions plays the key role for thermoelectric generator. In this paper the author has simultaneously worked to provide the numerical model for further analysis on net power output with relative to the fluid pressure across the heat exchanger.

L. Chen et al, in their paper "Effect of heat transfer on the performance of thermoelectric generators" (2002) have shown that the power output and efficiency expression for TEG

which is composed of multiple-elements are derived with consideration of heat transfer irreversibility in heat exchanger between the generator and the heat reservoirs. It was noted that the heat transfer irreversibility affects the performance of TEG. Further, as any practical TEG is composed of multiple elements hence there is variation in the power output with the number of modules and hence the heat transfer also varies very different when multiple elements are considered. They also pointed out that the load resistance and internal electrical resistance has to be properly optimized for creating a perfect balance between power and efficiency.

Emil J. Sandoz-Rosado presented a paper "On the Thomson effect in thermoelectric power devices" (2012). In this they have pointed out that most TE device modelling neglects the non-linear Thomson effect to develop a closed-form solution to the governing thermal energy transfer equation even if this effect is profoundly present in TEM and often contributes significantly to the power generation capabilities of a module. However, in contrast this effect has been assumed to be of negligible importance since decades. It was also pointed out that the effect earlier didn't played important role as high temperature application was not employed, but in present case scenarios, high temperature application are very dominant and existing models are not adequate to evaluate and determine the exact performance and statistical data of TEM. It was concluded that considering the Thomson effect has increased the accuracy of result significantly.

Robert J. Stevens et al. presented their paper **"Theoretical limits of thermoelectric power generation from exhaust gases"**, in which they have made a model to predict a theoretical limit to the optimum number of TE modules for maximum performance in a TEG system and also defined that adding any more modules will result in performance degradation. Further it was pointed out that in most cases, optimization of local thermoelectric efficiency leads to predictions close to that of the theoretical limit of maximum power generated by TEG. Further, their analysis pointed out that the theoretical figure of merit (ZT) is not sufficient parameter to determine the performance of an entire system. They have given a new algorithm which they showed is necessary to consider while determining performance of a system level TEG.

Chapter 3

Scope of the Study

Simplified models are usually incorporated to describe the behaviour of thermoelectric elements due to their low computational effort needed for solving the physical behaviour in a wide number of situations (e.g., in both heating/cooling mode i.e., TEH/TEC and in power generation mode - TEG). The accuracy of these models depends on different assumptions like: (i) Negligible Thomson effect (ii) the thermoelectric properties are assumed to be constant in the thermoelectric leg and are estimated from the mean temperature of its two sides. These assumptions make the model simpler to handle and solve but the accuracy of the model decreases significantly when large temperature difference is considered for other thermoelectric properties. A new mathematical model can be developed considering all the non-linear parameters in the phenomenological effects of a thermoelectric modules and not simplifying any of the parameters to get a much more accurate results when considering a thermoelectric module for any practical application in real world. A more accurate model can help determining the behaviour of the material when it is exposed to the condition as specified. Further it will be much easier to develop new materials in this field of engineering i.e., Thermoelectric materials, which are synthesised semiconductors, for specified field and application as and where required.

This solution of exhaustive modelling problem can be best achieved by considering all the phenomenological effects on a thermoelectric module and developing the energy balance by considering the differential forms of all the effects and combining them all into a single equation without omitting any effect by considering it negligible or small. Hence after, the equation has to be solved analytically to get an exact solution rather than an approximate solution as in case of numerical solution of any equation. Also, rather than taking average of the non-linear parameters the overall equations has to be considered while solving for result.

Chapter 4

Objectives of the Study

The main objective of this study is to incorporate the various thermoelectric phenomenological effects in the generator mode for thermoelectric module to the temperature profile in the legs of junction diodes. This temperature profile when incorporated in the energy transfer equation the accuracy of the energy transfer at high operating temperature difference increases as compared to the conventional model. So, the objectives of removing the limitation of inaccurate energy transfer at high temperature difference due to neglecting the various thermoelectric phenomenological effects. This will facilitate us to remove the limitation of analysis of thermoelectric materials because of consideration of non-linear thermoelectric properties with high temperature difference. Although the non-linear effect to be constant or average of it. But rather an interdependency of each parameter can be made in feasible way to make the study easier and more proper. It would further facilitate simplification of higher consideration of different characteristics and parameters like power development, efficiency etc. We can develop a more accurate mathematical model which will be as close to the practical observation as it can be.

Mathematical Modelling

A thermoelectric module in this work is considered to be a Thermal system. To develop a Mathematical model for a Thermal system it is the best practise to use the concept of Energy balance. The energy balance equation simply states that at any given location, or node, in a system, the heat into that node is equal to the heat out of the node plus any heat that is stored. Hence it can be expressed as

Heat in = Heat out + Heat stored

In this model for energy balancing, we have used the concept:

(Heat in - Heat out) + Heat generated due to (Thomson effect + Joule effect) = 0

The heat that is entering the module and leaving the module is the Fourier heat for heat source to heat sink respectively. These models are the most important ones in the designing of thermal systems because they provide considerable versatility in obtaining quantitative results that are needed as inputs for design.

