SIMULATION OF MULTISTAGE CASCADED THERMOELECTRIC GENERATORS WITH ADAPTIVE FINITE ELEMENT METHOD

By:

MUHAMMAD FARIS BIN MOHD FAIZAL

(Matric no: 141874)

Supervisor:

Dr. Ing. Muhammad Razi Abdul Rahman

July 2022

This dissertation is submitted to

Universiti Sains Malaysia

As partial fulfillment of the requirement of graduate with honors degree in

BACHELOR OF ENGINEERING (MECHANICAL ENGINEERING)

School of Mechanical Engineering

Engineering Campus

Universiti Sains Malaysia

DECLARATION

This work has not previously been accepted in substance for any degree and is not being concurrently submitted in candidature for any degree.

Signed……...… (MUHAMMAD FARIS BIN MOHD FAIZAL)

Date……

STATEMENT 1

This journal is the result of my own investigation, except where otherwise stated. Other sources are acknowledged by giving explicit reference. Bibliography/references are appended.

Signed……...… (MUHAMMAD FARIS BIN MOHD FAIZAL)

Date……

STATEMENT 2

I hereby give consent for my journal, if accepted, to be available for pgotocopying and for interlibrary loan, and for the title and summary to be made available outside organizations.

Signed……...… (MUHAMMAD FARIS BIN MOHD FAIZAL)

Date……

ACKNOWLEDGEMENT

First of all, I am grateful to the School of Mechanical Engineering for providing me with the required resources and knowledge to complete my Final Year Project (FYP). All the opportunity and knowledge that I gained during the four-year course in Mechanical Engineering will be helpful and useful for my future as an engineer.

Moreover, I want to express my utmost thank you to my supervisor, Dr. Razi Abdul Rahman for allowing me to gain the experience to study and do research about this thesis. With his kindness, a lot of patience, guidance, and vast knowledge, I am able to complete the research and write the thesis. There are a lot of things that seem new to me such as Salome software, PolyDE and many other things and he teaches to use that software with ease. He assists me in every possible way like communicating through Telegram and sharing file through Google Drive. This makes the interaction as easy as possible. He also allows doing meetings through Webex during the Covid-19 pandemic and while I am at home when I am not on campus. He always gives valuable feedback especially during the simulation result. Hence, I would like to show my full gratitude to my supervisor.

Last but not least, I want to thank my parents for always believing in me and supporting me emotionally and financially throughout my life. Their understanding of my passion for studying engineering has allowed me to pursue my dream and their faith encourages me to keep going until the end. Thank you so much for everything.

TABLE OF CONTENTS

DECLARATION ..... **ii**

ACKNOWLEDGEMENT ..... **iii**

TABLE OF CONTENTS ..... **iv**

LIST OF TABLES ..... **vii**

LIST OF FIGURES ..... **viii**

LIST OF SYMBOLS ..... **xi**

LIST OF ABBREVIATIONS ..... **xii**

LIST OF APPENDICES ..... **xiii**

ABSTRAK ..... **xiv**

ABSTRACT ..... **xvi**

CHAPTER 1 INTRODUCTION **1**

1.1 Research Background 1

1.2 Problem Statement 2

1.3 Objectives 2

1.4 Scope of Research 3

1.5 Thesis Organization 3

CHAPTER 2 LITERATURE REVIEW **4**

2.1 Introduction 4

2.2 Thermoelectric Generator 4

2.3 Finite Element Method & Analysis 5

2.4 TEG Working Principle 7

2.4.1 Seebeck Effect 7

2.4.2 Peltier Effect 8

2.4.3 Thomson Effect 8

2.5 Software Used for Thesis 9

2.6 Previous Works with Different Simulation Packages 9
2.6.1 MATLAB 9
2.6.2 ANSYS 10
2.6.3 COMSOL Multiphysics 13
CHAPTER 3 METHODOLOGY 15
3.1 Introduction 15
3.2 Theory of Cascaded TEG 15
3.3 Simulation of Cascaded TEG 17
3.3.1 Initial Planning and Sketching 17
3.3.2 3D Geometry Model in Salome Software 18
3.3.2(a) 3D Geometry of Single Thermocouple 18
3.3.2(b) 3D Geometry of Cascaded Thermocouple 22
3.3.2(c) 3D Geometry of Cascaded TEG 24
3.3.3 3D Mesh Model in Salome Software 25
3.4 Coding in PolyDE through HPC 27
3.4.1 Software 27
3.4.2 Files in WinSCP 29
3.4.3 Coding 31
3.5 Visualization in ParaView 31
3.6 Verification with Formulation 32
CHAPTER 4 RESULT & DISCUSSION 34
4.1 Introduction 34
4.2 Meshing of Materials and Boundary Conditions in Salome Software 34
4.3 Coding in PolyDE 36
4.4 Result in ParaView 38
4.4.1 Linear Solver of Single Thermocouple 38
4.4.2 Linear Solver of Cascaded Thermocouple 40

4.4.3 Linear Solver of Cascaded TEG 45
4.4.4 Non-Linear Solver of Single Thermocouple 50
4.4.5 Non-Linear Solver of Cascaded Thermocouple 52
4.4.6 Non-Linear Solver of Cascaded TEG 57
4.5 Summary for Obtained Values 62
4.6 Comparison of Output Power 64
4.6.1 Calculation for Single Thermocouple Element 65
4.6.2 Calculation for Cascaded Thermocouple Elements 66
4.6.3 Calculation for Cascaded TEG 67
4.6.4 Comparison with Analytical Formulas 68
CHAPTER 5 CONCLUSION AND FUTURE RECOMMENDATIONS 71
5.1 Conclusion 71
5.2 Recommendations for Future Research 72
REFERENCES 73
APPENDICES

LIST OF TABLES

Page

Table 3.1 Description of Important Setting in PolyDE 28

Table 3.2 Properties for Material 30

Table 4.1 All the Values of Maximum Temperature and Voltage for Single and Cascaded Thermocouple in Linear and Non-Linear Solver 63

Table 4.2 All the Values of Maximum Temperature and Voltage for Different Sets of Cascaded TEG in Linear and Non-Linear Solver ... 64

Table 4.3 Comparisons of Result with Other Authors 65

Table 4.4 Comparisons of Values Between Ideal Equation and Single and Cascaded Thermocouple 69

Table 4.5 Comparisons of Values Between Ideal Equation and Different Sets of Cascaded TEG 69

LIST OF FIGURES

Page

Figure 3.1 Illustration of Single and Cascaded Thermocouple 16

Figure 3.2 Sketching of Single and Cascaded Thermocouple and Cascaded TEG 18

Figure 3.3 First Box, Second Box, and Full Boxes of Copper Plate with Cold Surface at its Bottom 19

Figure 3.4 Third Box with n_doped Material and Full Boxes with Three Box .. 20

Figure 3.5 Fourth Box, Fifth Box and All Six Boxes 20

Figure 3.6 Seventh Box with p_doped material and All Seven Boxes 21

Figure 3.7 Eight and Ninth Box 21

Figure 3.8 3D Model of Single Thermocouple in Salome Software 22

Figure 3.9 Bottom Plate of Cascaded Thermocouple 22

Figure 3.10 Top Plate of Copper Plate and First Design of Cascaded Thermocouple 23