5.1. Assumptions

- The module is modelled as a 1-D unit.
- The entire module is working under steady state at given time.
- The entire thermoelectric module is considered as an insulation package, hence heat leakage through the lateral faces are neglected.
- The entire unit is working under a constant temperature difference.
- Temperature dependent thermoelectric properties, especially, the Thomson heat loss and non-linear Seebeck effect are taken in to account.

5.2. Modeling and problem formulation

For modelling and problem formulation we have used the concept developed above as

$$\dot{Q}_{Kin} - \dot{Q}_{Kout} + \dot{Q}_t + \dot{Q}_j = 0$$
 (5.1)

Where \dot{Q}_{Kin} & \dot{Q}_{Kout} are the Fourier heat in and out respectively.

 \dot{Q}_t : Thomson heat generated

& \dot{Q}_j : Joule heat generated

Hence we get,

$$kA\frac{d^2T}{dx^2} + Q_t + Q_j = 0 (5.2)$$

Where, $Q_t = \pi I \frac{dT}{dx} \& Q_j = \frac{I^2}{\sigma A}$

Hence, the equation becomes,

$$kA\frac{d^2T}{dx^2} + \pi I \frac{dT}{dx} + \frac{I^2}{\sigma A} = 0$$
(5.3)

Generalizing, we get,

$$C_1\frac{d^2T}{dx^2} + C_2\frac{dT}{dx} + C_3 = 0$$

We Use Non-dimensionalised terms as,

$$\theta = \frac{T - T_L}{T_H - T_L} \tag{5.4}$$

&

$$\bar{x} = \frac{x}{l} \tag{5.5}$$

Or

$$T = \theta(T_H - T_L) + T_L$$

&

 $x = \bar{x}l$

Now,

$$\frac{d^2T}{dx^2} = \frac{d}{dx} \left(\frac{dT}{dx} \right)$$

or $\frac{d^2T}{dx^2} = \frac{d}{dx} \left(\frac{d(\theta(T_H - T_L) + T_L)}{ld\bar{x}} \right)$
or $\frac{d^2T}{dx^2} = \frac{\Delta T}{l^2} \frac{d^2\theta}{d\bar{x}^2}$
&
 $\frac{dT}{dx} = \frac{(T_H - T_L)}{l} \frac{dT}{d\bar{x}}$

$$\frac{dT}{dx} = \frac{\Delta T}{l} \frac{dT}{d\bar{x}}$$

Hence, the equation after non- dimensionalizing becomes,

$$kA\frac{\Delta T}{l^2}\frac{d^2\theta}{d\bar{x}^2} + \pi I\frac{\Delta T}{l}\frac{d\theta}{d\bar{x}} + \frac{I^2}{\sigma A} = 0$$
(5.6)

Dividing throughout by $\frac{\Delta T}{l^2}$, we get

$$\frac{d^2\theta}{d\bar{x}^2} + \frac{\pi I l}{kA} \frac{d\theta}{d\bar{x}} + \frac{I^2 l^2}{\sigma k A^2 \Delta T} = 0$$
(5.7)

Let it be,

$$\frac{d^2\theta}{d\bar{x}^2} + m_1 \frac{d\theta}{d\bar{x}} + m_2 = 0$$
(5.8)

Where,

$$m_1 = \frac{\pi l l}{kA} \tag{5.9}$$

&

$$m_2 = \frac{I^2 l^2}{\sigma k A^2 \Delta T} \tag{5.10}$$

Now, for
$$m_1$$

$$m_1 = \frac{\pi l l}{kA}$$

We know that,

$$\frac{l}{kA} = R_{T}$$
 i. e., Thermal Resistance

Hence,

$$\frac{kA}{l} = K_{T}i. e.$$
, Thermal Conductance

Also for πI , unit of π is VK⁻¹

Hence

$$m_1 = \frac{\mathrm{VI}}{\mathrm{KK}_{\mathrm{T}}} = \frac{\mathrm{W}}{\mathrm{KK}_{\mathrm{T}}}$$

i.e., physically m_1 denotes the power generated per unit temperature per unit thermal conductance of the diode.

Now, for m_2

$$m_2 = \frac{I^2 l^2}{\sigma k A^2 \Delta T}$$

or

$$m_2 = I^2 \left(\frac{l}{\sigma A}\right) \left(\frac{l}{kA}\right) \left(\frac{1}{\Delta T}\right)$$

here,

$$\frac{l}{\sigma A} = R_e$$
: Internal electrical resistance

&

$$\frac{l}{kA} = R_{T}$$
: Thermal Resistance

Or

$$m_2 = I^2 R_e R_T \frac{1}{\Delta T}$$

 $\therefore m_2 = (I^2 R_e) \left(\frac{R_T}{\Delta T}\right)$

Now we know that $I^2 R_e = W$: Electrical power & $\left(\frac{R_T}{\Delta T}\right) = \frac{1}{Q}$ from Newton's law

Hence, $m_2 = \frac{W}{Q}$

i.e., physically m_2 denotes the electrical power generated per unit net heat conducted through diode junction.