Figure 3.11 Second and Third Design of Cascaded Thermocouple 23

Figure 3.12 2, 4, and 8 Sets of Cascaded TEG 24

Figure 3.13 Meshing For Single Thermocouple 25

Figure 3.14 Meshing for First, Second and Third Design of Cascaded Thermocouple 26

Figure 3.15 Meshing for 2, 4, and 8 Sets of Cascaded TEG 26

Figure 3.16 Setting for ‘FEMsetting’ in PolyDE 28

Figure 3.17 All Boundary Conditions for PolyDE 30

Figure 4.1 Boundary Condition for Current In, Earth, Hot, Cold and Free 35

Figure 4.2 Material for n_doped, p_doped and Copper 36

Figure 4.3 Result for Coding in PolyDE using ‘solver3d’ 37

Figure 4.4 Result for Coding in PolyDE using ‘post3d’ 37

Figure 4.5 Temperature Distribution of Single Thermocouple (Linear Solver) 38

Figure 4.6 Voltage Distribution of Single Thermocouple (Linear Solver) 39

Figure 4.7 Temperature plot through line at single thermocouple (Linear Solver).....39

Figure 4.8 Voltage plot through line at single thermocouple (Linear Solver) 40

Figure 4.9 Temperature Distribution for First, Second and Third Design of Cascaded Thermocouple (Linear Solver).....41

Figure 4.10 Voltage Distribution for First, Second and Third Design of Cascaded Thermocouple (Linear Solver).....42

Figure 4.11 Temperature plot through line for First, Second and Third Design of Cascaded Thermocouple (Linear Solver) 43

Figure 4.12 Voltage plot through line for First, Second and Third Design of Cascaded Thermocouple (Linear Solver).....44

Figure 4.13 Temperature Distribution for 2, 4 and 8 Sets of Cascaded TEG (Linear Solver) 46

Figure 4.14 Voltage Distribution for 2, 4 and 8 Sets of Cascaded TEG (Linear Solver).....47

Figure 4.15 Temperature plot through line for 2, 4 and 8 Sets of Cascaded TEG (Linear Solver) 48

Figure 4.16 Voltage plot through line for 2, 4 and 8 Sets of Cascaded TEG (Linear Solver) 50

Figure 4.17 Temperature distribution for single themocouple (Non-Linear Solver).....50

Figure 4.18 Voltage distribution for single themocouple (Non-Linear Solver)....51

Figure 4.19 Temperature plot through line at single thermocouple (Non-Linear Solver).....51

Figure 4.20 Voltage plot through line at single thermocouple (Non-Linear Solver) 52

Figure 4.21 Temperature Distribution for First, Second and Third Design of Cascaded Thermocouple (Non-Linear Solver) 53

Figure 4.22 Voltage Distribution for First, Second and Third Design of Cascaded Thermocouple (Non-Linear Solver) 54

Figure 4.23 Temperature plot through line for First, Second and Third Design of Cascaded Thermocouple (Non-Linear Solver) 55

Figure 4.24 Voltage plot through line for First, Second and Third Design of Cascaded Thermocouple (Non-Linear Solver) 56

Figure 4.25 Temperature Distribution for 2, 4 and 8 Sets of Cascaded TEG (Non-Linear Solver) 58

Figure 4.26 Voltage Distribution for 2, 4 and 8 Sets of Cascaded TEG (Non-Linear Solver) 59

Figure 4.27 Temperature plot through line for 2, 4 and 8 Sets of Cascaded TEG (Non-Linear Solver) 60

Figure 4.28 Voltage plot through line for 2, 4 and 8 Sets of Cascaded TEG (Non-Linear Solver) 62

LIST OF SYMBOLS

A	Cross Sectional Area (m^2)
I	Current (A)
T_c	Cold Temperature
σ	Electrical Conductivity (Ω /m)
T_h	Hot Temperature
R	Internal Resistance (Ω)
L	Length (m)
R_L	Load Resistance (Ω)
n	Number of Thermocouple
ΔV	Potential Difference
P_{out}	Power Output (W)
α	Seebeck Coefficient (V/K)
T	Temperature (°C)
ΔT	Temperature Gradient
k	Thermal Conductivity (W/m.K)
V	Voltage (V)

LIST OF ABBREVIATIONS

3D	3 Dimensional
CAD	Computer-Aided Design
CEA	Atomic Energy Commission
EDF	Electrical of France
FEA	Finite Element Analysis
FEM	Finite Element Method
FYP	Final Year Project
HEX	Heat Exchanger
HPC	High-Performing Computer
TEM	Thermoelectric Module
MPP	Maximum Power Point
NDOF	Number Degree of Freedom
PDE	Partial Differential Equation
STEG	Solar Thermoelectric Generator
TE	Thermoelectric Effect
TEG	Thermoelectric Generator
UNV	Universal File Format
USM	Universiti Sains Malaysia
VTK	Visualization Toolkit

LIST OF APPENDICES

Appendix A Example for UNV Files Used in PolyDE

Appendix B Example for Result of Errors in PolyDE Using Other Settings

SIMULASI PENJANA TERMOELEKTRIK BERTINGKAT DENGAN KAEDAH ELEMEN TERHINGGA BERADAPTIF

ABSTRAK

Penjana termoelektrik merupakan suatu peranti yang menukar tenaga haba kepada tenaga elektrik menggunakan kesan Seebeck. Lebih banyak tingkat dan banyak termokopel dalam penjana termoelektrik, lebih tinggi keberkesanan peranti tersebut dalam menghasilkan nilai voltan dan kuasa. Ramai penyelidik telah menjalankan simulasi termoelektrik dengan menggunakan kaedah yang berbeza termasuklah dengan menggunakan analisis penuh dalam kaedah unsur terhingga, namun analisis penuh untuk model tingkat ini tidak ada dalam sastera. Salah satu masalah utama adalah simulasi yang tepat agak susah untuk dicapai disebabkan oleh ketidaklurusan dalam kesan termoelektrik. Oleh sebab itu, matlamat projek ini adalah untuk membuat analisis penuh untuk penjana termoelektrik menggunakan adaptif kaedah unsur terhingga kerana ia diterima secara amnya untuk mendapat hasil yang tepat termasuk dalam kesan ketidaklurusan. Banyak bentuk geometri dengan tahap kesusahan yang berbeza telah dibuat dalam projek ini, di mana kaedah unsur terhingga dibuat dengan menggunakan lurus and ketidaklurusan penyelesai termasuk dengan hp adapti. Hasil ini akan dilihat dan diproses untuk menilai ketepatannya. Pencarian terbesar dalam projek ini adalah penilaian dalam ketepatan dalaman FEM kod yang dibuat untuk membanding kuasa pengeluaran dari simulasi dengan hasil teori ramalan. Walaupun hasil untuk suhu agak tepat, ketepatan untuk voltan berbeza bergantung dengan bentuk kompleks geometri. Sebagai contoh, hasil voltan dari satu termokopel adalah 0.033V padahal hasil voltan dari 8 set penjana termoelektrik bertingkat ialah 0.44V. Secara amnya, bentuk yang lebih kompleks dengan banyak termokopel akan menghasilkan

nilai tinggi untuk maksimum voltan dan kuasa pengeluaran, di mana ia agak selari dengan teori untuk penjana termoelektrik bertingkat. Oleh itu, objektif utama untuk project ini telah dicapai.

SIMULATION OF MULTISTAGE CASCADED THERMOELECTRIC GENERATORS WITH ADAPTIVE FINITE ELEMENT METHOD

ABSTRACT

A thermoelectric generator (TEG) is a device to convert the thermal energy to electrical energy using the Seebeck effect. The more cascaded or more thermocouples in TEG, the more efficient the device is in terms of producing voltage and power. Modelling efforts have been done by many researchers using different approaches including a full-field analysis with the finite element method, but full analysis of a cascaded model is not present in the literature. One of the main reasons is that accurate simulation of cascaded TEG is hard to achieve due to the nonlinearity of thermoelectric effect. For this purpose, this project aims to construct a full analysis of TEG using the adaptive finite element method (FEM) as it is generally accepted to attain highly accurate results with nonlinear effects. Various geometrical models with different level of complexity are considered in the study, where the finite element models are solved using linear and non-linear solvers combined with an hp-adaptivity. The results are visualised and post-processed to assess the accuracy. The major outcome for the project is the assessment of the accuracy of in-house adaptive FEM code used by comparing the power output from the simulation with the theoretical prediction. Although the results obtained for temperature are mostly accurate, the accuracy of voltage potential and power output varies according to geometrical complexities. For example, the voltage for single thermocouple is 0.033V while the voltage for 8 sets of cascaded TEG is 0.44V. In general, a more complex design with more thermocouples produces a higher value of maximum voltage and power output, which is consistent

with the theory for cascaded TEG. In this respect, the main objective of the project has been achieved.

CHAPTER 1

INTRODUCTION

1.1 Research Background

Harnessing thermal energy is quite common in the electronics sensor and thermoelectric generator (TEG) is one of them. TEG are made of different thermocouples which refer to the Seebeck effect where the thermoelectric elements are connected in series for electrical and parallel for thermal (Piggott, 2018). There are many finite element method (FEM) software packages that can simulate the physics of thermoelectricity but to achieve the accurate result is still difficult, particularly when it involves the nonlinear effects.

Hence, this project is about to create a 3D modelling of the TEG by using the Salome software package. This will include relevant input such as the materials, the boundaries condition, and others. Then, the 3D model of the TEG will be transferred to the high-performance computing (HPC) server. After that, it will undergo some programming using PolyDE software and see the result using ParaView software. The finite element method will be considered using nonlinear adaptive methods.

In the adaptive method for finite element analysis, there are h, p, and h-p versions of adaptivity. The h-adaptivity refines the mesh by dividing the element into two or more elements. The p-adaptivity refines the mesh by increasing the number of degrees of freedom (NDOF). NDOF is the values that are free to vary in the final calculation of statistics. Moreover, the hp-adaptivity refers to a systematic combination of refinement of mesh size h and extension of the polynomial approximation order p for a selected element that gives high local errors (Kamaludin

& Abdul-Rahman, 2015). From that, the accuracy of the results can be achieved by comparing it with analytical formulas where applicable.

1.2 Problem Statement

Improving energy harvesting power generators is one of the main concerns in alternative energy systems. One of the examples are cascaded thermoelectric generators that can convert thermal energy into electrical energy via the Seebeck effect. With complex geometry of cascaded TE generators and nonlinearity of the TE effect, accurate simulations with the finite element method (FEM) remain a problem. The fully automatic adaptive finite element solver in the form of in-house code PolyDE is expected to overcome this challenge. Hence, this project aims to verify the efficacy of PolyDE in complex simulations of cascaded TEG devices.

1.3 Objectives

There are two main objectives for this study.

i. To implement a comprehensive finite element simulation of a full 3D model of a cascaded TEG using Salome, PolyDE and ParaView software.

ii. To develop the finite element analysis by using nonlinear adaptive methods, and the accuracies will be assessed by comparing with closed form formulations.

1.4 Scope of Research

The main scope of this project is about simulations. To obtain it, the geometry model of TEG must be created in Salome with certain materials on the top plate and both n-type and p-type legs. Then, the model will be transferred to PolyDE with some thermoelectric problems and solve it with finite element methods and different adaptive strategies. Non-linear problems were expected to occur due to the complex geometry of cascaded TEG. Hence, PolyDE will be used to solve all these problems and check its accuracy.

1.5 Thesis Organization

For this thesis, it contains five chapters with a segment that shows the list of tables, figures, abbreviations, references, appendix and many more. The first chapter primarily reviews the research background of thermoelectric generators, its objective and scope of research for this thesis. The second chapter shows the literature review which was done by a lot of researchers in many aspects such as the software and theory. The third chapter reviews the methodology on how the study has been done. It also shows the procedure inside Salome, PolyDE, and ParaView software. The result will be discussed, analysed, and compared in chapter four. Lastly, chapter five governed the conclusion of the thesis and what the future work could have been.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

This chapter focuses on a review of some well-known concepts regarding computational approaches in this study. In particular, it emphasizes a detailed approach in modelling thermoelectric generators (TEG), finite element method and analysis, the working principle of TEG, the relevant software packages that have been used and many more. Since there are no previous researchers on doing full simulation for cascaded TEG using adaptive FEM, I did research on how other researchers perform the computations although most of them only studied for single thermocouple and TEG by using other software packages. Some of their results will be used to verify my simulations especially for single thermocouple.

2.2 Thermoelectric Generator

In physical principle, a thermoelectric generator (TEG) is utilized to directly convert heat energy into electrical energy. TEG is different compared to dynamic heat engines as it does not have shifting components and is thoroughly mute. When a temperature gradient is imposed on solid, an electric potential is produced. This is because of the distribution of charge carriers in the material. This phenomenon is known as the Seebeck effect. The inversion phenomenon, in which a temperature difference is produced across a material by an electric current due to the lattice cooling or heating at the interfaces, is called the Peltier effect. These two effects can be utilized in numerous power generation and refrigeration applications via the thermal-to-electric (or vice versa) energy conversion (Kang et al., 2015).

TEG have been used reliably for more than 30 years of maintenance-free operation in deep space probes such as the Voyager missions of NASA (Fisk, 2005). Compared to big traditional heat engines, TEGs have lower efficiency. However, for simple and small applications, TEG can become competitive as it is compact, inexpensive, and scalable. Thermoelectric systems can be designed to operate with diminutive heat sources and minuscule temperature differences. This small generator can be mass produced so it can be used in automotive waste heat recovery or home co-generation of heat and electricity (Snyder, 2008).

2.3 Finite Element Method & Analysis

The finite element method (FEM) is a computational method that is being used to gain approximated solutions of boundary value problems in engineering. To summarize, a boundary value problem is a mathematical problem in which one or more dependent variables need to meet a differential equation everywhere within a known domain of independent variables and exact conditions on the boundary of the domain. Commonly, boundary value problems are recognized as field problems. The field variables are the dependent variables of interest directed by the differential equation. Depending on the classification of physical problems that need to be analysed, the field variables may include physical displacement, temperature, heat flux, and many other things (Hutton, 2004).

The constant work out for FEM are:

1) Parting the domain of the problem into a set of subdomains, with each subdomain expressed by a set of element equations to the original problem.