Now,

$$\frac{d^2\theta}{d\bar{x}^2} + m_1 \frac{d\theta}{d\bar{x}} + m_2 = 0$$

This is a simple linear differential equation of second degree

Where,

$$C.F. = C_1 + C_2 e^{m_1 \bar{x}}$$

&

$$P.I. = -\frac{m_2}{m_1}\bar{x}$$

Hence on solving we get,

$$\theta = C_1 + C_2 e^{-m_1 \bar{x}} - \frac{m_2}{m_1} \bar{x}$$

Now, the boundary conditions are

$$at \ \bar{x} = 0, \theta = 1 \ \&$$
$$at \ \bar{x} = 1, \theta = 0$$

Now, substituting the boundary conditions in the solution, we get

$$C_{1} = \frac{\binom{m_{2}}{m_{1}} - e^{-m_{1}}}{1 - e^{-m_{1}}}$$

&,
$$C_{2} = \frac{1 - \binom{m_{2}}{m_{1}}}{1 - e^{-m_{1}}}$$

Hence, the final complete equation becomes:

$$\theta = \frac{\binom{m_2}{m_1} - e^{-m_1}}{1 - e^{-m_1}} + \frac{1 - \binom{m_2}{m_1}}{1 - e^{-m_1}} e^{-m_1 \bar{x}} - \frac{m_2}{m_1} \bar{x}$$
(5.11)

Where,

$$m_1 = \frac{\pi I l}{kA}$$

&

$$m_2 = \frac{I^2 l^2}{\sigma k A^2 \Delta T}$$

Now differentiating the equation (5.11) with respect to \bar{x} we get

$$\frac{d\theta}{d\bar{x}} = -m_1 \frac{1 - \binom{m_2}{m_1}}{1 - e^{-m_1}} e^{-m_1 \bar{x}} - \frac{m_2}{m_1}$$
(5.12)

Now, the equation (5.12) is substituted in the energy equation in form of temperature gradient in the Fourier heat transfer to include the various thermoelectric effects in the final energy equation.

$$\dot{Q}_{L} = \alpha T_{L} I + 0.5 I^{2} R_{l} + 2kA \frac{\Delta T}{l} \left| \frac{d\theta}{d\bar{x}} \right|_{\bar{x}=1}$$
(5.13)

$$\dot{Q}_{H} = \alpha T_{\rm H} I - 0.5 I^{2} R_{l} + 2kA \frac{\Delta T}{l} \left| \frac{d\theta}{d\bar{x}} \right|_{\bar{x}=0}$$
(5.14)

The equations (5.13) and (5.14) have been modified accordingly to accommodate the nondimensional parameters of my analysis. Hence, in the final equation of energy transfer, the derived temperature profile is just an additional term when compared to the conventional heat transfer equation, i.e.,

$$\dot{Q}_L = \alpha T_L I + 0.5 I^2 R_l + 2kA \frac{dT}{dx}$$
$$\dot{Q}_H = \alpha T_H I - 0.5 I^2 R_l + 2kA \frac{dT}{dx}$$

Where:

Here,

Combined Seebeck coefficient:
Internal electrical resistance:

$$\alpha = |\alpha_p| + |\alpha_n| \qquad (5.15)$$

$$R = \rho_n \left(\frac{l_n}{A_n}\right) + \rho_p \left(\frac{l_p}{A_p}\right) \qquad (5.16)$$

Applied temperature difference:

The electric current is given by:
$$I = \frac{\alpha \Delta T}{R_e + R_l}$$
(5.17)

 $\Delta T = T_H - T_L$

 R_l : Load resistance

Hence, the output electric power is given by: $P_o = I^2 R_l = VI$ (5.18)

And therefore the thermal efficiency can be given $\eta = P_o/\dot{Q}_H$ (5.19) by

The major properties i.e., Thermal conductivity, Electrical resistivity, Seebeck coefficient and Thomson coefficient were considered as a quadratic function on temperature. However the entire function couldn't be incorporated so a more appropriate value determined from these functions was considered. The operating temperature difference is between $T_h \& T_c$ hence the temperature at which the properties were determined was:

$$T = (T_{\rm H} - T_L)/2$$

As the Seebeck coefficient was not considered to be a constant value, the Thomson coefficient henceforth is to be considered as a derivative function of Seebeck coefficient as

$$\pi = T \frac{d\alpha}{dT}$$

Simulation Model

Any analytical model is not considered worthy enough if it has not been validated by simulation or experimental method. Hence for checking the validity of the equation developed for energy transfer analytically, ANSYS workbench 14.5 was used for simulation of the similar setup and then the results so obtained were compared for drawing the final conclusion regarding the model developed.

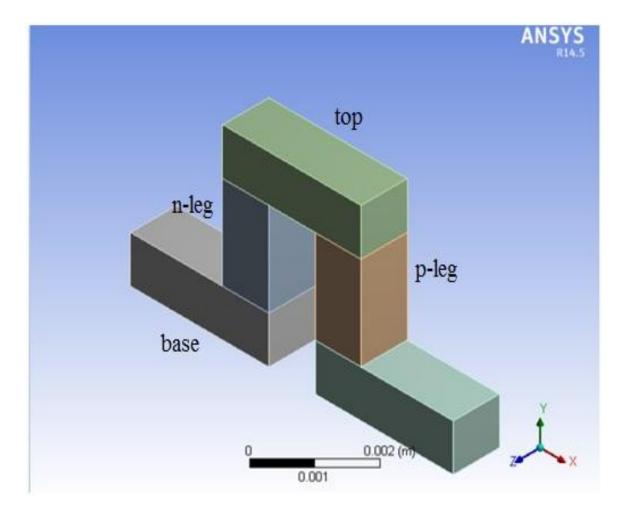


Figure 1: Simulation model setup

The simulation model was modelled for two different setups. One was for benchmark or the best possible result, the non-linear analysis model with temperature dependent thermoelectric, thermal and electrical properties. These properties were a quadratic function of temperature and were taken from a standard data book. The values of the properties, Seebeck coefficient, thermal conductivity and electrical resistivity were fed into the model at 100 different temperature points between the operating temperature range.

The other simpler model was made with just a single value of each property. The Seebeck coefficient, Thermal conductivity and electrical resistivity was determined from the same relation at the average operating temperature and then fed into the model. This gave the simulation a linear model for solution. This modelling though inherently not as accurate as above, gave a perfect mode to compare the result that will be obtained from the analytical model that was developed earlier.

As shown in figure, the model consisted of 5 parts:

- i. p-leg,
- ii. n-leg,
- iii. Top, connecting the two legs,
- iv. Base of p-leg &
- v. Base of n-leg.

The entire analysis is on the p-leg and n-leg, the semiconductor pair for thermoelectric power generation module. All the properties were fed manually for these both legs only. The leg's material was taken to be based on Bismuth material as it is the base material of the thermoelectric material (Bismuth telluride) for our numerical model and validation. The top and base were taken to be standard copper alloy that is required for electrical conductivity between legs and also for good thermal conductivity between source to legs and between legs to sink.

For the Thermal-electrical analysis in ANSYS Workbench 14.5, SOLID226 element was used for modelling. It is a brick element with 6 faces and has 20 nodes per element for accurate analysis. The entire model was meshed into a fine 13000 elements and 60401 nodes overall, with 2000 elements and 9581 nodes per leg. Such high number of elements and nodes assured that the model is as close to accuracy as possible.

To determine the various values on heat transfer and current generated, two Heat reaction probes and one current reaction probe were used in the model. One heat reaction probe was at the top surface and another was at the bottom surface of the base of the model. The current reaction probe was set at the right face of base of p-leg so that we can get the current that has been generated in the model.

The temperature profile was than plotted and then was compared to the temperature profile of the analytical model that was made. These profiles gave a very good perspective for comparison of various types of models and relative accuracy of all the models. The heat reaction probes gives us heat input to the legs and the heat output of the legs, hence giving the overall heat transfer that has been taking place through the system.

Result and Discussion

Any research work is not worth anything until and unless useful results are not got from it. A research is more or less like a thriller mystery whose end remains unknown until and unless results are discussed. No matter the result may be negative or positive in nature; it serves the purpose in any way. If the results derived are positive it's an indication that there is a scope better serving the society with the research. Whereas, if the results are not as expected then it clearly indicates that no one in future should try to work on similar approach as it is not of use hence saving a lot of time which would have otherwise wasted.

7.1. Numerical data

In the following numerical example the following data are used. Commercial thermoelectric material, Bismuth Telluride, is widely acceptable as most used thermoelectric material for power generation. It's various property data, physical properties, physical size, etc. are easily available in data book. One such standard data was selected for analysis which included the various values as follows:

Length: 2mm

Area: (1mm x 1mm)

Source temperature: $T_H = 600 \text{ K}$

Sink Temperature: $T_C = 300 \text{ K}$

Seebeck Coefficient: α (T) = (22 224.0 + 930.6 T - 0.9905 T²)10⁻⁹ VK⁻¹

Electrical resistivity: ρ (T) = (5112.0 + 163.4 T + 0.6279 T²)10⁻¹⁰ Ω m,

Thermal conductivity: $k(T) = (62\ 605.0 - 277.7\ T + 0.4131\ T^2)10^{-4}\ Wm^{-1}\ K^{-1}$

Thomson coefficient can be determined by second Kelvin relationship: $\pi(T) = T(d\alpha/dT)$

Also it is known that $\alpha_p = -\alpha_n$

For all practical application and ease of manufacturing it is taken that both the legs are of same area, same length, same electrical resistivity and same thermal conductivity with only

exception of the Seebeck coefficient, which only changes it's sign from positive to negative keeping the magnitude of the value same as it moves from p-leg to n-leg respectively.