2) Methodically recombining all sets of element equations into an all-around system of equations for the final calculation.

For step (1), the element equations are simple equations that are narrowly close to the original complex equations, where the original equations are regularly partial differential equations (PDE). To explain the closeness in this process, the finite element method is frequently introduced as a special case of Galerkin method. The process, in mathematical language, is to create an integral of the inner product of the residual and the weight functions and set the integral to zero. In simple terms, it is a method that reduces the inaccuracy of approximation by fitting trial functions into the PDE. In step (2), a global system of equations is produced from the element equations through a transformation of coordinates from the subdomains' local nodes to the domain's global nodes. This spatial transformation encloses suitable orientation improvement as applied in relation to the reference coordinate system. This procedure has normally been done by FEM software as it is using coordinate data generated from the subdomains (Reddy, 2006).

This FEA is very important to design and create something especially for engineers. This is because with FEA, the engineer can check and evaluate the impact in different conditions like stress, vibration, buckling, fatigue, creep, heat, and many more in the design. Having FEA as part of the development process, the engineer can simulate the effects of any variables on the design before they create a physical prototype. With the simulation results, it can cut a lot of time and money by reducing the amounts of physical prototypes needed. Currently, the FEA is being used in many departments of engineering such as aerospace, automotive, biomedical, chemicals, electronics, and much more (CaliberDesign, 2020). Therefore, the FEM or FEA is taken into consideration in order to create a simulation of a cascaded thermoelectric generator.

2.4 TEG Working Principle

Normally, TEG has three main elements. First, the heat exchanger (HEX) that functions to absorb heat and move the heat into thermoelectric modules. Second, a thermoelectric module (TEM) which generates electricity when a temperature difference occurs between their ends. It consists of many pairs of thermoelectric couples which each couple having a pair of n- and p- type semiconductors. The third is a heat sink as it functions to remove additional heat from the TEM. In theory of TEG, when one of the pieces of metal were heated while simultaneously cooling the other side, the electrons surrounding the metal atoms at the hot side will have more energy than the equivalent electrons at the cooler side. This shows that the hot electron will have more kinetic energy than those in cooler side. This also makes the hot electron travel more quickly toward the cold side than the cold electrons move toward the hot side. The TEG has three effects which are Seebeck, Peltier and Thomson effect (Jouhara et al., 2021).

2.4.1 Seebeck Effect

Seebeck effect discusses the anticipation of a potential gap (ΔV) through a semiconductor as the diffusion of its load carriers over a temperature gradient (ΔT). It is encountered by the substance if one side of it is heated or cooled. The Seebeck coefficient sign shows that the material is a p-type or n-type conductor, the positive sign indicates the p-type, the negative indicates the n-type material. The Seebeck coefficient (S), which is responsible for allowing the current to move while the temperature gradient is present, is the relation between the theoretical differential created and the temperature gradient applied which may be seen in Equation 1 (Jouhara et al., 2021).

$$S = -\frac{\Delta V}{\Delta T} \tag{1}$$

2.4.2 Peltier Effect

This effect is believed to be the opposite of the Seebeck effect. The Peltier effect appears because the average energy of the electrons involved in the transmission of electrical current in the various conductors is different. Numerous considerations, such as the energy range of electrons, their distribution in the conductor and the atoms scattering them under the effect of applied voltage at the junction of two dissimilar conductors, will have an effect on the conductor. The electrons move from one electrode to another based on the path of the electrical charge wave, then pass their extra energy to the surrounding atoms (exude) or consume energy from the surrounding atoms (Jouhara et al., 2021).

2.4.3 Thomson Effect

Thomson indicated that as the current passes into unequally heated conductors, the thermal energy is either consumed or formed in the metal structure. In other words, the Thomson effect is the generation of reversible heat when an electrical current is passed through a conductive material subjected to a temperature gradient. The Thomson effect therefore describes the heat loss of a substance with a current through it and this transfer of heat is immediately observable. It is different from the effects of Peltier and Seebeck, for which only the net effect of two different materials can be measured. the amount of heat absorbed or evolved when one ampere of current flows for one second (one Coulomb) in a metal between two points which differ in temperature by one degree Celsius is known as the Thomson coefficient (Jouhara et al., 2021).

2.5 Software Used for Thesis

Salome software developed by French Alternative Energies and Atomic Energy Commission (CEA) and Electrical of France (EDF). This software provides tools for building complex and integrated applications in terms of numerical simulations. The software makes it easy to plug in core numerical code, define and mesh geometry, define boundary conditions, run solvers, visualize results, and analyse data. The advantage of Salome software is it can generate input or output files or produce mesh from computer-aided design (CAD). Moreover, it is able to run large numerical simulations. For instance, industrial studies performed by CEA and EDF use Salome in the cast sector like nuclear reactor physics, structural mechanics and many more (Ribés et al., 2017).

PolyDE is a software which is based on an open-source FE research code. It works as an extension of the code to solve 3D thermoelectric problems. The solution method includes p-adaptivity and high order tetrahedral elements. ParaView is a software that has a powerful visualization framework which is built based on the visualization toolkit (VTK) developed by Kitware. It has unique features to create robust visualization from scientific data such as slicing and streamline representation of vector fields. It also can be used for big data visualization by using HPC which is useful for parallel visualization techniques (Farahani, 2018).

2.6 Previous Works with Different Simulation Packages

2.6.1 MATLAB

Elzalik et al. did a TEG with simulation and experiment investigation. In experiments, they use a lot of TEG theory and equations such as Seebeck coefficient, Peltier coefficient, Thomson effect, first law of thermodynamics, Ohm’s law, and

maximum power point (MPP). For simulation, they used MATLAB and Simulink at continual and different temperatures to estimate the performance of TEG. Using the designed MATLAB software and some TEG equation, the model for Simulink will be obtained. In the end, they got the result for experimental value and simulation value and then they compared it in terms of TEG power, voltage and current (Elzalik et al., 2019).

The advantages of other software like MATLAB for previous workers is it is easy to use due to its command line interface and file-oriented structure. This software is platform independent and can be installed in many different operating systems. Furthermore, its error is easier to solve because it is interpreted language and this software is not expensive and can be obtained through student license. The drawback is since this software is interpreted language; it will consume more time to execute. It also requires a fast computer with sufficient memory (*Advantages of MATLAB | Disadvantages of MATLAB*, n.d.).

2.6.2 ANSYS

Abubakar et al. had done the simulation for TEG as an ambient source by using ANSYS software. Commonly, the ANSYS software is used to get some value on electromagnetic and thermal analysis. The methodology they took has three fundamental processes which are pre-processing, solving and post-processing. For the pre-processing phase, it has five stages that includes modelling 3D geometry using ANSYS, selecting of the thermal-electric, inputting of the TEG engineering data, the building of solid-state model that allows field temperature evaluation and generation of finite element by ANSYS meshing. For thermal boundary conditions, it was kept constant on the subtract T_h and T_c. For the TEG performance, it will show the images of ANSYS simulation. The red and blue colour parts show higher and lower temperatures. As a result, the maximum temperature achieved is 27.575 °C while the

minimum temperature is 26.109 °C. Not only that, they also get a result for density, voltage across TEG, the graph of variation of hot and cold side temperature, graph for voltage and power (Abubakar et al., 2021).