The load resistance was taken: $R_L = 0.1$ ohm

7.2. Calculation

The mean effective average temperature for numerical model was taken to be 450 K, and at this same temperature the various values were calculated. The values found were as follows:

Seebeck Coefficient: $\alpha_p = 2.4041 \times 10^{-4} \text{ VK}^{-1} \& \alpha_n = -2.4041 \times 10^{-4} \text{ VK}^{-1}$

Electrical resistivity: $\rho_p = \rho_n = 2.0579 \times 10^{-5} \Omega m$

Thermal conductivity: $k = 2.1293 \text{ Wm}^{-1} \text{ K}^{-1}$

Thomson coefficient: $\pi = 1.7617 \times 10^{-5} \text{ VK}^{-1}$

Now, using equation (5.15), equation (5.16) and equation (5.17), we calculate the following

Combined Seebeck coefficient: $\alpha = 4.8082 \times 10^{-4} \text{ VK}^{-1}$

Internal electrical resistance: $R = 8.2316 \times 10^{-2}$

Applied temperature difference: $\Delta T = 300 \text{ K}$

The electric current is: I = 0.79115 amp

From equation (5.9) and equation (5.10), values of m_1 and m_2 are calculated as

$$m_1 = 0.01309 \&$$

 $m_2 = 0.08065$

Now, substituting the values obtained above in the equation (5.11), we get the function of the temperature profile in the semiconductor leg of the Thermoelectric generator. The function is derived as: $\theta(\bar{x}) = 398.015 - 397.015 e^{-0.01309 \bar{x}} - 6.1612 \bar{x}$

From equation (5.12), we get the differential function,

$$\frac{d\theta}{d\bar{x}} = 5.1969 \ e^{-0.01309 \ \bar{x}} - \ 6.1612$$

This function gives us the temperature gradient at any point of the function, which will be subsequently used in the heat transfer equation to determine the rate of heat transfer at source and sink of the semiconductor leg of the TEG. Now, using equation (5.13) and equation (5.14) with the values determined above, we find the values of heat transfer at source and at sink $\dot{Q}_c = 0.8213 W$

$$\dot{Q}_{\rm h} = 0.8413 W$$

Electrical power is given by equation (5.18): P = 0.0626 W

Hence, the conversion efficiency is given by equation (5.19): $\Pi = 0.0749$

7.3. Graphical representation of temperature profile

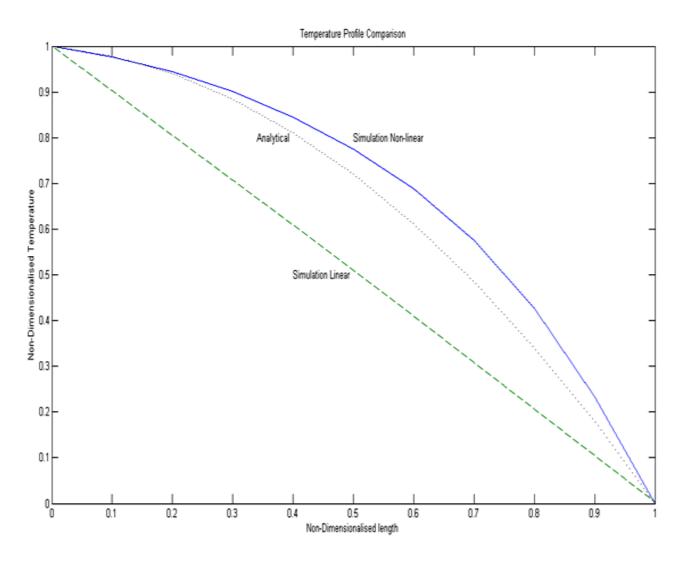


Figure 2: comparison of the temperature profile plots

The temperature profile determined from the various models is shown in the figure above. There are total three plots in the graph shown above:

- i. Simulation Non-linear: This is the plot of the case when the simulation was carried out with non-linear solution. In this the various properties were fed manually as function of temperature within the temperature range of 600 K and 300 K. As it evaluates the model at more number of intervals and at more number of points at various temperatures and successive and simultaneous value of the property, it is the most accurate result that can be obtained and hence provide us with the benchmark and ideal model to compare the other models.
- ii. Analytical: This is the plot of the temperature profile that was developed in the earlier chapter from the energy balance equations and the subsequent derivation that was performed on it. The various numerical data when substituted in the model of temperature profile, i.e., the function between temperature and length and was fed in the MATLAB software for plotting of graph between the defined temperature range of 600 K and 300 K, it yielded the plot as is shown in the graph above.
- iii. Simulation Linear: This is the temperature profile that was obtained from the simulation model of ANSYS when it solved the model as a linear solution. In this numerical example of Finite element solution, the properties were fed in the simulation software as constant and then the solution was carried on. The model was linear, so as expected, the plot was also obtained as a linear graph between the temperature and length of the module.

From the three graphs above it is clear that when compared to the model where same values of properties were fed in simulation and in analytical solution, the analytical solution derived in this paper is more accurate and is more near to the near exact non-linear solution than the linear solution of the simulation. So, it is clear that the temperature profile that has been derived in this paper is accurate than the present existing model of temperature profiles where the values of various thermal, electric and thermoelectric properties are fed at a single point of mean operating temperature as it is much closer to the non-linear solution's plot of the simulation done in ANSYS.

7.4.Pictorial representation of temperature variation

The simulation model was developed as steady state thermal-electric conduction model and boundary conditions were defined for hot and cold temperature across the legs as 600 K and 300 K respectively. For electric boundary condition, potential difference was applied across

the base of the semiconductor. The low and high potential difference was applied to facilitate the flow of electrons and ions for conduction of electric current. The high and low potential was applied as 0.08V and 0V respectively for the purpose. Now, as the entire module is a sealed package in commercial setups, it is insulated from all the sides except from the sides where from where it accepts heat and from where it rejects heat. Hence, it can be said that the entire TEG is an insulated package except from the junction to accept and reject heat. This way the entire heat transfer is uni-directional and there is no loss of heat from the sides of the leg. Further, the heat probes were set at the top and the base of the model to determine the heat transfer taking place from the module. Also, from this setup the temperature variation across the legs were determined as shown further:

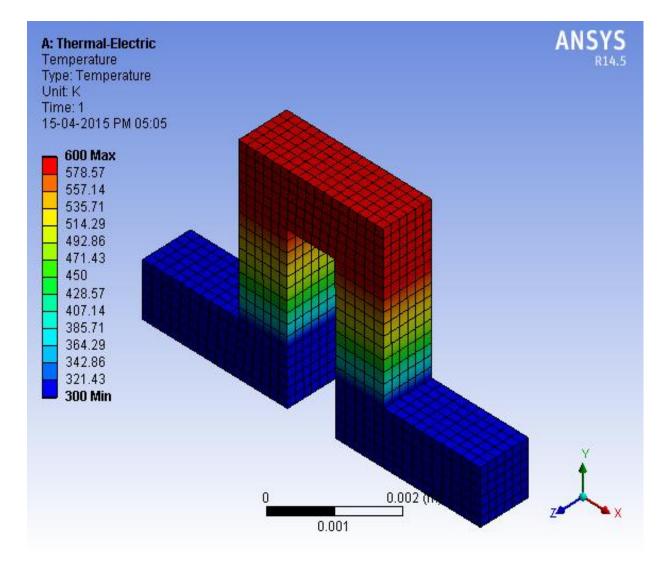


Figure 3 : Non-linear solution temperature variation

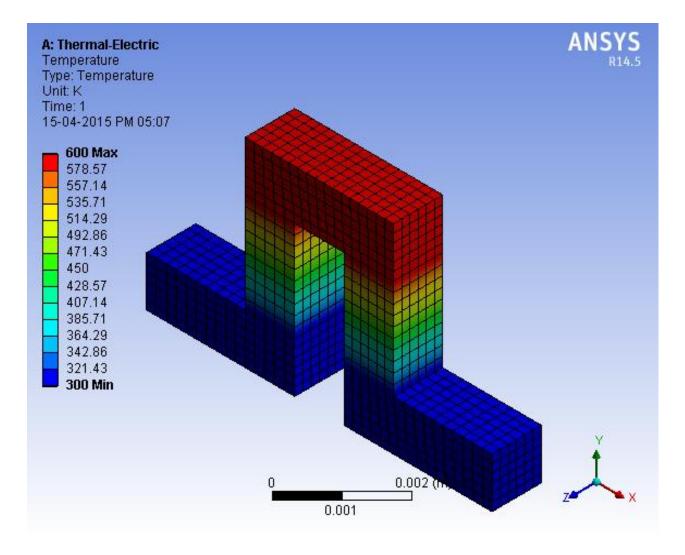


Figure 4: Linear solution temperature variation

As can be seen from the above two figures, Figure 2 shows the temperature variation across the entire system when the model was solved as non-linear solution. This was the case when properties were inserted in the simulation model at 100 different steps and hence the three properties: thermal conductivity, electrical resistivity and Seebeck coefficient were fed properly as the functions of temperature. Figure 3 is the temperature variation when the properties were taken as constant values. These values were determined at the average operating temperature from the same function, which was used to insert the values in the non-linear model of solution.

It is clear from the figures and temperature profile graph that in the non-linear model, initially at the source side of the system the temperature stays at higher end for longer length and then suddenly decreases at the sink side, remaining almost constantly varying in between. Whereas it is clearly visible in the figure 3 that in the linear model of simulation the temperature is constantly decreasing in almost linear fashion and hence the plot is linear. It is clear that practically it is not the case, where the linear temperature variation is there in the legs. Hence it can be easily said that the analytical model plot in the graph above is more accurate than the linear solution model approach on simulation.