Next, for Dhoopagunta, she did the analytical modelling and numerical simulation of TEG that includes contact resistance. The modelling of TEG can be divided into many steps like 3D CAD model of the TEG, specify material, meshing, provide input and simulation. First, the 3D model was created using ANSYS that have a ceramic top plate and P-leg and N-leg. The module has 32 thermoelectric couples. Then, the model was studied using heatsink and a numerical simulation was done by integrating the CFD-CFX model in ANSYS. After that, assign material for each geometry. In order to solve the model accurately, meshing must be done next. A fine mesh would give a better accuracy of the result. After meshing, input must be given into the module in terms of load resistance and hot and cold side temperature. As a result, he wants to know the value of analytical modelling with and without heatsink. He also got numerous results from ANSYS such as a graph of power output at constant leg length, a graph of power output at constant load resistance, a graph of power output at optimum load resistance, a graph on effect of thermal and electric contact resistance and much more (Dhoopagunta, 2016).

Furthermore, Hadi Ali Madkhali and Ho-Sung Lee did a modelling and simulation of a high performance solar thermoelectric generator. Their method was to compare the theoretical value with simulated value. Solar thermoelectric generator (STEG) is a renewable energy technique which converts sunlight directly into current. For experiments, they need to know first some of the values that were needed like solar flux, surrounding temperature, convection coefficient on glass, and many more. After that, they substitute those values into the equation that they derived. For simulations,

they do it using ANSYS and key in some important parameters like temperature difference, contact resistance and many more. After they compare both theoretical and simulated values, they came in conclusion that by using solar absorber with absorptivity of 0.95 and emissivity of 0.1, the optimized STEG obtain efficiency of 21.6% with 5.7W of power output (Madkhali & Lee, 2019).

In other research, Geppert et al. did a finite element simulation of TEG and their experimental validation. For experimental setup, in order to know the characteristics of TEG, the TEG was placed between a heat source and a heat sink, and the device will be fixed with clamping a force of 0.6 kN. They obtained some data like power output, specific thermal energy resistivity, current and others and tabulated it in a table. Each value is obtained for different components such as TE leg (n, p), electric connector and cover plates. For simulation, they did it using ANSYS software. The modelled devices have 72,048 elements and each leg of TEG is built up by 36 elements. This makes the total number of elements for the whole TEG leg are 5,112. As a result, the developed model can predict some properties for TEG and the regarded system can be changed with ease. Thus, it makes the FEM tools very reliable and flexible for predicting characteristics (Geppert et al., 2015).

Antonova and Looman did research about the finite element for thermoelectric device analysis in ANSYS. Their design is almost similar to mine for the single TEG. The materials that they applied also the same as mine and it is the reason why their result for power output will be used to compare with my result via PolyDe. The result is 1.05 W for power output, 11.07 W for heat produced, and 9.5% for efficiency. They also have a model for multi-stage cooler and the result for response surface for the cold side (Antonova & Looman, 2005).

For ANSYS software, the main benefits are it is easy to link with different simulations especially for mechanical and multi-physics problems. It also offers a lot of mesh options which allow the researcher to control the mesh and subsequent elements to a high degree (Malik, n.d.). Moreover, other benefits are that it has unequalled depth in the simulation domain, comprehensive multiphysics, engineered scalability and many more. This software also can be obtained easily by using student licenses. The disadvantage of this software is it usually harder to program and it relies heavily on numerical integration (Ozen, n.d.).

2.6.3 COMSOL Multiphysics

Firstly, Su and Engel did a modelling and simulation of a segmented TEG by using different software. She used software COMSOL Multiphysics software to run on the cascaded TEG. By using COMSOL, the simulation can be done without averaging the thermoelectric properties as needed by manual calculation. Hence, a more accurate distribution of temperature and potential can be achieved. Then, she used MATLAB to analyse it more. For the initial step, a TEG model with eight pairs of segmented legs is produced. Since the geometry model is taken from S. Li ‘s work, then the result of the COMSOL model will be compared to Li’s model in order to verify whether the simulation is accurate. After that, some optimizations were made to prototype models so the conversion efficiency can be increased. These methods include raising the working temperature, replacing couple materials, and reconfiguring the TEG geometry. Material that has been used for the model is thermoelectric materials which are Bi2Te3, PbSe0.5Te0.5, Bi0.3Sb1.7Te3, Zn4Sb3). For computation and result, she got a temperature distribution diagram with the top plate unseen and the value obtained is 296K for hot side temperature and 592K for cold side temperature. She also got a potential distribution diagram of an open circuit with the top plate unseen and much

more. For comparison with Li's result, the percentage error that she got for open-circuit voltage, inherent resistance, output power and maximum efficiency are under 12%. Thus, her result is pretty accurate (Su & Engel, 2017).

Moreover, other research is about a simulation that was done on a flexible TEG which used polymer based and pyroelectric material which is studied by Bakhari et al. The design geometry of their TEG has eight thermoelectric couples which are in red and blue colour. The n-type and p-type legs were made from different materials. The simulation software that has been used is COMSOL Multiphysics to examine the effect of parameter and material changing in determining the temperature differences and value of electrical energy produced. For the result, they got the analysis of TEG design using Polyimide and pyroelectric material, analysis of temperature difference by varying the input temperature at hot side and analysis of temperature different by changing the input voltage. To sum up, the best material is Polyimide as the substrate while Graphene for p-type leg and Bismuth Telluride for n-type leg (Bakhari et al., 2020).

For COMSOL Multiphysics software, one of the advantages is it is very easy to use and has a seamless interface between heat transfer. It also has the ability to change governing equations and have flexibility in solver in the form of direct, iterative, or mixed solvers, and many more (Elabbasi, n.d.). This software is heavily involved with finite elements so if the project of another researcher is heavily involved with finite elements, then COMSOL is the most suitable software to use. The disadvantage of this software is the software must be bought and need to contact them (*Comsol Vs Ansys Fluent?,* n.d.).

CHAPTER 3

METHODOLOGY

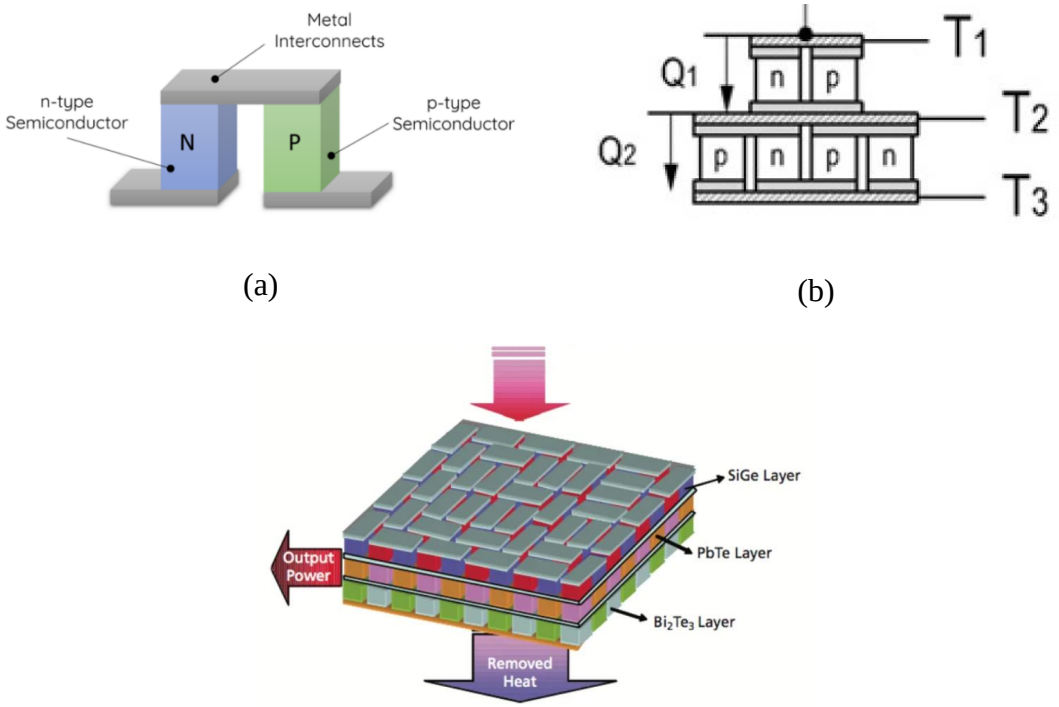
3.1 Introduction

For this project, one of the first things to plan is to do some research, especially in scientific theory of TEG and FEM. Then, the study about Salome software package is needed as the 3D model had to be done in that software. The sketch of cascaded TEG must be done first so it will be easy to draw in Salome. After that, the simulation file needs to be run by using PolyDE as it is connected to a high-performance computer (HPC). With an appropriate coding, the result of error and simulations such as temperature and voltage can be obtained. To observe the file, ParaView software is needed as the distribution of temperature and voltage can be seen clearly. Furthermore, the graph of temperature and voltage over line also can be obtained. This means the value for certain places can be identified. Last but not least, by using the formulation of power output, the comparison of power values can be made in order to determine the efficacy of PolyDE. Since there is no previous worker that has done the cascaded TEG geometry in any software, a single thermocouple needs to be made first so it can compare the result with the previous researcher. After that, several designs of cascaded thermocouple will be made and then the design of cascaded TEG will be created.

3.2 Theory of Cascaded TEG

To create a complete complex shaped of true TEG is complicated, so this project will focus on much simpler shape starts with single (2 copper plate, 2 bismuth telluride semiconductor and 1 copper plate at the top), cascaded thermocouple (multiple bottom copper plate, 6 bismuth telluride and top copper plate) and cascaded TEG (multiple bottom and copper and multiple bismuth telluride) which can be seen in Figure 3.1.

There are many components in cascaded TEG which consist of electric conductors, and pellets. For electric conductors, it provides serial electric contact of pellets with each other and contact with leading wires. It is a thin copper (Cu) structure which is embedded onto ceramic plates in real-life TEG. As for pellets, semiconductors like Bismuth Telluride (Bi_2Te_3) are usually used because of optimal TE performance and technological properties (*Thermoelectic Coolers Introduction - the Basics*, n.d.). In theory, the cascaded shape of thermocouple or TEG will produce more voltage and power compared to single, and plate shape.



(a) (b)

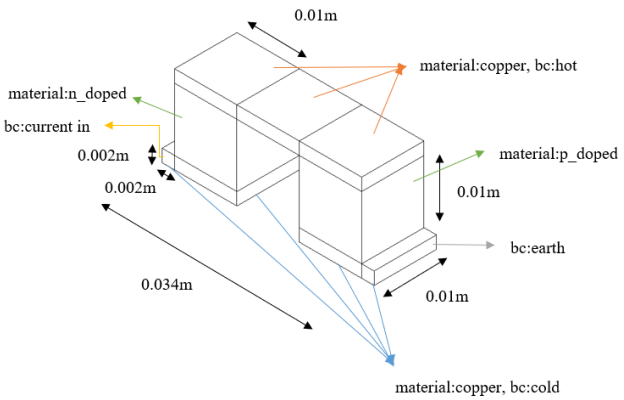
(c)

Figure 3.1 (a) Illustration of Single Thermocouple (Piggott, 2018) (b) Illustration of Cascaded Thermocouple (Karimi et al., 2011) (c) Illustration of Cascaded TEG (Sang H. Choi, James R. Elliott, Glen C. King, Yeonjoon Park, Jae-Woo Kim, n.d.)

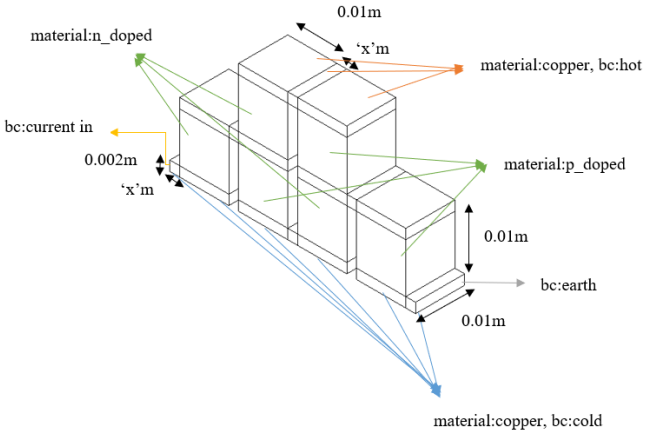
3.3 Simulation of Cascaded TEG

3.3.1 Initial Planning and Sketching

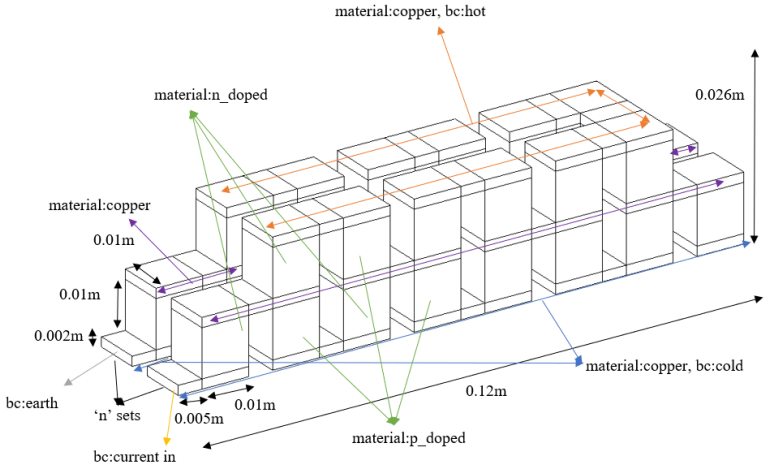
Based on the theory of cascaded TEG, most of its components and materials have become a reference for the 3D geometry and simulations. The next step is to draw the cascaded TEG to determine the dimensions. Figure 3.2 shows the 3D geometry of single and cascaded TEG with all its material and boundary conditions. Figure 3.2 (a) shows the dimensions of a single thermocouple with all its material and boundary conditions. The rest of boundary condition face which has not been mentioned is assigned as 'free'. This design also follows with Antonova design. With these, a comparison can be made whether the value is accurate or not. For Figure 3.2 (b), it is an example of design for cascaded thermocouple. The 'x' value is the only different dimension when creating another 2 designs. For the first, second and third design, the 'x' value is 0.002m, 0.005m and 0.01m. The third design dimension for 'current in' is 0.002m. Lastly, Figure 3.2 (c) shows the dimension of cascaded TEG. The 'n' represents the number of sets. The first, second and third designs have 'n' values of 2, 4, and 8 sets respectively. The material for n-dope and p-dope will be picked repeatedly to another.