7.5.Heat Transfer

In the simulation model, as mentioned above, that two heat reaction probes were setup in the model for measuring the total heat transfer taking place in the model. The heat input through the hot junction and the heat rejected at the cold junction were noted from the result generated from the simulation. Also from the equation (5.13) and equation (5.14), the heat transfers were calculated from the analytical model that was derived earlier in this paper. The various findings and results are tabulated in the table below for better comparison:

Γ	Heat input (Watts)	Heat output (Watts)
	Q_h	Q_c
Non-Linear simulation	0.88269	0.83195
Linear Simulation	0.83227	0.77079
Analytical model	0.84129	0.8213

Table1: Rate of heat transfer

As is seen from the table above, the heat transfer in Non-linear model when considered as the benchmark for comparison, linear simulation results variation is of greater extent. The heat transfer rate here is considered here only for one module, but it should be noted that in practical case scenarios, the entire TEG is made up of hundreds and even thousands of modules sometimes, so in general this variation which may not look like too much of a big value in this example, but when the entire system of TEG is considered the variation will seem to be significantly large and hence the requirement of accurate mathematical model arises to reduce this variation. For solving this problem, the model developed in this paper comes into play. As is seen in the table above, the heat transfer from the analytical model is much closer than the similar linear solution approach taken by the simulation model. Hence, validating the accuracy of the model even further, this was evident earlier with the temperature profile model also.

7.6.Conversion efficiency

While modelling the simulation model, the current reaction probe was also set to determine the current generated. This generated current is used to determine the electric power output which is put across the electrical load (Load resistance), which will give the useful output power from the TEG. This is determined to calculate the net conversion efficiency of the TEG module. The various results were compiled in a tabulated form for better comparison as shown below:

	Efficiency I
Non-Linear Simulation	5.75%
Linear Simulation	7.38%
Analytical model	7.49%

 Table 2: Conversion efficiency

As seen in the above table, the non-linear simulation model as expected is giving the least efficiency, as calculated from the equation (5.18) and equation (5.19). The other two results i.e., Linear simulation and analytical, vary to a greater extent from the Non-Linear simulation model is acceptable as the current calculation in non-linear solution was carried out by considering the Seebeck coefficient and the Internal resistance to be a function of temperature, whereas the linear model and analytical model, the Seebeck coefficient and the internal resistance was taken as a constant value. Hence, anyways the comparison of analytical model with non-linear simulation model was not valid, and the simulation model for linear solution must be considered in this case for comparison and validation. So, when compared to the Linear simulation model, the analytical model is in accordance with the result.

Conclusion and Future Scope

The equation of temperature profile was derived from the energy balance equation for a thermoelectric module in TEG mode. This modelling was carried out by considering all the properties of thermoelectric phenomena. The Thomson coefficient was also considered as the Seebeck coefficient was taken as the function of temperature. The simulation of a similar setup is carried out by modelling it in ANSYS software. The equation of temperature profile derived was used in the heat transfer equation of a TEG to determine the rate of heat transfer to the module and rate of heat transfer from the module. The graphs were plotted between the non-dimensionalised length and non-dimensionalised temperature and it was observed that the similar approach taken in this paper of single valued property yielded a better result than the single valued property approach taken by simulation model. Also the heat transfer rate was in accordance to the complicated non-linear solution model and was more accurate than the linear simulation model. The conversion efficiency included the current generation term which was not modelled in this paper, hence it was not close to the non-linear model, but was in accordance to the linear simulation model. Hence, it can be said that the model developed in this paper is better than the conventional model when compared to high temperature applications as all the phenomenological effects were considered.

This paper can be further extended in future for modelling the temperature profile in differential form of energy balance by taking the complete function of the properties to further refine the result and make it even more accurate than the model developed in this paper. Also, there is a scope of electrical current transfer modelling and optimization for better accuracy. Further, this model has to be validated experimentally to determine the accuracy of the result.

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Appendices

A.10.1. Values of Seebeck coefficient at various temperatures

Temp	Value	534	2.37E-04	465	2.41E-04
600	2.24E-04	531	2.37E-04	462	2.41E-04
597	2.25E-04	528	2.37E-04	459	2.41E-04
594	2.26E-04	525	2.38E-04	456	2.41E-04
591	2.26E-04	522	2.38E-04	453	2.41E-04
588	2.27E-04	519	2.38E-04	450	2.40E-04
585	2.28E-04	516	2.39E-04	447	2.40E-04
582	2.28E-04	513	2.39E-04	444	2.40E-04
579	2.29E-04	510	2.39E-04	441	2.40E-04
576	2.30E-04	507	2.39E-04	438	2.40E-04
573	2.30E-04	504	2.40E-04	435	2.40E-04
570	2.31E-04	501	2.40E-04	432	2.39E-04
567	2.31E-04	498	2.40E-04	429	2.39E-04
564	2.32E-04	495	2.40E-04	426	2.39E-04
561	2.33E-04	492	2.40E-04	423	2.39E-04
558	2.33E-04	489	2.40E-04	420	2.38E-04
555	2.34E-04	486	2.41E-04	417	2.38E-04
552	2.34E-04	483	2.41E-04	414	2.38E-04
549	2.35E-04	480	2.41E-04	411	2.37E-04
546	2.35E-04	477	2.41E-04	408	2.37E-04
543	2.36E-04	474	2.41E-04	405	2.37E-04
540	2.36E-04	471	2.41E-04	402	2.36E-04
537	2.36E-04	468	2.41E-04	399	2.36E-04