(a)



(b)



(c)

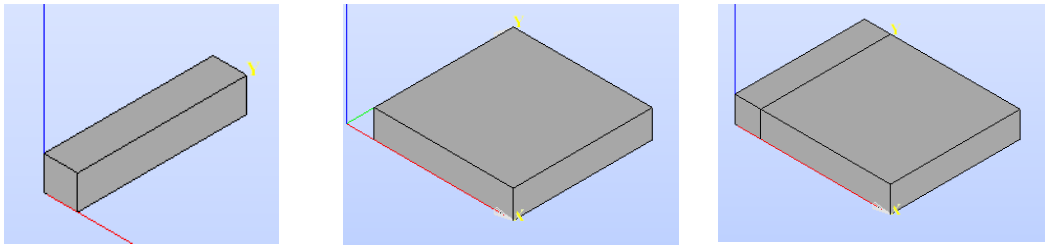
Figure 3.2 (a) Sketching of Single Thermocouple (b) Sketching of Cascaded Thermocouple (c) Sketching of Cascaded TEG

3.3.2 3D Geometry Model in Salome Software

3.3.2(a) 3D Geometry of Single Thermocouple

First of all, the Salome software must be installed first from the internet. Before doing anything, I need to study on how to use the software from YouTube before start designing all the TEG designs (Calculix09, n.d.). After learned from the YouTube, I start draw the geometry by clicking on the top tab 'Geometry' to open the window.

Create a box with certain coordinates depending on the dimension by clicking ‘Primitive’ under ‘New entity’. The material has been set to ‘copper’ and multiple boundary conditions must be set. For example, the left side of the face has been set as ‘current in’, the bottom side face has been set as ‘cold’ while the rest face except the right face been set as ‘free’. After that, create a second box located next to the first box by using the same steps. Both boxes material’s been defined as ‘copper’. The boundary condition for the bottom face needs to be set as ‘cold’ and the rest face has been set to ‘free’ except the face that meet with the pellet. These two boxes are known as copper conductors for the bottom side which has the cold side.



(a) (b) (c)

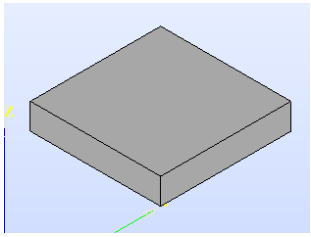
Figure 3.3 (a) First Box (b) Second Box (c) Full Boxes of Copper Plate with Cold Surface at Its Bottom

Next, create the third box with the material being defined as ‘n_doped’ and its boundary condition been set to ‘free’ for front, back, right, and left face. This box is known as pellet as shown in Figure 3.4.

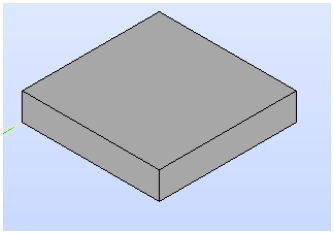
(a) (b)

Figure 3.4 Third Box with ‘n_doped’ Material (b) Full Boxes with Three Boxes

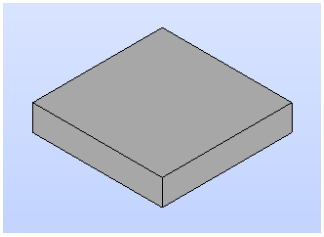
Then, create the fourth, fifth and sixth boxes using the same steps. Its material has been set as ‘copper’. For its boundary conditions, the front, left, and back face have been defined as ‘free’. The top surface has been defined as ‘hot’. These three boxes are known as copper conductors for the top side. All images can be seen in Figure 3.5.



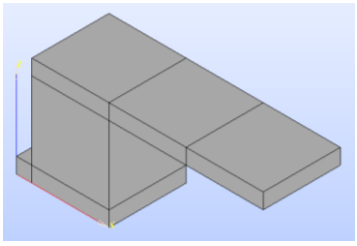
(a)



(b)



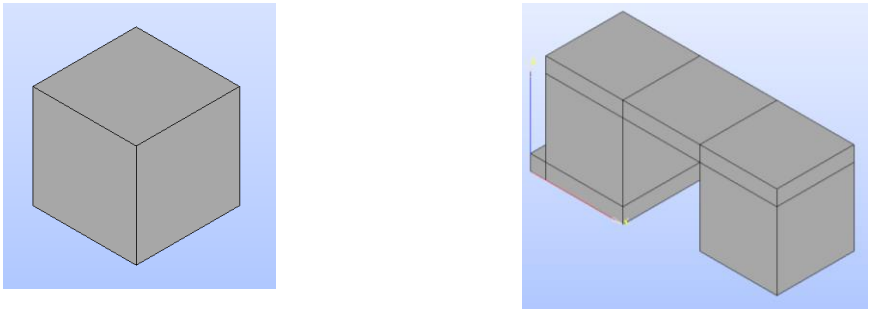
(c)



(d)

Figure 3.5 (a) Fourth box (b) Fifth box (c) Sixth box (d) All six boxes

The seventh box was created like the third box. The material has been defined as ‘p_doped’ and its boundary condition has been set to ‘free’ for front, back, right, and left face. This box is known as pellet as shown in Figure 3.6.



(a) (b)

Figure 3.6 (a) Seventh Box with ‘p_doped’ Material (b) All Seven Boxes

The steps for eight and ninth boxes are the same as the first and second boxes. The material was set as ‘copper’. The boundary condition for the right-hand side is assigned as ‘earth’ and the bottom side is defined as ‘cold’. The boxes can be seen in Figure 3.7.

(a) (b)

Figure 3.7 (a) Eight box (b) Ninth box

After done with all the 9 boxes, the single thermocouple geometry will look like Figure 3.8 and almost the same as the design with Antonova. This model is not final as the objective is to create a cascaded TEG. The result for a single thermocouple will be compared with previous researchers that used other software. When the value is almost identical and has a reasonable value or percentage error, then we can start the 3D geometry for cascaded thermocouple.

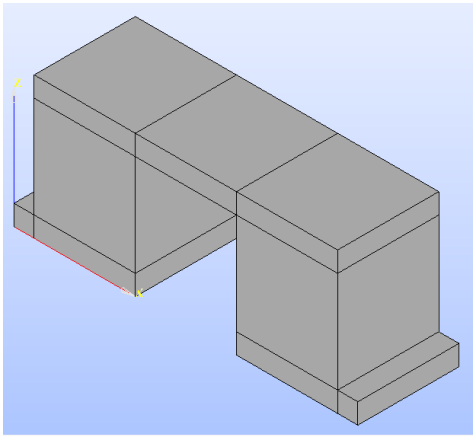


Figure 3.8 3D Model of Single Thermocouple in Salome Software

3.3.2(b) 3D Geometry of Cascaded Thermocouple

The steps for single TEG have been repeated but this time, the boxes must be added until it has 17 boxes. The material and boundary conditions also follow the steps in a single thermocouple except ‘hot’ as it will be removed. Hence, the bottom side of boxes will look like in Figure 3.9.