396	2.35E-04	363	2.30E-04	330	2.22E-04
393	2.35E-04	360	2.29E-04	327	2.21E-04
390	2.35E-04	357	2.28E-04	324	2.20E-04
387	2.34E-04	354	2.28E-04	321	2.19E-04
384	2.34E-04	351	2.27E-04	318	2.18E-04
381	2.33E-04	348	2.26E-04	315	2.17E-04
378	2.33E-04	345	2.25E-04	312	2.16E-04
375	2.32E-04	342	2.25E-04	309	2.15E-04
372	2.31E-04	339	2.24E-04	306	2.14E-04
369	2.31E-04	336	2.23E-04	303	2.13E-04
366	2.30E-04	333	2.22E-04	300	2.12E-04

A.10.2. Values of electric resistivity at various temperatures

Temp.	Value	528	2.66E-05	453	2.08E-05
600	3.29E-05	525	2.64E-05	450	2.06E-05
597	3.27E-05	522	2.62E-05	447	2.04E-05
594	3.24E-05	519	2.59E-05	444	2.01E-05
591	3.21E-05	516	2.57E-05	441	1.99E-05
588	3.18E-05	513	2.54E-05	438	1.97E-05
585	3.16E-05	510	2.52E-05	435	1.95E-05
582	3.13E-05	507	2.49E-05	432	1.93E-05
579	3.10E-05	504	2.47E-05	429	1.91E-05
576	3.08E-05	501	2.45E-05	426	1.89E-05
573	3.05E-05	498	2.42E-05	423	1.87E-05
570	3.02E-05	495	2.40E-05	420	1.85E-05
567	3.00E-05	492	2.38E-05	417	1.82E-05
564	2.97E-05	489	2.35E-05	414	1.80E-05
561	2.94E-05	486	2.33E-05	411	1.78E-05
558	2.92E-05	483	2.31E-05	408	1.76E-05
555	2.89E-05	480	2.28E-05	405	1.74E-05
552	2.87E-05	477	2.26E-05	402	1.72E-05
549	2.84E-05	474	2.24E-05	399	1.70E-05
546	2.82E-05	471	2.21E-05	396	1.68E-05
543	2.79E-05	468	2.19E-05	393	1.66E-05
540	2.76E-05	465	2.17E-05	390	1.64E-05
537	2.74E-05	462	2.15E-05	387	1.62E-05
534	2.71E-05	459	2.12E-05	384	1.60E-05
531	2.69E-05	456	2.10E-05	381	1.59E-05

378	1.57E-05	351	1.40E-05	324	1.24E-05
375	1.55E-05	348	1.38E-05	321	1.22E-05
372	1.53E-05	345	1.36E-05	318	1.21E-05
369	1.51E-05	342	1.34E-05	315	1.19E-05
366	1.49E-05	339	1.33E-05	312	1.17E-05
363	1.47E-05	336	1.31E-05	309	1.16E-05
360	1.45E-05	333	1.29E-05	306	1.14E-05
357	1.44E-05	330	1.27E-05	303	1.12E-05
354	1.42E-05	327	1.26E-05	300	1.11E-05

A.10.3. Values of Thermal conductivity at various temperatures

Temp	Value	534	4 3.2111	465	2.2797
600	4.4701	53	1 3.1624	462	2.2481
597	4.4051	523	8 3.1145	459	2.2173
594	4.3408	52:	5 3.0673	456	2.1872
591	4.2772	522	2 3.0209	453	2.1579
588	4.2144	51	9 2.9752	450	2.1293
585	4.1524	51	5 2.9302	447	2.1014
582	4.091	513	3 2.886	444	2.0743
579	4.0305	51	0 2.8425	441	2.0479
576	3.9706	50	7 2.7998	438	2.0223
573	3.9116	504	4 2.7578	435	1.9974
570	3.8532	50	1 2.7166	432	1.9733
567	3.7956	498	8 2.6761	429	1.9499
564	3.7388	49:	5 2.6363	426	1.9273
561	3.6827	492	2 2.5973	423	1.9053
558	3.6273	489	9 2.5591	420	1.8842
555	3.5727	480	5 2.5215	417	1.8638
552	3.5188	483	3 2.4848	414	1.8441
549	3.4656	480	0 2.4487	411	1.8252
546	3.4133	47′	7 2.4134	408	1.807
543	3.3616	474	4 2.3789	405	1.7895
540	3.3107	47	1 2.3451	402	1.7728
537	3.2605	46	8 2.312	399	1.7569

396	1.7416	363	1.6234	330	1.5951
393	1.7272	360	1.6171	327	1.5969
390	1.7135	357	1.6115	324	1.5996
387	1.7005	354	1.6067	321	1.603
384	1.6882	351	1.6027	318	1.6071
381	1.6767	348	1.5993	315	1.6119
378	1.666	345	1.5968	312	1.6175
375	1.656	342	1.5949	309	1.6239
372	1.6467	339	1.5939	306	1.631
369	1.6382	336	1.5935	303	1.6388
366	1.6304	333	1.5939	300	1.6474