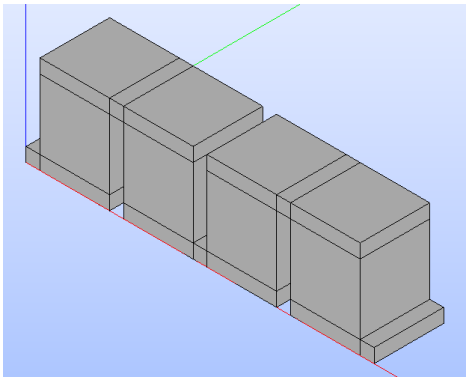
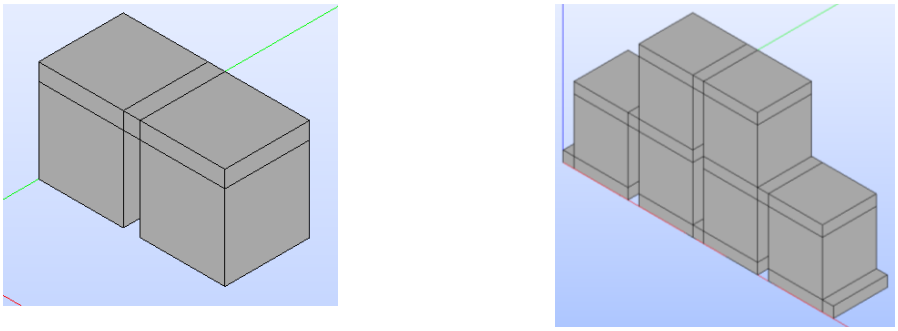


Figure 3.9 Bottom Plate of Cascaded Thermocouple

Next, repeat again the step for the five boxes but this time, place it above the bottom copper plate with 17 boxes. The difference from previous boxes is it need to remove the boundary condition of ‘cold’ at bottom side and replace it with ‘hot’ at top

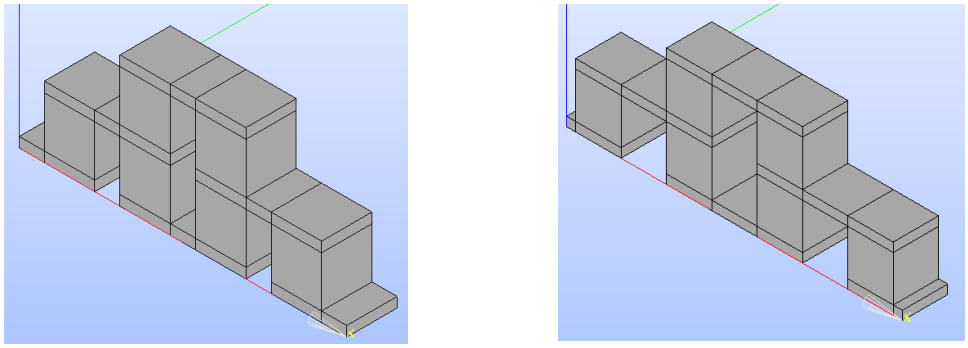
face. No need to put ‘current in’ and ‘earth’ for boundary conditions. Figure 3.10 shows the first design of cascaded thermocouple.



(a) (b)

Figure 3.10 (a) Top Plate on Copper Plate (b) First Design of Cascaded Thermocouple

Since the dimensions of bottom copper and top copper plate of a single thermocouple from Antonova are not equal, another two designs with different dimensions were created in order to check whether the changes in dimension of copper plate will affect the result. Figure 3.11 shows the design of another two cascaded thermocouple. The result of these three cascaded thermocouples were obtained in chapter 4 and the second design was chosen to create the design of complex cascaded TEG.

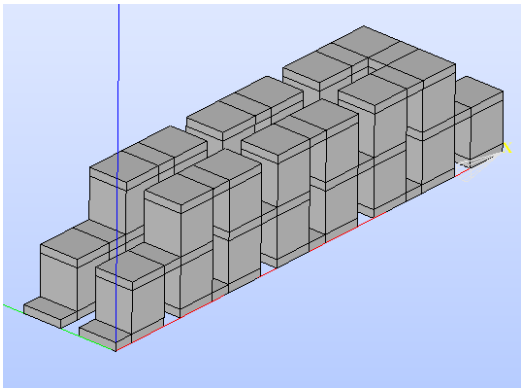


(a) (b)

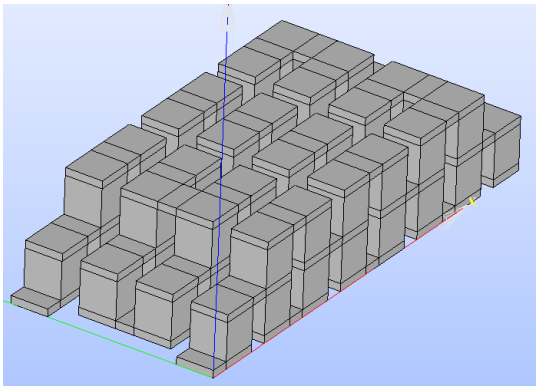
Figure 3.11 (a) Second Design of Cascaded Thermocouple (b) Third Design of Cascaded Thermocouple

3.3.2(c) 3D Geometry of Cascaded TEG

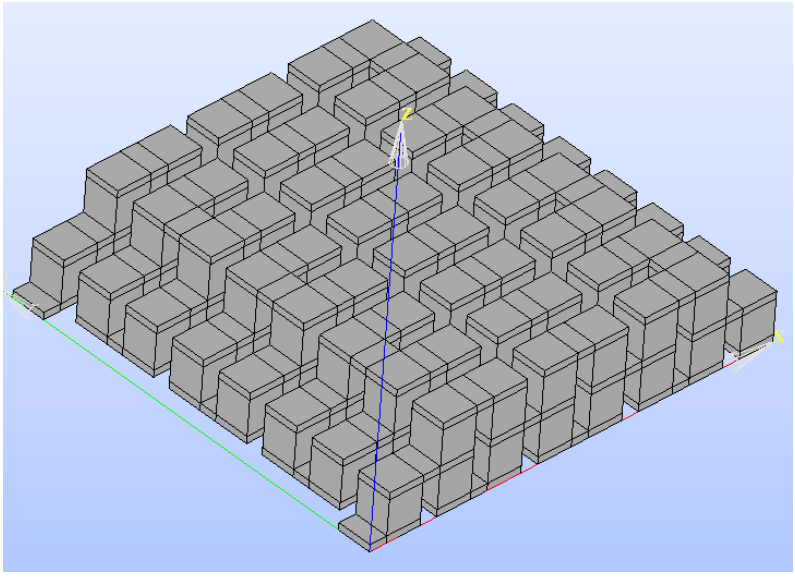
Since the geometry of cascaded of thermocouple has been made, the creation of the box needs to continue multiple times so it can become many like the actual TEG. Follows the same steps as creating the box with all the materials and boundary conditions until three iterations of cascaded TEG design were created like in Figure 3.12.



(a)



(b)



(c)

Figure 3.12 (a) 2 Sets of Cascaded TEG (b) 4 Sets of Cascaded TEG (c) 8 Sets of Cascaded TEG